

**APPROACHES FOR THE APPLICATION OF  
PHYSIOLOGICALLY -BASED PHARMACOKINETIC  
DATA AND MODELS IN RISK ASSESSMENT**

**APPENDIX 3:  
Partition coefficients  
and metabolic rate  
constants for PBPK  
modeling of  
environmental**

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<b>Acetone</b>			
Species	Rat	Human	Human
Reference	<b>18</b>	<b>18</b>	<b>81</b>
Partition coefficients			
Blood/air	275	260	245
Brain/blood	0.5	0.69	
Fat/blood	0.31	0.44	0.44
Liver/blood	0.6	0.58	0.58
Kidney/blood			0.74
Rapidly perfused/blood	0.53	0.69	0.69
Slowly perfused/blood	0.55	0.7	
Muscle and skin/blood			0.77
Mucus/air	275	260	
Biochemical Parameters			
V <sub>max</sub> C (mg/h/kg)	7.5	3.5	18.6
K <sub>m</sub> (mg/L)	75	10	83.5
Clearance into upper respiratory tract (L/h/kg)	11	11	
Urinary clearance (L/h)		0.004	
Fecal clearance (h <sup>-1</sup> )	0.25	0	
Skin permeability coefficient (cm/h)	0.008		
First-order absorption stomach/peritoneum (h <sup>-1</sup> )	2.0	1.0	
Transfer from stomach to duodenum (h <sup>-1</sup> )	3.0	10.0	
First-order absorption from duodenum (h <sup>-1</sup> )	0.5	8.0	

<b>Acrylonitrile</b>			
Species	Rat	Rat	Human
Reference	<b>52</b>	<b>69</b>	<b>127</b>
Partition coefficients			
Blood/air	512	512	154
Liver/blood	0.46	0.46	1.51
Stomach/blood		0.46	1.34
Brain/blood	0.40	0.40	1.34
Fat/blood	0.28	0.28	
Rapidly perfused/blood	0.46	0.46	1.34
Slowly perfused/blood	0.35	0.35	1.16
Biochemical parameters			
Oxydation			
VmaxC (mg/h/kg)	6.5	5	15.6
Km (mg/L)	1.5	1.5	0.8
GSH conjugaison			
KFC enzymatic (h <sup>-1</sup> . kg <sup>-1</sup> )	30	73	
KFC enzymatic (L/h/kg)			113
KSO spontaneous (L/mmol/hr)		0.2584	0.2584
Binding to blood (h <sup>-1</sup> )	2.54	2.54	
Binding to blood RSH (h <sup>-1</sup> )			0.0008
Binding to hemoglobin (h <sup>-1</sup> )	1.245	1.245	1.245
Oral absorption rate in water (h <sup>-1</sup> )	2.0	8.0	8

<b>2-Cyanoethylene Oxyde (acrylonitrile metabolite)</b>			
Species	Rat	Rat	Human
Reference	<b>52</b>	<b>69</b>	<b>127</b>
Partition coefficients			
Blood/air	1658	1658	1658
Liver/blood	0.27	0.27	0.27
Stomach/blood		0.27	0.27
Brain/blood	1.40	1.40	1.40
Fat/blood	0.78	0.78	???
Rapidly perfused /blood	0.27	0.27	0.27
Slowly perfused/blood	1.84	1.84	1.84
Biochemical parameters			
Hydrolysis			
VmaxC (mg/h/kg)			841
Km (mg/L)			113
Elimination ( $h^{-1} \cdot kg^{-1}$ )			
<i>KFC2</i> (liver)	750	500	
<i>KFCBrC</i> (brain)	8.4	11.5	
<i>KFSIC</i> (stomach)		27	
<i>KFSC</i> (slowly perfused)	9.3	4.4	
<i>KFRSC</i> (rapidly perfused)	9.3	15.5	
GSH conjugaison (L/h/kg)			
<i>KFC2</i> (liver)			197
<i>KFCBrC</i> (brain)			10.4
<i>KFSIC</i> (stomach)			12.6
<i>KFSC</i> (slowly perfused)			3.9
<i>KFRSC</i> (rapidly perfused)			9.0
Binding to blood ( $h^{-1}$ )	0.68	0.68	
Binding to blood RSH ( $h^{-1}$ )			0.84
Binding to hemoglobin ( $h^{-1}$ )	1.134	1.134	1.134

**ARSENIC**

<b>As(V) Pentavalent arsenate</b>				
Species	Rabbit	Hamster	Human	Human
Reference	<b>99</b>	<b>99</b>	<b>100</b>	<b>147</b>
Body weight (kg)	3.5	0.1		
Partition coefficients				
Liver/plasma	1.0	1.0	1.0	
Kidneys/plasma	40	40	40	
Lungs/plasma	1.0	1.0	1.0	
Skin/plasma	1.0	1.0	1.0	
RBC/plasma			0.2	
Others/plasma	10	10	10	
Large intestine/blood				2.8
Skin/blood				2.5
Fat/blood				0.3
Muscle/blood				2.6
Kidney-VRG/blood				4.15
Liver/blood				5.3
Lung/blood				4.15
Biochemical parameters				
Reduction first-order rate in plasma As(V) to As(III) (l/h)	3000	100		
Reduction first-order rate in plasma As(V) to As(III) (h-1)			1.37	
Oxydation first-order rate in plasma (l/h)	6000	400		
Oxydation first-order rate in plasma (h-1)			1.83	
Reduction first-order rate in kidney As(V) to AS(III) (l/h)	30	1.0		
Reduction first-order rate in kidney As(V) to AS(III) (h-1)			1.8	
KR GSH reduction As(V) to As(III) all perfused tissues (mol/min)				**
Clearance GFR (ml/min)	10	0.6	156	
Urinary excretion rate of As(V) (% of GFR)	75	75		
Urinary excretion rate of As(V) (min-1)				1,25 x 10 <sup>-3</sup>
Fecal excretion rate of As(V) (min-1)				2,00 x 10 <sup>-5</sup>
Biliary excretion rate of As(V) (min-1)				3,00 x 10 <sup>-4</sup>
Absorption rate constant GI (Arsenic acid) (h <sup>-1</sup> )			2.5	
Absorption rate constant GI (Drinking water) (h <sup>-1</sup> )			2.5	
Absorption rate Small Intestine (min <sup>-1</sup> )				2,00 x 10 <sup>-2</sup>
Absorption rate Large Intestine (min <sup>-1</sup> )				2,00 x 10 <sup>-2</sup>
	*	*	*	

\* Transfer from plasma to the tissues is also dependent on the permeability of the capillaries.

\*\* Chemical reaction with tissue glutathione (GSH concentrations reported in Table 5 of the article)



<b>As(III) Trivalent Arsenite</b>					
Species		Rabbit	Hamster	Human	Human
Reference		<b>99</b>	<b>99</b>	<b>100</b>	<b>147</b>
Partition coefficients					
	Liver/plasma	200	200	200	
	Kidneys/plasma	20	20	20	
	Lungs/plasma	1.0	1.0	1.0	
	Skin/plasma	60.0	60.0	60.0	
	RBC/plasma			1.5	
	Others/plasma	40	40	40	
	Large intestine/blood				2.8
	Skin/blood				2.5
	Fat/blood				0.3
	Muscle/blood				2.6
	Kidney-VRG/blood				4.15
	Liver/blood				5,3
	Lung/blood				4.15
Biochemical parameters					
	Liver				
	Vmax As(III) to MMA 1st methylation (μmol/ml/h)	4.0	0.12	0.0004	
	Vmax As(III) to MMA (mol/min)				5.20 x 10 <sup>-7</sup>
	Km As(III) to MMA 1st methylation (μmol/ml)	0.05	0.12	0.00015	0.10
	Vmax As(III) to DMA (mol/min)				1.04 x 10 <sup>-6</sup>
	Km As(III) to DMA (mol/L)				1.00 x 10 <sup>-4</sup>
	Kidney-VRG				
	Vmax As(III) to MMA (mol/min)				3.47 x 10 <sup>-7</sup>
	Km As(III) to MMA (mol/L)				1.00 x 10 <sup>-4</sup>
	Vmax As(III) to DMA (mol/min)				4.63 x 10 <sup>-7</sup>
	Km As(III) to DMA (mol/L)				1.00 x 10 <sup>-4</sup>
	Urinary excretion rate of AS(III) (% of GFR)	>100	>100		
	Urinary excretion rate of AS(III) (min <sup>-1</sup> )				8.33 x 10 <sup>-4</sup>
	Absorption rate constant Gi tract ( NaAsO <sub>2</sub> ) (h <sup>-1</sup> )			1.8	
		*	*	*	

\* Transfer from plasma to the tissues is also dependent on the permeability of the capillaries.

<b>MMA Monomethylarsenic (Arsenic Metabolite)</b>						
Species		Rabbit	Hamster	Human	Human	
Reference		<b>99</b>	<b>99</b>	<b>100</b>	<b>147</b>	
Partition coefficients						
	Liver/plasma	10	10	10		
	Kidneys/plasma	100	100	100		
	Lungs/plasma	1.0	1.0	1.0		
	Skin/plasma	50	50	50		
	RBC/plasma			0.2		
	Others/plasma	1	1	1		
	Large intestine/blood				1.2	
	Skin/blood				1.25	
	Fat/blood				0.3	
	Muscle/blood				1.8	
	Kidney-VRG/blood				1.8	
	Liver/blood				2.35	
	Lung/blood				1.8	
Biochemical parameters						
	Liver					
		Vmax MMA to DMA 2st methylation (μmol/ml/h)	1.5	0.12	0.0005	
		Vmax MMA to DMA (mol/min)				7.41 x 10 <sup>-7</sup>
		Km MMA to DMA methylation (μmol/ml)	0.9	0.08	0.00015	0.10
	Kidney-VRG					
		Vmax MMA to DMA in kidney-VRG (mol/min)				2.31 x 10 <sup>-7</sup>
		Km MMA to DMA in kidney-VRG (mol/L)				1.00 x 10 <sup>-4</sup>
	Urinary excretion rate of MMA (% of GFR)	100	100			
	Urinary excretion rate of MMA (min <sup>-1</sup> )					0.07
	Absorption rate constant Gi tract (h <sup>-1</sup> )			5.1		

<b>DMA Dimethylarsenic (Arsenic Metabolite)</b>					
Species		Rabbit	Hamster	Human	Human
Reference		<b>99</b>	<b>99</b>	<b>100</b>	<b>147</b>
Partition coefficients					
	Liver/plasma	1	1	1	
	Kidneys/plasma	5	5	5	
	Lungs/plasma	20	20	20	
	Skin/plasma	1	1	1	
	RBC/plasma			0.2	
	Others/plasma	1	1	1	
	Large intestine/blood				1.4
	Skin/blood				1.25
	Fat/blood				0.3
	Muscle/blood				2.8
	Kidney-VRG/blood				2.075
	Liver/blood				2.65
	Lung/blood				2.075
Biochemical parameters					
	Urinary excretion rate of DMA (% of GFR)	100	100		
	Urinary excretion rate of DMA ( $\text{min}^{-1}$ )				0.04
	Absorption rate constant Gi tract ( $\text{h}^{-1}$ )			4.4	

<b>Benzene</b>							
Species	Mouse	Mouse	Rat	Rat	Rat	Human	Human
Reference	<b>103</b>	<b>135</b>	<b>103</b>	<b>135</b>	<b>58</b> <b>59</b>	<b>135</b>	<b>60</b>
Partition coefficients							
Blood/air	18.0	22	18.0	15	15	7.4	7.4
Liver/blood	1	0.91	1	1.13	1.13	1.49	1.49
Fat/blood	28	22.73	28	33.33	33.33	54.86	54.86
Bone marrow/blood		2.27		2.00		16.22	
Rapidly perfused /blood	1.0	0.91	1.0	1.13	1.13	1.49	1.49
Slowly perfused /blood	0.6	1.73	0.6	1.00	1.00	2.03	2.03
Biochemical parameters							
Liver							
Vmax (mg/h)		0.39		3.65		29.04	
VmaxC (mg/h/kg)	9.54		15.64		2.11		2.11
Km (mg/L)	3.13	0.35	0.0782	0.35	0.10	0.35	0.10
Bone Marrow							
VmaxC (mg/h/kg)		0.21		0.36		0.05	
Km (mg/L)		0.35		0.35		0.35	
Gastric absorption constant (min <sup>-1</sup> )		0.032		0.01			
<b>Inhibition constants (mg/L)</b>							
<i>Ki</i> competitive (dichloromethane)					0.084		0.08
<i>Ki</i> competitive (toluene)					0.223		0.22
<i>Ki</i> competitive (ethylbenzene)					0.626		0.63
<i>Ki</i> competitive (m-xylene)					0.226		0.23

<b>Benzoic acid</b>	
Species	Guinea Pig (Hairless)
Reference	<b>98</b>
Partition coefficients	
Liver/plasma	0.956
Rapidly perfused/plasma	0.956
Slowly perfused/plasma	0.511
Biochemical parameters	
Vmax ( $\mu\text{g/hr}$ )	3767
Km ( $\mu\text{g/ml}$ )	4460
Transdermal input function **	
<i>K</i> Elimination rate from skin	0.2245 - 0.1808
<i>Ka</i> Absorption rate into skin	0.1787 - 0.1790
Scaling parameter	12.35 - 38.45

\* Optimized with different doses of BA

<b>Bromochloromethane</b>		
Species	Rat	Rat
Reference	<b>101</b>	<b>49</b>
Partition coefficients		
Blood/air	41.5	41.5
Liver/blood	0.70	0.70
Fat/blood	7.83	7.83
Slowly perfused/blood	0.27	
Rapidly perfused/blood	0.70	
Skin/blood	2.53	
Muscle/blood		0.27
Biochemical parameters		
VmaxC (mg/h/kg)	7	7
Km (mg/L)	0.4	0.4
Kf First order hepatic metabolism (h <sup>-1</sup> .kg <sup>-1</sup> )	0.7	3.4
Skin permeability constant (cm/h)	0.79	

<b>Bromodichloromethane</b>		
Species	Rat	Rat
Reference	<b>92</b>	<b>27</b>
Partition coefficients		
Blood/air	31.4	31.4
Liver/blood	0.97	0.97
Kidney/blood	1.05	1.05
Fat/blood	16.75	16.75
Slowly perfused/blood	0.4	0.4
Rapidly perfused/blood	0.97	0.97
Biochemical parameters		
Vmax liver (mg/h/kg)	12.8	8.01
Km liver (mg/L)	0.5	0.30
Kidney/liver metabolic activity ratio	0.052	0.052
<i>Ka</i> Oral absorption in water vehicle (h <sup>-1</sup> )	0.28 – 3.1	
Bioavailability term for aqueous dose	0.6 -1.0	
Emptying time for aqueous dose(h)	0.13- 6.0	
<i>Ka</i> Oral absorption in oil vehicle (h <sup>-1</sup> )	0.20 - 0.85	
Bioavailability term for oil dose	0.3 – 0.99	
Emptying time for oil dose (h)	0.22 - 6.0	
<i>Ka</i> Oral absorption in Alkalamus vehicle (h <sup>-1</sup> )		0.41
<b>Bromide Ion Submodel</b>		
<i>Kec</i> Br Elimination constant (h <sup>-1</sup> .kg <sup>-1</sup> )	0.007	
<i>Kw1c</i> Br constant transfer blood to water (h <sup>-1</sup> . kg <sup>-1</sup> )	6.52	

<b>2-Bromo,2-chloro-1,1,1-trifluoroethane (Halothane)</b>		
Species	Rat	Human
Reference	<b>145</b>	<b>145</b>
Partition coefficients		
Blood/air	6.1	3.3
Liver/blood	1.15	2.42
Rapidly perfused/blood	1.15	2.42
Poorly perfused/blood	0.77	2.91
Fat/blood	29.18	44.24
Gut/blood	1.21	0.94
Biochemical parameters		
V <sub>maxC</sub> (mg/h/kg)	7.4	7.4
K <sub>m</sub> (mg/L)	0.1	0.1
K <sub>s</sub> Suppression constant (mg/L)	18.1	18.1
V <sub>d</sub> Volume of distribution for TFA (L/kg)	0.35	0.34
K <sub>l</sub> Elimination rate constant for TFA (h <sup>-1</sup> .kg <sup>-1</sup> )	0.01	0.03



<b>Bromoform</b>	
Species	Rat
Reference	<b>27</b>
Partition coefficients	
Blood/air	198.1
Liver/blood	1.06
Fat/blood	20.84
Richly perfused/blood	1.06
Slowly perfuseds/blood	0.58
Kidney/blood	0.88
Biochemical parameters	
Vmax (mg/h/kg)	10.4
Km (mg/L)	0.42
<i>Ka</i> Oral absorption in Alkalamus vehicle (h <sup>-1</sup> )	0.421

<b>Bromotrifluoromethane (Halon1301)</b>		
Species		Human
Reference		<b>140</b>
Partition coefficients		
	Blood/air	0.34
	Liver/blood	2.50
	Rapidly perfused/blood	2.50
	Poorly perfused/blood	1.74
	Fat/blood	11.62
	Gut/blood	2.03
Biochemical parameters		
	VmaxC (mg/h/kg)	0
	Km (mg/L)	N/A

<b>Butadiene (1,3-)</b>						
Species	Mouse	Mouse	Mouse	Mouse	Mouse	Mouse
Reference	<b>66</b>	<b>78</b>	<b>37</b>	<b>105</b>	<b>84</b>	<b>126</b>
Partition coefficients						
Blood/air	3.03	1.5	1.184	1.34	1.6	1.34
Liver/blood		5.49	2.675	1.01	0.94	1.01
Kidney/blood			1.69			
Brain/blood			2.355			
Rapidly perfused/blood		5.34	2.02		1.0	
Slowly perfused/blood					2.3	
Muscle/blood		5.26	1.871	2.99		2.99
Fat/blood	7.23	118.2	32.362	14.33	11.4	14.33
Lung/blood			1.272	1.10		1.10
Lung & arterial , muscle &VRG, liver /blood	0.251					
Biochemical						
Vmax total ( $\mu\text{mol/h/kg}$ )			465			
Km ( $\mu\text{M}$ )			8			
Vmax liver ( $\mu\text{mol/h/kg}$ )			318	338	485	338
Km liver ( $\mu\text{M}$ )				2	11.0	2
Vmax bronchial ( $\mu\text{mol/h/kg}$ )			77			
Vmax lung ( $\mu\text{mol/h/kg}$ )			70	21.6		21.6
Km lung ( $\mu\text{M}$ )				5.01		5.01
LIVER						
Vmax cyt1 (nmol/h/mg)	193.2	155.4				
Km cyt1 (mM)	0.005	0.002				
Vmax cyt2 (nmol/h/mg)		12				
Km cyt2 (mM)		0.0156				
LUNG						
Vmax cyt1 (nmol/h/mg)		138.6				
Km cyt1 (mM)		0.00501				
LIVER						
Vmax Oxydation to BMO ( $\mu\text{mol/h/kg}$ )						97
Km Oxydation to BMO ( $\mu\text{M}$ )						0.88
Vmax Oxydation to other volatiles ( $\mu\text{mol/h/kg}$ )						243
Km Oxydation to other volatiles ( $\mu\text{M}$ )						2.72
LUNG						
Vmax Oxydation to BMO ( $\mu\text{mol/h/kg}$ )						6.4
Km Oxydation to BMO ( $\mu\text{M}$ )						1.6
Vmax Oxydation to other volatiles ( $\mu\text{mol/h/kg}$ )						16.1
Km Oxydation to other volatiles ( $\mu\text{M}$ )						9.5

<b>Butadiene monoepoxide (1,3-) ( 1,2-epoxy-3-butene)</b>					
Species		Mouse	Mouse	Mouse	Mouse
Reference		<b>66</b>	<b>105</b>	<b>126*</b>	<b>78</b>
Partition coefficients					
	Blood/air	83.4	36.6	36.6	60
	Liver/blood		1.150	1.150	0.6545
	Kidney/blood				
	Brain/blood				
	Rapidly perfused/blood				0.6348
	Muscle/blood		0.645	0.645	0.6533
	Fat/blood	1.859	2.492	2.492	1.8083
	Lung/blood		1.538	1.538	
	Lung & arterial , muscle &VRG, liver /blood	0.71			
Biochemical parameters					
LIVER					
	Vmax Oxidation (one enzyme) (µmol/h/kg)		26	176.6	
	Km Oxydation (one enzyme) (µM)		15.6	145	
	Vmax Oxidation <sup>-1</sup> (two enzyme) (µmol/h/kg)			32.5	
	Km Oxydation <sup>-1</sup> (two enzyme) (µM)			15.6	
	Vmax Oxidation <sup>-2</sup> (two enzyme) (µmol/h/kg)			144.1	
	Km Oxydation <sup>-2</sup> (two enzyme) (µM)			145	
	Vmax hydrolysis (liver) (µmol/h/kg)		754	754	
	Km (µM)		1590	1590	
	Vmax GSH conjugation (liver) (µmol/h/kg)		154000	154000	
	Km (µM)		35300	35300	
	K (L/kg/hr)		4.36		
LIVER					
	Vmax Epoxide hydrolase (nmol/h/mg)	1020			347.4
	Km Epoxide hydrolase (mM)	0.7			1.59
	Km intrinsic (% of apparent Km)	20			
	Vmax GST (nmol/h/mg)				30000
	Km GST (mM)	100			35.3
	Vmax/Km GST (µl. min <sup>-1</sup> .mg <sup>-1</sup> )	17			
LUNG					
	<i>k</i> Apparent first-order rate for epoxide hydrolysis (h <sup>-1</sup> /mg)				0.112
	Vmax GST (nmol/h/mg)				16380
	Km GST (mM)				36.5
	<i>k</i> Apparent first-order rate for GST (h <sup>-1</sup> /mg)				

\* Nonenzymatic reaction rate constants in tissues ( blood, liver, lung and fat)

<b>Butanol (tertiary)</b>	
Species	Rat
Reference	<b>12</b>
Partition coefficients	
Blood/air	481
Kidney/blood	1.13
Liver/blood	0.83
Fat/blood	0.40
Muscle/blood	1.02
Biochemical parameters	
VmaxC pathway A (μmol/h/kg)	54
Km pathway A (μM)	379

Butoxyethanol (2-)									
Species	Mouse Male	Mouse Female	Rat	Rat	Rat Male	Rat Female	Human	Human	Human
Reference	86	86	122	21	86	86	66	21	86
Partition coefficients:									
Blood/air	7965	7965	8000	7965	7965	7965	**	7965	7965
Liver/blood	1.46	1.46	0.9	1.46	1.46	1.46	1.0	1.46	1.46
Kidney/blood	1.83	1.83		1.83	1.83	1.83		1.83	1.83
Lung/blood	11.3	11.3		11.3	11.3	11.3		11.3	11.3
Fat/blood	2.03	2.03	0.7	2.03	2.03	2.03		2.03	2.03
Muscle/blood			0.9	0.64			1.0	0.64	
Gut/blood	4.33	4.33	0.9	4.33	4.33	4.33	1.0	4.33	4.33
Skin/blood	2.9	2.9	0.9	2.9	2.9	2.9		2.9	2.9
Skin/air	7965	7965		7965	7965	7965		7965	7965
Rapidly perfused/blood	1.46	1.46	0.9	1.46	1.46	1.46	1.0	1.46	1.46
Slowly perfused blood	0.64	0.64		0.64	0.64	0.64	1.0	0.64	0.64
Biochemical parameters									
V <sub>max</sub> (μmol/min/g liver)							0.73		
K <sub>m</sub> (μM)							2.28		
ZEE to butoxyacetic acid (2BAA) in liver									
V <sub>max</sub> C (ng/h/g)	206.9	206.9	102.15	37.5	103.4	206.9		37.5	103.4
K <sub>m</sub> (mg/L)	20.1	20.1	37.47	26.9	20.1	20.1		26.9	20.1
ZEE to others in liver									
V <sub>max</sub> C (ng/h/g)				5				5	
K <sub>m</sub> (mg/L)				0.5				0.5	
ZEE to ethylene glycol (EG) in liver									
V <sub>max</sub> C (ng/h/g)	2.4	2.4	2.33		2.4	2.4			2.4
K <sub>m</sub> (mg/L)	2.7	2.7	2.74		2.7	2.7			2.7
ZEE to BE-glucuronide (2BEG) in liver									
V <sub>max</sub> C (ng/h/g)	14.5	14.5	14.31		14.5	14.5			14.5
K <sub>m</sub> (mg/L)	55.8	55.8	55.79		55.8	55.8			55.8
ZEE-glucuronide (2BEG) to 2BE in liver									
V <sub>max</sub> C (ng/h/g)			0.59						
K <sub>m</sub> (mg/L)			118.20						
BE to BE-glucuronide in skin comp.									
Skin 1 V <sub>max</sub> C (ng/h/g)			0.15						
Skin 1 K <sub>m</sub> (mg/L)			55.79						
Skin 2 V <sub>max</sub> C (ng/h/g)			2.97						
Skin 2 K <sub>m</sub> (mg/L)			55.79						
Protein binding									
P <sub>binding sites</sub> (mg/L)	*	*		164	*	*		164	*
K <sub>D</sub> dissociation constant (mg/L)	*	*		48	*	*		48	*
First-order transfer rate (θ) to feces (h <sup>-1</sup> )									
			1						
First-order transfer rate of metabolite to urine (h <sup>-1</sup> )									
			5						
BE skin absorption in dermal exposures (h <sup>-1</sup> )									
			5						
			5.76 (0.34E-0)						
BE to GI in drinking water exposures									
k <sub>a</sub> Oral absorption constant (h <sup>-1</sup> )	1	1		1	1	1		1	1
k <sub>p</sub> Dermal permeability constant (cm/h) for	3	3		3	3	3		3	3

\* Corley et al (1994) TAP 129:61-79 adjusted on plasma albumin concentrations

\*\* Blood/air partition coefficient replace by relative pulmonary uptake set to 60% of the pulmonary ventilation

<b>Carbon tetrachloride</b>							
Species	Rat	Rat	Rat	Rat	Rat	Monkey	Human
Reference	<b>109</b>	<b>51</b>	<b>47</b>	<b>36</b>	<b>133</b>	<b>109</b>	<b>109</b>
Partition coefficients							
Blood/air	4.52	4.52	4.52	5.49	4.52	4.52	2.64
Liver/blood		3.14	3.14	2.95	3.14		
Fat/blood	79.4	79.42	79.5	51.24	79.4	100	136
Richly perfused/blood			3.14	2.95	3.14		
Slowly perfuseds/blood		1.01		2.43	2		
Muscle/blood	2		1.01			2	1.74
Lung/blood			3.14				
Biochemical parameters							
Vmax (mg/h)			0.178				
VmaxC (mg/h/kg)	0.64	0.40		0.37	0.828	0.66	0.65
Km (mg/L)	0.25	0.25	0.25	1.3	0.25	0.25	0.25
Lung:alveolar mass transfer coefficient (ml/min)			500				
VmaxC (mg/h/kg) after 24hr methanol exposure				1.6			
VmaxC (mg/h/kg) after 48hr methanol exposure				0.6			

<b>Chlordecone</b>		
Species		Rat
Reference		<b>13</b>
Partition coefficients		
	Fat/blood	15
	Liver/blood	55
	Muscle/blood	5.0
	Skin/blood	6.0
	Gastrointestinal tract	
	Stomach/blood	7
	Small Intestine 1 /blood	8
	Small Intestine 2 /blood	7
	Small Intestine 3 /blood	6
	Cecum/blood	5
	Large Intestine/blood	4
	Lumen/Stomach	1
	Lumen/Small Intestine 1	0.5
	Lumen/Small Intestine 2	0
	Lumen/Small Intestine 3	0.3
	Lumen/Cecum	0.2
	Lumen/Large Intestine	0.2
Biochemicals parameters		
	Permeability-area products (ml/min)	
	Liver/blood	11
	Skin/blood	0.54
	Stomach/blood	0.2
	Small Intestine 1 /blood	0.3
	Small Intestine 2 /blood	0.26
	Small Intestine 3 /blood	0.25
	Cecum/blood	0.09
	Large Intestine/blood	0.1
	Lumen/Stomach	0.002
	Lumen/Small Intestine 1	0.05
	Lumen/Small Intestine 2	0.04
	Lumen/Small Intestine 3	0.02
	Lumen/Cecum	0.006
	Lumen/Large Intestine	0.004
	Biliary excretion (ml/h)	3.6



<b>Chlorobiphenyl (4-)</b>			
Species		Mouse	Rat
Reference		<b>136</b>	<b>3</b>
Partition coefficients			
Parent compound			
	Muscle/blood	1	1
	Skin/blood	10	10
	Fat/blood	30	30
	Liver/blood	1	1
	Gut lumen/blood	1	1
Metabolite			
	Muscle/blood	0.14	0.14
	Skin/blood	0.25	0.25
	Fat/blood	0.6	0.6
	Liver/blood	2	2
	Gut lumen/blood	1	1
Biochemical parameters			
	<i>km</i> Metabolic clearance PCB (ml/min)	2.43	10
	<i>kB</i> Biliary clearance of metabolite (ml/min)	0.05	0.2
	<i>kK</i> Kidney clearance of metabolite (ml/min)	0.05	0.2
	<i>KG</i> Gut reabsorption of metabolite (h <sup>-1</sup> )	0.12 (0.016)	0.0096
	<i>kF</i> Fecal transport of metabolite (h <sup>-1</sup> )	0.08	0.048

<b>1-Chloro-1,1-difluoroethane</b>	
Species	Rat
Reference	<b>95</b>
Partition coefficients	
Blood/air	1.21
Liver/blood	1.22
Fat/blood	14.4
Rapidly perfused /blood	1.22
Lean tissue/blood	0.54
Biochemical parameters	
<i>K<sub>f</sub></i> First order metabolism rate constant (h <sup>-1</sup> . kg <sup>-1</sup> )	2.59

<b>Chloroethane</b>	
Species	Rat
Reference	<b>51</b>
Partition coefficients	
Blood/air	4.08
Liver/blood	0.88
Fat/blood	9.46
Rapidly perfused /blood	
Slowly perfused /blood	0.79
Biochemical parameters	
V <sub>max</sub> C (mg/h/kg)	4.0
K <sub>m</sub> (mg/L)	0.1
K <sub>f</sub> First order metabolism (h <sup>-1</sup> .kg <sup>-1</sup> )	1.0

<b>Chloroform</b>									
Species	Mouse	Mouse	Rat	Rat	Rat	Rat	Human	Human	Human
Reference	20	122	20	51	122	27	20	Male	Female
Reference	20	122	20	51	122	27	20	22	22
Partition coefficients									
Blood/air	21.3	21.3	20.8	20.8	20.8	20.8	7.43	7.43	7.43
Liver/blood	0.90	0.90	1.01	1.01	1.01	1.01	2.29	2.29	2.29
Kidney/blood	0.52	0.52	0.53		0.53	0.53	1.48	1.48	1.48
Fat/blood	11.36	11.36	9.76	9.76	9.76	9.76	37.69	37.69	37.69
Rapidly perfused /blood	0.90	0.90	1.01	1.01	1.01	1.01	2.29	2.29	2.29
Slowly perfused /blood	0.61	0.61	0.67	0.67	0.67	0.67	1.62	1.62	1.62
Skin/blood								1.62	1.62
Skin/water								3.85	3.85
Biochemical parameters									
VmaxC (mg/h/kg)	22.8	15	6.8	6.8	7	9.31	15.7	15.7	15.7
Km (mg/L)	0.352	0.1	0.543	0.25	1.0	0.422	0.448	0.448	0.448
Kgs Second-order rate constant GSH conjugaison ( $\mu\text{M}^{-1}\cdot\text{h}^{-1}$ )				0.009					
Kresyn Enzyme destruction ( $\text{h}^{-1}$ )	0.125		0				0	0	0
A Proportionality metabolism constant kidney/liver	0.153	0.153	0.052		0.052	0.052	0.033	0.033	0.033
fMMB Macro molecular binding fraction (liver)	0.003	0.0022	0.00104		0.0015		0.002		
fMMB Macro molecular binding fraction (kidney)	0.01	0.011	0.0086		0.013		0.0093		
Ka Oral absorption in water vehicle ( $\text{h}^{-1}$ )	5	8	5		2.45		5		
Ka Oral absorption in corn oil vehicle ( $\text{h}^{-1}$ )	0.6	1.2	0.6		0.35		0.6		
Ka Oral absorption in Alkalamus vehicle ( $\text{h}^{-1}$ )						0.586			
Kp Skin permeability coefficient (cm/h) 40 C								0.059	0.059
Kp Skin permeability coefficient (cm/h) 35 C								0.05	0.015
Kp Skin permeability coefficient (cm/h) 30 C								0.01	0.003

<b>Chloromethane</b>	
Species	Rat
Reference	<b>51</b>
Partition coefficients	
Blood/air	2.47
Liver/blood	1.40
Fat/blood	5.47
Rapidly perfused /blood	1.40
Slowly perfused /blood	0.39
Biochemical parameters	
VmaxC (mg/h/kg)	5.0
Km (mg/L)	1.0

<b>Chloropentafluorobenzene</b>						
Species	Mouse	Rat	Monkey (rhesus)	Monkey	Human	Human
Reference	<b>19</b>	<b>19</b>	<b>23</b>	<b>19</b>	<b>23</b>	<b>19</b>
Partition coefficients						
Blood/air	12.3	12.3	7	7.0	7	7.0
Liver/blood	2.77	2.77	8	8.0	8	8.0
GI tract/blood	2.55	2.55		3.65		3.65
Slowly perfuseds/blood	1.07	1.07	2.1	1.07	2.1	1.07
Richly perfuseds/blood	2.55	2.55	3.5	3.65	3.5	3.65
Fat/blood	75	75	104.1	93	104.1	93
Bone marrow/blood	11.6	11.6		16.0		16.0
Biochemical parameters						
<i>KFC</i> First order metabolism rate constant (h <sup>-1</sup> · kg <sup>-1</sup> )	2.0	2.0	2.0	2.0	2.0	2.0

<b>CHLOROFLUOROHYDROCARBONS</b>			
<b>2-Chloro-1,1,1,2-tetrafluoroethane (HCFC-124)</b>			
Species	Mouse	Rat	Hamster
Reference	<b>94</b>	<b>94</b>	<b>94</b>
Partition coefficients			
Blood/air	1.15	1.52	0.76
Liver/blood	1.11	1.47	4.55
Fat/blood	5.25	6.42	14.62
Rapidly perfused /blood	1.11	1.47	4.55
Lean tissue/blood	0.59	0.52	2.63
Biochemical parameters			
VmaxC (mg/h/kg)	1.78	0.35	
Km (mg/L)	1.2	1.2	
Kf First order metabolism rate constant (h <sup>-1</sup> . kg <sup>-1</sup> )	4.08	1.25	1.47

<b>Cyclohexane</b>	
Species	Human
Reference	<b>111</b>
Partition coefficients	
Blood/air	1.3
Liver/blood	8.5
Vessel-rich group/blood	7
Muscle/blood	7.7
Poorly perfused/blood	2
Fat/blood	200
Biochemical parameters	
Vmax (mg/min)	5.0
Km (mg/L)	0.43
Synthesis rate constant 1,2-DIOL (min <sup>-1</sup> )	0.25
Synthesis rate constant 1,4-DIOL (min <sup>-1</sup> )	0.11
Urinary excretion rate (ml/min)	1.0



<b>Chlorpyrifos</b>			
Species		Rat	Human
Reference		<b>134</b>	<b>134</b>
Partition coefficients			
Parent compound			
	Brain/blood	33	33
	Diaphragm/blood	6	6
	Fat/blood	435	435
	Liver/blood	22	22
	Rapidly perfused/blood	10	10
	Poorly perfused/blood	6	6
	Skin/blood	6	6
Metabolite (CPF-oxon)			
	Brain/blood	26	26
	Diaphragm/blood	4.9	4.9
	Fat/blood	342	342
	Liver/blood	17	17
	Rapidly perfused/blood	8.1	8.1
	Poorly perfused/blood	4.9	4.9
Biochemical parameters			
CYP450 CPF to oxon (liver)			
	VmaxC1 (µmol/h/kg)	80	80
	Km1 (µmol/L)	2.86	2.86
CYP450 CPF to TCP			
	VmaxC2 (µmol/h/kg)	273	273
	Km2 (µmol/L)	24	24
A-EST oxon to TCP (liver)			
	VmaxC3 (µmol/h/kg)	74421	74421
	Km3 (µmol/L)	240	240
A-EST oxon to TCP (blood)			
	VmaxC4 (µmol/h/kg)	57003	57003
	Km4 (µmol/L)	250	250
Oral absorption parameters			
	<i>Ka</i> S stomach (h <sup>-1</sup> )	0.01	0.01
	<i>Ka</i> I intestine (h <sup>-1</sup> )	0.5	0.5
	<i>Ks</i> I transfer stomach-intestine (h <sup>-1</sup> )	0.5	0.5
	Fractional absorption (%)	0.8	0.72
	<i>Kp</i> Permeability coefficient (cm/h)		4,81 x 10 <sup>-5</sup>
	<i>Ke</i> Elimination rate (h <sup>-1</sup> )	0.017	1,70x 10 <sup>-2</sup>
	Plasma protein binding CPF (%)	97	97
	Plasma protein binding CPF-oxon (%)	98	98

<b>Dibromochloromethane</b>	
Species	Rat
Reference	<b>27</b>
Partition coefficients	
Blood/air	116
Liver/blood	1.09
Fat/blood	16.53
Richly perfused/blood	1.09
Slowly perfuseds/blood	0.48
Kidney/blood	1.09
Biochemical parameters	
Vmax (mg/h/kg)	13.7
Km (mg/L)	0.72
Ka Oral absorption in Alkalamus vehicle (h <sup>-1</sup> )	0.55

<b>Dibromomethane</b>		
Species	Rat	Rat
Reference	<b>101</b>	<b>49</b>
Partition coefficients		
Blood/air	74.1	74.1
Liver/blood	0.92	0.92
Fat/blood	10.69	10.69
Richly perfused/blood	0.92	
Slowly perfuseds/blood	0.55	
Skin/blood	3.59	
Muscle/blood		0.55
Biochemical parameters		
Vmax (mg/h/kg)	12.5	12.5
Km (mg/L)	0.4	0.4
<i>K<sub>f</sub></i> First order hepatic metabolism (h <sup>-1</sup> .kg <sup>-1</sup> )	3.4	0.7
Skin permeability constant (cm/h)	1.32	

Dichlorobiphenyl (4,4'-)							
Species		Mouse	Mouse	Rat	Rat	Monkey	Dog
Reference		136	97	3	97	97	97
Partition coefficients							
Parent compound							
	Muscle/blood	2 (2)	2.0	2	2.0	5.0	4.0
	Skin/blood	10 (10)	10	10	10	50	12
	Fat/blood	70 (70)	70	70	70	300	40
	Liver/blood	5 (3)	5	3	3	20	6
	Gut lumen/blood			1			
Metabolite							
	Muscle/blood	0.4 (0.4)	0.4	0.4	0.4	0.3	0.16
	Skin/blood	0.8 (0.3)	0.8	0.3	0.3	1	0.8
	Fat/blood	1 (0.6)	1	0.6	0.6	9	0.6
	Liver/blood	4 (5)	4	5	5	2	0.4
	Gut lumen/blood			1			
Biochemical parameters							
	<i>km</i> Metabolic clearance PCB (ml/min)	0.365 (0.487)	0.37	2	2	7	470
	<i>kB</i> Biliary clearance of metabolite (ml/min)	0.1465 (0.085)	0.15	0.35	0.35	0.083	10.2
	<i>kK</i> Kidney clearance of metabolite (ml/min)	0.069 (0.0325)	0.069	0.133	0.133	1.5	2.7
	<i>KG</i> Gut reabsorption of metabolite (h <sup>-1</sup> )	0.454 (0.016)		0.0096	0	0	0
	<i>kF</i> Fecal transport of metabolite (h <sup>-1</sup> )	0 (0.08)		0.048		0.04	0.04
	<i>F</i> Fraction of preferential excretion by the liver ( <i>km</i> *(1- <i>F</i> ))					0.1	0.4

<b><i>p,p'</i>-Dichlorodiphenylsulfone</b>		
Species		Rat
Reference		<b>108</b>
Partition coefficients		
Parent compound (DDS)		
	Fat/blood	106.0
	Kidney/blood	4.64
	Liver/blood	22.1
	Muscle/blood	3.84
	Skin/blood	16.1
Metabolites		
	Kidney/blood	1.09
	Liver/blood	2.21
	Muscle/blood	0.728
Biochemical parameters		
Metabolic rate constant (male) (h <sup>-1</sup> )		0.142
Metabolic rate constant (female) (h <sup>-1</sup> )		0.0989
Urinary excretion rate constant DDS (h <sup>-1</sup> )		2.70
Biliary excretion rate constant DDS (h <sup>-1</sup> )		4.83
Biliary excretion rate constant for metabolites (h <sup>-1</sup> )		2.01
Capillary permeability (liver and kidney)		0.441
Capillary permeability (other tissues)		0.793
Maximum rate of absorption from gut (mg/L.h)		3.83 x 10 <sup>+3</sup>
Michaelis-Menten parameter for absorption from gut (mg/L)		5.61 x 10 <sup>+3</sup>

<b>Dichloroethane (1,1-)</b>	
Species	Rat
Reference	<b>51</b>
Partition coefficients	
Blood/air	11.2
Liver/blood	0.96
Fat/blood	14.64
Rapidly perfused /blood	
Muscle/blood	0.46
Biochemical parameters	
Vmax Oxidation (mg/h/kg)	7.5
Km (mg/L)	0.2

<b>Dichloroethane (1,2-)</b>				
Species		Mouse	Rat	Rat
Reference		<b>26</b>	<b>26</b>	<b>51</b>
Partition coefficients				
	Blood/air	30	28	30.4
	Liver/blood	1.2	1.2	1.17
	Fat/blood	12	12	11.32
	Rapidly perfused /blood	1.2	1.2	
	Muscle/blood	0.8	0.8	0.77
Biochemical parameters				
	Vmax Oxidation (mg/h/kg)	3.24	3.24	3.25
	Km (mg/L)	0.25	0.25	0.25
	<i>Kf</i> First-order rate constant GSH conjugaison (h <sup>-1</sup> .kg <sup>-1</sup> )	9.0 *	9.0 *	
	<i>Kgs</i> Second-order rate constant GSH conjugaison (μM <sup>-1</sup> .h <sup>-1</sup> )			0.0014**
	<i>Kgs</i> Second-order rate constant GSH conjugaison (μM <sup>-1</sup> .h <sup>-1</sup> .kg <sup>-1</sup> )	0.0012**	0.0012**	

\* Low exposure concentrations

\*\* High exposure concentrations

<b>Dichloroethylene (1,1-)</b>			
Species		Rat	Rat
Reference		<b>48</b>	<b>25</b>
			<b>51</b>
Partition coefficients			
	Blood/air	5.0	5
	Liver/blood	2.84	1.1
	Fat/blood	0.88	18.4
	Muscle/blood	0.41	
	Poorly perfused/blood		0.6
	Rapidly perfused/blood		1.1
	Kidney/blood		0.884
Biochemical parameters			
	Vmax (mg/h)		2.6
	VmaxC (mg/h/kg)	7.5	
	Km (mg/L)	0.2	0.25
	<b>Metabolite detoxification</b>		
	<i>Kgsm</i> Reaction with GSH ( $\mu\text{M}^{-1} \cdot \text{h}^{-1}$ )		0.33
	<i>Kfee</i> Reaction with 'everything else' ( $\text{h}^{-1}$ )		50
	<i>Kinm</i> Conversion of epoxide to CAC met. ( $\text{h}^{-1}$ )		9000
	<i>KCO2</i> Reaction of epoxide with water ( $\text{M}^{-1} \cdot \text{h}^{-1}$ )		$1.82 \times 10^{-5}$
	<i>H<sub>2</sub>O</i> Water concentration in liver (M)		55



<b>Dichloroethylene (1,2-) (cis)</b>	
Species	Rat
Reference	<b>51</b>
Partition coefficients	
Blood/air	21.6
Liver/blood	0.71
Fat/blood	10.51
Muscle/blood	0.28
Rapidly perfused/blood	0.71
Biochemical parameters	
VmaxC (mg/h/kg)	3
Km (mg/L)	0.5
Kd Enzyme inhibition second-order rate constant	1.2

<b>Dichloroethylene (1,2-) (trans)</b>	
Species	Rat
Reference	<b>51</b>
Partition coefficients	
Blood/air	9.58
Liver/blood	0.94
Fat/blood	15.45
Muscle/blood	0.37
Rapidly perfused/blood	0.94
Biochemical parameters	
VmaxC (mg/h/kg)	3
Km (mg/L)	0.1
Kd Enzyme inhibition second-order rate constant	400

<b>1,1-Dichloro-1-fluoroethane</b>	
Species	Rat
Reference	<b>95</b>
Partition coefficients	
Blood/air	2.11
Liver/blood	1.59
Fat/blood	17.1
Rapidly perfused/blood	1.59
Lean tissue/blood	0.50
Biochemical parameters	
First order metabolism rate constant (h <sup>-1</sup> . kg <sup>-1</sup> )	3.15

<b>Dichloromethane</b>						
Species	Mouse	Hamster	Human	Human	Human	Human
Reference	<b>3</b>	<b>3</b>	<b>34</b>	<b>4</b>	<b>5</b>	<b>60</b>
<b>Partition coefficients</b>						
Blood/air	8.29	22.5	9.7	9.7	8.94	8.94
Red blood cell/plasma						
Liver/blood	1.71	0.84	1.460	1.464	1.46	1.47
Lung/blood	1.71	0.84	1.460			
Richly perfused/blood	1.71	0.84	1.460		0.82	1.47
Slowly perfuseds/blood	0.96	1.196	0.82	0.814	0.82	0.82
Fat/blood	14.5	6	12.4	12.37	12.4	12.42
Kidney/blood						
Gut/blood						
Cacass/blood						
Skin/blood						
<b>Biochemical parameters</b>						
<b>MFO pathway</b>						
Vmax (mg/h)	1.054	2.047	118.9	78.0		
Vmax (mg/h/kg)				3.36	6.25	6.25
Vmax (nmol/ml/min)						
Km (mg/L)	0.396	0.649	0.58	0.4	0.75	0.75
Km (nmol/ml)						
A1 Distribution of MFO activity between lung and liver	0.416	0.0638	0.00143			
<b>GSH pathway</b>						
Kf First-order hepatic metabolism (h <sup>-1</sup> )	4.017	1.513	0.53			
Kf First-order hepatic metabolism (h <sup>-1</sup> . kg <sup>-1</sup> )					2.0	2.0
A2 Distribution of GSH activity between lung and liver	0.137	0.0774	0.0473			
<b>Inhibition constants (mg/L)</b>						
Ki competitive (benzene)						0.3
Ki competitive (toluene)						0.35
Ki competitive (ethylbenzene)						0.99
Ki competitive (m-xylene)						0.45

<b>Dichlorophenoxyacetic acid (2,4-)</b>			
Species	Rat	Rabbit	Rabbit
Reference	<b>73</b>	<b>74</b>	<b>72</b>
Partition coefficients			
Brain/plasma	1.42	1.42	1.42
Brain plasma/plasma	1.0	1.0	1.0
CSF/ plasma	1.0	1.0	1.0
Body/plasma	0.17	0.17	0.17
Biochemical parameters			
Vmax1 choroid plexus (mg/h)	2.1	2.1	2.1
Km1 choroid plexus (mg/l)	17	17	17
Vmax2 kidney (mg/h)	3.45	3.45	3.45
Km2 kidney (mg/l)	86	86	86
Transfert between body and deep compartment (l/h)	0.013	0.017	0.017
Transfert between deep compartment and body (l/h)	0.048	0.05	0.05
Transfer constant between plasma and brain (l/h)	0.017		
Transfer constant between brain and CSF (l/h)	0.29		
First-order rate of ip dose absorption (h <sup>-1</sup> )	5.0	5.0	
First-order rate of oral dose absorption (h <sup>-1</sup> )	0.8		
Mass transfer rate constants in areas of the brain			
Plasma to cerebellum (l/h)		0.017	0.017
Plasma to hypothalamus (l/h)		0.017	0.017
Plasma to caudate nucleus (l/h)		0.017	0.017
Plasma to hippocampus (l/hr)		0.017	0.017
Plasma to brainstem (l/h)		0.017	0.017
Plasma to forebrain (l/h)		0.017	0.017
Cerebellum to CSF (l/h)		0.7	0.8
Hypothalamus to CSF (l/h)		1.1	1.2
Caudate nucleus to CSF (l/h)		1.8	1.2
Hippocampus to CSF (l/h)		1.6	1.2
Brainstem to CSF (l/h)		1.6	1.0
Forebrain to CSF (l/h)		1.1	1.0

**CHLOROFLUOROHYDROCARBONE****2,2-Dichloro-1,1,1-trifluoroethane (HCFC-123)**

Species	Rat	Rat	Rat	Rat	Human	Human
Reference	<b>139</b>	<b>145</b>	<b>93</b>	<b>94</b>	<b>140</b>	<b>145</b>
Partition coefficients						
Blood/air	3.2	3.2	4.06	4.06	1.9	1.9
Liver/blood	1.03	1.03	1.15	1.15	1.58	1.58
Rapidly perfused/blood	1.03	1.03	1.15	1.15	1.58	1.58
Poorly perfused/blood	0.66	0.66			1.58	1.58
Fat/blood	21.97	21.88	15.4	15.4	25.79	25.79
Gut/blood	0.97	0.97			0.84	0.84
Lean tissue/blood			1.2	1.2		
Biochemical parameters						
VmaxC (mg/h/kg)	8.8	8.8	7.2	7.97	8.8	8.8
Km (mg/L)	0.7	0.7	1.2	1.2	0.7	0.7
<b>Metabolite (TFA)</b>						
Ks Suppression constant (mg/L)	65	65				65
Vdc Volume of distribution (L/kg)	0.345	0.35				0.34
Klosc Elimination rate constant (h <sup>-1</sup> .kg <sup>-1</sup> )	0.01	0.01				0.03

<b>Diethylether</b>	
Species	Rat
Reference	<b>48</b>
Body weight (kg)	0.225
Partition coefficients	
Blood/air	12.2
Liver/blood	0.56
Fat/blood	3.91
Muscle/blood	0.43
Biochemical parameters	
Vmax (mg/h)	1.9
Km (mg/L)	0.2
<i>K<sub>f</sub></i> First order hepatic metabolism (h <sup>-1</sup> )	1.60

<b>Difluoromethane (HFC32)</b>	
Species	Rat
Reference	<b>35</b>
Partition coefficients	
Blood/air	1.25
Liver/blood	1.304
Rapidly perfused/blood	1.304
Poorly perfused/blood	1.152
Fat/blood	1.432
Biochemical parameters	
<i>K<sub>f</sub></i> First order metabolic rate constant (h <sup>-1</sup> )	8.98



<b>Diisopropylfluorophosphate</b>		
Species	Mouse	Rat
Reference	<b>54</b>	<b>54</b>
Partition coefficients		
Blood/air	12.57	12.57
Brain/blood	0.67	0.67
Liver/blood	1.53	1.53
Kidney/blood	1.63	1.63
Richly perfused/blood	0.67	0.67
Fat/blood	17.6	17.6
Slowly perfuseds/blood	0.77	0.77
Diaphragm/blood	0.77	0.77
Biochemical parameters		
<b>Hydrolysis of DFP in tissues</b>		
Vmax Brain (mg/h)	2.28	9.18
Km Brain (mg/L)	439.8	439.8
Vmax Liver (mg/h)	256.58	1380
Km Liver (mg/L)	237.36	237.36
Vmax Kidney(mg/h)	25.61	103.32
Km Kidney (mg/L)	134.3	134.3
Vmax Richly perfused (mg/h)	2.73	11.04
Km Richly perfused (mg/L)	50.89	50.89
Vmax Venous blood (mg/h)	79.38	320.18
Km Venous blood(mg/L)	198.7	198.7
Vmax Arterial blood (mg/h)	26.46	106.73
Km Arterial blood (mg/L)	198.7	198.7
<b>Bimolecular inhibition rate constants (<math>\mu\text{M}^{-1} \cdot \text{h}^{-1}</math>)</b>		
Acetylcholinesterase	14.16	14.16
Butyrylcholinesterase (Fast)	354	354
Butyrylcholinesterase (Slow)	30	30
Carboxylesterase (Fast)	1.1	1.1
Carboxylesterase (Slow)	0.52	0.52

<b>Dioxane (1,4)</b>					
Species	Mouse	Rat	Rat	Human	Human
Reference	<b>117</b>	<b>117</b>	<b>88</b>	<b>117</b>	<b>88</b>
Partition coefficients					
Blood/air	2750	1850	1850	3650	1825
Liver/blood	0.566	0.842	0.85	0.427	0.85
Fat/blood	0.309	0.460	0.4	0.233	0.4
Richly perfused/blood	0.566	0.842	0.85	0.427	0.85
Slowly perfuseds/blood	0.566	0.842	0.54	0.427	0.2
Saline/air	0.751	1.117		0.566	
Biochemical parameters					
Vmax (mg/h)			1.9 **		300
VmaxC (mg/h/kg)	10.0	13.7		6.35	
Km (mg/L)	16.2	29.4	7.5	3.0	15
Ka Oral absorption in water vehicle (h <sup>-1</sup> )	5	5		5.0	

\*\*Vmax =3.5mg/h at doses greater than 300 mg/kg

<b>Ethoxyethanol (ethylene glycol monoethyl ether)</b>			
Species		Rat	Human
Reference		<b>53</b>	<b>53</b>
Partition coefficients			
<b>Parent compound</b>			
	Blood/air	22093	22093
	Liver/blood	1.00	1.00
	Rapidly perfused/blood	1.10	1.10
	Poorly perfused/blood	0.94	0.94
	Fat/blood	0.04	0.04
<b>Metabolite (2-EAA)</b>			
	Liver/blood	1.10	1.10
	Rapidly perfused/blood	1.05	1.05
	Poorly perfused/blood	0.50	0.50
	Fat/blood	0.32	0.32
Biochemical parameters			
	First order rate EGEE to 2-EAA (L blood/h/kg liver)	223	76,6
	First order rate EGEE to EG (L blood/h/kg liver)	66.9	41.4
	Urinary excretion rate of 2-EAA (h <sup>-1</sup> )	0.015	0.4

<b>Ethoxyethylacetate (ethylene glycol monoethyl ether acetate)</b>		
Species	Rat	Human
Reference	<b>53</b>	<b>53</b>
Partition coefficients		
Blood/air	3822	3822
Liver/blood	1.0	1.0
Rapidly perfused/blood	1.1	1.1
Poorly perfused/blood	0.94	0.94
Fat/blood	1.3	1.3
Biochemical parameters		
First order rate EGEEA to EGEE (L blood/h)	2.3	2.3

### Ethyl acrylate

Species		Rat
Reference		<b>45</b>
Coefficients partition		
	Blood/air	367
	Lung/blood	0.29 ± 0.07
	Liver/blood	0.40 ± 0.09
	Skin/blood	0.18 ± 0.09
	Kidney/blood	0.31 ± 0.07
	Muscle/blood	0.33 ± 0.13
	Fat/blood	0.63 ± 0.27
	Forestomach/blood	0.19 ± 0.06
	Glandular stomach/blood	0.28 ± 0.07
	Duodenum/blood	0.28 ± 0.07
	Small intestine/blood	0.47 ± 0.12
	Cecum/blood	0.41 ± 0.12
	Large intestine/blood	0.40 ± 0.16
	Colon/blood	0.30 ± 0.10
Biochemicals parameters		
Metabolic constants		
VmaxC (µmol/ml tissue/min) Hydrolysis rate		
	Lung	5.3
	Liver	31.7
	Skin	0.86
	Kidney	3.5
	Muscle	0.17
	Fat	1.6
	Other perfused tissues	0.79
	Venous blood	0.18
	Arterial blood	0.18
	Forestomach	0.26
	Glandular stomach	0.32
	Duodenum	0.55
	Small intestine	0.71
	Cecum	0.79
	Large intestine	0.54
	Colon	0.83
Km (µmol/ml tissue) Hydrolysis rate		
	Lung	1.88
	Liver	1.9
	Skin	5.45
	Kidney	15.18
	Muscle	4.47
	Fat	5.02
	Other perfused tissues	3.93
	Venous blood	4.6
	Arterial blood	4.6
	Forestomach	3,15
	Glandular stomach	4.4
	Duodenum	8.23
	Small intestine	5.9
	Cecum	3.93
	Large intestine	4.75
	Colon	4.21
GSH rate ( M-1.min-1)		
		33.0

<b>Ethylbenzene</b>					
Species	Rat	Rat	Human	Human	Human
Reference	<b>129</b>	<b>58</b>	<b>129</b>	<b>60</b>	<b>63</b>
Partition coefficients					
Blood/air	42.7	42.7	28	28	28.4
Liver/blood	1.96	1.96	2.99	2.99	3.49
Slowly perfuseds/blood	0.61	0.61	0.93	0.93	
Richly perfused/blood	1.41	1.41	2.15	2.15	
Fat/blood	36.44	36.44	55.57	55.57	93.73
Muscle and skin/blood					1.86
Brain/blood					3.80
Kidneys/blood					1.90
Others/blood					2.43
Biochemical parameters					
VmaxC (mg/h/kg)	7.3	6.39	7.3	6.39	7.3
Km (mg/L)	1.39	1.04	1.39	1.04	1.39
<b>Inhibition constants (mg/L)</b>					
<i>Ki</i> competitive (dichloromethane)		0.112		0.11	
<i>Ki</i> competitive (toluene)	0.33	0.168	0.33	0.17	
<i>Ki</i> competitive (m-xylene)	0.23	0.505	0.23	0.51	1.5
<i>Ki</i> competitive (benzene)		0.256		0.26	
Urinary excretion rate mandelic acid (h-1)					0.231

<b>Ethylene dibromide</b>		
Species	Rat	Human
Reference	<b>112</b>	<b>112</b>
Partition coefficients		
Blood/air	74.1	74.1
Liver/blood	0.92	0.92
Fat/blood	10.69	10.69
Richly perfused/blood	0.92	0.92
Slowly perfuseds/blood	0.55	0.55
Biochemical parameters		
Vmax CYP2E1 ( $\mu\text{mol/h/kg liver}$ )	414	503
Km CYP2E1 ( $\mu\text{M}$ )	19	42
First order rate constant GST pathway ( $\mu\text{mol/h/kg liver at } 1\mu\text{M}$ )	3.7	2.7

<b>Ethylene oxide</b>	
Species	Rat
Reference	<b>80</b>
Partition coefficients	
Blood/air	64.14
Liver/blood	0.96
Slowly perfuseds/blood	0.75
Testis/blood	1.29
Fat/blood	0.69
Brain/blood	0.92
Lung/blood	0.95
Richly perfuseds/blood	1.05
Biochemical parameters	
Hydrolysis (h <sup>-1</sup> , whole body except fat)	0.62
GSH conjugation (L. mmol GSH <sup>-1</sup> .h <sup>-1</sup> )	
Liver	2.04
Lung	1.31
Testis	0.98
Other tissues	0.21
Hemoglobin binding (L.mg Hb <sup>-1</sup> .h <sup>-1</sup> )	
N-hydroxyethyl valine	3,3 x 10 <sup>-8</sup>
N <sup>1</sup> -hydroxyethyl histidine	3, x 10 <sup>-8</sup>
N <sup>3</sup> -hydroxyethyl histidine	2,0 x 10 <sup>-8</sup>
N-hydroxyethyl cysteine	3,3 x 10 <sup>-7</sup>
DNA binding (L.mg DNA <sup>-1</sup> h <sup>-1</sup> )	
Testis	1,7E-08
All other tissues	2,8E-08



<b>Fluoride</b>		
Species	Rat	Human
Reference	<b>115</b>	<b>115</b>
Partition coefficients		
Plasma/blood	1.333	1.333
Liver/plasma	0.98	0.98
Kidneys/plasma	4.16	4.16
Rapidly perfused/plasma	0.83	0.83
Slowly perfused/plasma	0.63	0.63
Bone/plasma	1000-4000	1000
Kinetic constants		
Bone clearance	Variable	Variable
Renal clearance (youth)	*	*
Renal clearance (adult) (ml/min/kg)	7.2	2.9
<i>K<sub>bpl</sub></i> (bone to plasma) (kg <sup>-1</sup> . hr <sup>-1</sup> ) * age factor	0.016	0.016

\* Clearance = 30.6\*exp(-0.166\*age)

<b>Furan</b>			
Species	Mouse	Rat	Human
Reference	<b>68</b>	<b>68</b>	<b>68</b>
Partition coefficients			
Blood/air	6.59	6.59	6.59
Liver/blood	0.901	0.901	0.901
Fat/blood	9.721	9.721	9.721
Rapidly perfused/blood	0.901	0.901	0.901
Slowly perfused/blood	0.642	0.642	0.642
Biochemical parameters			
VmaxC ( $\mu\text{mol/h/kg}$ )	112	60.8	242.7 - 560.8
Km ( $\mu\text{M}$ )	1	0.4	2.1 - 3.3

<b>Heptafluoropropane (HFC-227ea)</b>	
Species	Human
Reference	<b>140</b>
Partition coefficients	
Blood/air	0.23
Liver/blood	1.83
Rapidly perfused/blood	1.83
Poorly perfused/blood	1.57
Fat/blood	6.87
Gut/blood	1.96
Biochemical parameters	
VmaxC (mg/h/kg)	0
Km (mg/L)	N/A

<b>Hexabromobiphenyl (2,2',4,4',5,5'-)</b>		
Species	Rat	Human
Reference	<b>137</b>	<b>137</b>
Partition coefficients		
Liver/blood	17	17
Muscle/blood	5	5
Fat/blood	340	340
Skin/blood	56.5	57
Intestine tissue/blood	1	1
Biochemical parameters		
<i>K<sub>b</sub></i> Biliary clearance(ml/hr)	0.074	5.06
<i>K<sub>G</sub></i> Permeability constant (h <sup>-1</sup> )	0.7	0.7
<i>K<sub>s</sub></i> Stomach transport (h <sup>-1</sup> )	0.87	0.82
<i>K<sub>f</sub></i> Fecal transport (h <sup>-1</sup> )	0.095	0.05

<b>Hexachlorobenzene</b>			
<b>Species</b>	<b>Rat</b>	<b>Rat (female)</b>	<b>Human (female)</b>
<b>Reference</b>	<b>46</b>	<b>146</b>	<b>146</b>
<b>Partition coefficients</b>			
Muscle + skeleton/plasma	3.16		
Lung/plasma	7.7		
Liver/plasma	11.4		
Kidney/plasma	8.67		
Fat/plasma	258		
Colon/plasma	7.17		
Spleen/plasma	4.16		
Skin/plasma	25.7		
Centralnervous system/plasma	6.47		
Heart/plasma	6.86		
GI tract/plasma	8.25		
Colon/feces	0.9		
Kidney/urine	16.0		
Systemic circulation/blood		0.25	0.25
Brain/blood		7.7	7.7
Kidney/blood		5.3	5.3
Liver/blood		13.1	13.1
Intestinal lumen/blood		1	1
Richly peRfused tissues/blood		10	10
Poorly perfused tissues/blood		267	267
Breast/blood		60	60
<b>Biochemicals parameters</b>			
Unavailable HCB upper limits (µg/g)			
Systemic circulation		4	4
Brain		200	200
Kidney		100	100
Liver		300	300
Intestinal lumen		0	0
Richly pefused tissue		200	200
Poorly perfused tissue		$6.0 \times 10^{+3}$	$6,0 \times 10^{+3}$
Breast		$1.0 \times 10^{+6}$	$1,0 \times 10^{+6}$
Factors modulating rate of uptake /Kidney		0.75	0.75
Factors modulating tissues clearance / Poorly perfused tissues		0.9	0.9
First order metabolic constant in liver (h-1)		0.2310	0.2310
First order absorption rate Intestinal lumen/blood (h-1)		0.3466	0.3466
First order secretion rate bile/lumen (h-1)		4.1586	4.1586
First order elimination constant / feces (h-1)		0.0289	0.0289
First order excretion constant / urine (h-1)		0.1155	0.1155

Hexachlorobiphenyl (2,2',3,3',6,6'-)				
Species		Rat	Monkey	Dog
Reference		<b>97</b>	<b>97</b>	<b>97</b>
Coefficients partition				
Parent compound				
	Muscle/blood	10.0	4.0	4.0
	Skin/blood	20	40	8
	Fat/blood	200	250	30
	Liver/blood	10	20	2
Metabolite				
	Muscle/blood	0.3	0.1	0.1
	Skin/blood	1	0.5	0.2
	Fat/blood	1	1	0.25
	Liver/blood	3	5	10
Biochemical parameters				
	<i>km</i> Metabolic clearance HCB (ml/min)	5	15	183
	<i>kB</i> Biliary clearance of metabolite (ml/min)	1	0,5	7
	<i>kK</i> Kidney clearance of metabolite (ml/min)	0.03	0.4	2
	<i>kF</i> Fecal transport of metabolite ( $h^{-1}$ )		0.04	0.04
	<i>F</i> Fraction of preferential excretion by the liver ( $km^*(1-F)$ )		0.4	0.3

Hexachlorobiphenyl (2,2',4,4',5,5'-) (PCB153)								
Species		Mouse	Mouse	Mouse	Rat	Rat	Monkey	Dog
Reference		136	97	86	3	97	97	97
Coefficients partition								
Parent compound								
	Muscle/blood	5 (4)	5.0	5.0	4.0	4.0	7.0	6.0
	Skin/blood	35 (30)	35	35	30	30	70	30
	Fat/blood	300 (400)	300	300	400	400	500	300
	Liver/blood	10 (12)	10	10	12	12	30	10
	Gut lumen/blood				1			
	Brain/blood			2.5				
Metabolite								
	Muscle/blood	3 (0.3)	3		0.3	0.3	1	0.2
	Skin/blood	5 (2)	5		2	2	3	0.7
	Fat/blood	1 (2)	1		2	2	9	2
	Liver/blood	10 (4)	10		4	4	5	10
	Gut lumen/blood				1			
Biochemical parameters								
	<i>km</i> Metabolic clearance HCB (ml/min)	0.01 (0.011)	0.01	0.01	0.045	0.045	0.67	16
	<i>kB</i> Biliary clearance of metabolite (ml/min)	0.074 (0.073)	0.074		0.3	0.3	0.7	1.8
		0.018						
	<i>kK</i> Kidney clearance of metabolite (ml/min)	(0.0074)	0.018		0.03	0.03	0.041	0.15
	<i>KG</i> Gut reabsorption of metabolite (h <sup>-1</sup> )	(0.016)	0		0.0096	0	0	0
	<i>KAS</i> Absorption coefficient upper GI			0.415				
	<i>KAD</i> Absorption coefficient Lower GI			0.077				
	<i>KT</i> Elimination coefficient upper GI			10				
	<i>KE</i> Elimination coefficient lower GI			0.073				
	<i>kF</i> Fecal transport of metabolite (h <sup>-1</sup> )	(0.08)			0.048		0.04	0.04
	<i>F</i> Fraction of preferential excretion by the liver ( <i>km</i> *(1- <i>F</i> ))						0.4	0.4
	<i>PAFC</i> Diffusion permeation constant in fat			10				

<b>Hexachloroethane</b>	
Species	Rat
Reference	<b>50</b>
Partition coefficients	
Blood/air	62.7
Liver/blood	5.88
Slowly perfused/blood	1.2
Fat/blood	52.9
Biochemical parameters	
VmaxC (mg/h/kg)	1.97
Km (mg/L)	0.8



<b>Isoprene</b>			
Species	Mouse	Rat	Human
Reference	<b>40</b>	<b>40</b>	<b>40</b>
Partition coefficients			
Blood/air	2.04	2.33	0.75
Muscle/blood	0.73	0.64	1.97
Fat/blood	30.2	26.4	82.0
Liver/blood	0.95	0.83	2.57
Kidney/blood	0.86	0.75	2.33
Richly perfused/blood	0.91	0.79	2.45
Biochemical parameters			
Liver metabolism			
Vmax mo1 ( $\mu\text{mol/h}$ )	9.18	24.8	1060 and 1690
Km (mmol/l)	0.004	0.002	0.002
Richly perfused tissues metabolism			
Vmax mo2 ( $\mu\text{mol/h}$ )	1.02	2.75	118 and 188
Km (mmol/l)	0.004	0.002	0.002
Endogenous production rate ( $\mu\text{mol/h}$ )			
			23.8

<b>Isopropanol</b>		
Species	Rat	Human
Reference	<b>18</b>	<b>18</b>
Partition coefficients		
Blood/air	1290	848
Brain/blood	0.88	1.33
Fat/blood	0.21	0.32
Liver/blood	0.76	1.16
Rapidly perfused/blood	0.79	1.25
Slowly perfused/blood	0.85	1.3
Saline/air	1500	1500
Mucus/air	1290	848
Biochemical parameters		
VmaxC (mg/h/kg)	150	300
Km (mg/L)	500	10
<i>CL<sub>muc</sub></i> Clearance into upper respiratory tract (L/h/kg)	11	11
<i>Cl<sub>ur</sub></i> Urinary clearance (L/h)		0.004
<i>KTD</i> Fecal clearance (h <sup>-1</sup> )	0.25	0
<i>P</i> Skin permeability coefficient (cm/h)	0.008	
<i>KAS</i> First-order absorption stomach/peritoneum (h <sup>-1</sup> )	2.0	1.0
<i>KTSD</i> Transfer from stomach to duodenum (h <sup>-1</sup> )	3.0	10.0
<i>KAD</i> First-order absorption from duodenum (h <sup>-1</sup> )	0.5	8.0

<b>Lead</b>				
Species	Rat (absence of As-Ac)	Rat (presence of As-Ac)	Rat	Human
Reference	<b>31</b>	<b>31</b>	<b>106</b>	<b>107</b>
Partition coefficients				
RBC/plasma	46.3	43.8		
Liver/plasma	2094.1	1632.4	75	100
Lung/plasma	800	732.4		
Bone/plasma	5756	4051	6000	1000
Kidney/plasma	2445.6	2305	variable	100
Carcass/plasma	200	539.3		
Well-perfused/plasma			75	100
Poorly perfused/plasma			20	20
Mass transfer coefficient of drug from plasma to lung	500	516		
Mass transfer coefficient of drug from plasma to bone	1216.2	445.7		
Mass transfer coefficient of drug from plasma to kidney	803	449.5		
Mass transfer coefficient of drug from bone to plasma	2860	1369		
Mass transfer coefficient of drug from kidney to plasma	569	536.5		
Biochemical parameters				
Max binding capacity in blood (mg/L)			10	2.7
Half-saturation concentration of binding in blood (mg/L)			0.067	0.0075
Fractional Cl of lead into forming bone (liters plasma cleared/liter new bone formed)			15000	15000
Elimination clearance (liter/day/kg)			14	Var
Within-bone movement permeability coefficient (cm/day/unit)			$8.0 \times 10^{-7}$	$1.0 \times 10^{-7}$
Bone-to-plasma transfer permeability coefficient (cm/day/unit)			$8.0 \times 10^{-7}$	$1.0 \times 10^{-7}$
Plasma-to-bone transfer permeability coefficient (cm/day/unit)			0.1	0.08

<b>Lindane</b>	
Species	Rat
Reference	<b>33</b>
Coefficients partition	
Liver/blood	4.2
Fat/blood	95.3
Slowly perfused/blood	1.6
Brain/blood	4.1
Biochemical parameters	
Biotransformation rate ( $\text{hr}^{-1} \cdot \text{kg}^{-1}$ )	4.5
Oral /intraperitoneal uptake rate ( $\text{h}^{-1}$ )	0.035
Oral /intraperitoneal uptake efficiency	0.8

<b>Methyl Mercury</b>		
Species		Rat
Reference		<b>38</b>
Partition coefficients		Rat
		<b>55</b>
Liver/blood		0.18
Liver/plasma		14.2
Kidney/blood		1.5
Kidney/plasma		164
Brain/blood		0.08
Brain/plasma		11.1
Skin/blood		0.08
Skin/plasma		14.2
GI tissue/blood		0.1
GI lumen/tissue		0.28
Urine/blood		0.008
Carcass/blood		0.1
RBC/plasma		302
Muscle/plasma		14.5
Transport process		
	Blood to brain(ml blood/min/g tissue)	$3.50 \times 10^{-5}$
	Blood to carcass (ml blood/min/g tissue)	$7.70 \times 10^{-4}$
	Blood to liver (ml blood/min/g tissue)	$9.10 \times 10^{-4}$
	Blood to kidney (ml blood/min/g tissue)	$2.00 \times 10^{-2}$
	Blood to skin (ml blood/min/g tissue)	$1.00 \times 10^{-3}$
	Blood to GI tissues (ml blood/min/g tissue)	$8.60 \times 10^{-3}$
	GI tissue to lumen(ml tissue/min/g tissue)	$1.00 \times 10^{-2}$
	Skin to hair (ml skin/min/g skin)	$1.20 \times 10^{-4}$
Membrane transfer constants ( $\text{min}^{-1}$ )		
	Liver	0.506
	Kidney	1.55

	Brain	0.028
	RBC	1.0
	Muscle	0.063
	Skin	0.506
Biochemical parameters		
Biliary clearance ratio of NPSH compounds from liver to mercury from liver	0.5	
Biliary secretion rate kB (excr. rate/liver MeHg mass) ( $\text{min}^{-1}$ )		0.0021
Demethylation in GI lumen ( $\text{min}^{-1}$ )	$3.00 \times 10^{-3}$	
Demethylation in liver ( $\text{min}^{-1}$ )	$2.00 \times 10^{-4}$	
Loss of mercuric mercury from kidney via exfoliation of tubular cells ( $\text{min}^{-1}$ )	$2.80 \times 10^{-6}$	
Loss of mercury in hair to surroundings ( $\text{min}^{-1}$ )	$2.40 \times 10^{-6}$	
Ingestion of mercury in hair during grooming ( $\text{min}^{-1}$ )	$3.40 \times 10^{-6}$	
Gut reabsorption rate kA (reabsorption rate/excr. rate x gut vol./fecal flow rate) ( $\text{min}^{-1}$ )		0.0026
Excretion rate (average over 10 days) (mg/min)		$8.68 \times 10^{-6}$
Reabsorption rate (average over 10 days) (mg/min)		$7.99 \times 10^{-6}$

<b>Inorganic Mercury</b>	
Species	Rat
Reference	<b>38</b>
Partition coefficients	
Liver/blood	11.5
Kidney/blood	600
Brain/blood	0.8
Skin/blood	2.7
GI tissue/blood	0.45
GI lumen/tissue	10
Urine/blood	
Carcass/blood	0.45
Biochemical parameters	
Transport process	
Blood to brain(ml blood/min/g tissue)	$3.20 \times 10^{-5}$
Blood to carcass (ml blood/min/g tissue)	$3.10 \times 10^{-4}$
Blood to liver (ml blood/min/g tissue)	$9.10 \times 10^{-2}$
Blood to kidney (ml blood/min/g tissue)	$8.40 \times 10^{-3}$
Blood to skin (ml blood/min/g tissue)	$4.20 \times 10^{-4}$
Blood to GI tissues (ml blood/min/g tissue)	$3.50 \times 10^{-3}$
GI tissue to lumen(ml tissue/min/g tissue)	$2.00 \times 10^{-4}$
Skin to hair (ml skin/min/g skin)	$1.20 \times 10^{-4}$
Renal filtration clearance of mercuric mercury (ml blood/min/g kidney)	$3.50 \times 10^{-4}$
Biliary clearance ratio of NPSH compounds from liver to mercury from liver	3
Loss of mercuric mercury from kidney via exfoliation of tubular cells	$2.80 \times 10^{-6}$

<b>Methanol</b>							
Species		Mouse	Rat	Rat	Monkey	Human	
Reference		<b>143</b>	<b>61</b>	<b>143</b>	<b>61</b>	<b>61</b>	
Partition coefficients							
	Blood/air		1349		1349	1349	
	Liver/blood	1.06	1.6	1.6	1.6	1.6	
	Kidney/blood	0.731	1.3	1.3	1.3	1.3	
	Rapidly perfused /blood	1.06	1.3	1.6	1.3	1.3	
	Slowly perfused /blood	0.649	1.1		1.1	1.1	
	Fat/blood	0.083		1.1			
	Conceptus/blood	1.12					
Biochemical parameters							
	Methanol						
		VmaxC 1 (mg/h/kg)	134	15.41	63.2	15.41	15.41
		Km1 (mg/L)	48.7	33.92	44.8	33.92	33.92
		VmaxC 2 (mg/h/kg)		7		33.43	33.43
		Km2 (mg/L)		15		394	384
	Formaldehyde						
		VmaxC (mmol/h/kg)		7.69		7.69	7.69
		Km (mmol/L)		0.127		0.127	0.127
	Formate						
		VmaxC (mmol/h/kg)		0.995		0.995	0.995
		Km (mmol/L)		1.97		4.86	4.86
	Renal extraction efficiencies						
		Methanol		0.007		0.007	0.007
		Formate		0.25		0.25	0.25
	First-order pathway for MeOH elimination ( $h^{-1}$ )						
	<i>K<sub>af</sub></i> Fast oral absorption constant ( $h^{-1}$ )		16.8		8.18		
	<i>K<sub>as</sub></i> Slow oral absorption constant ( $h^{-1}$ )		4.53		0.2		
	<i>K<sub>f</sub></i> % of MeOH absorbed via fast oral absorption		68		50.4		



<b>Methoxyethanol (2-)</b>				
Species	Mouse	Mouse	Rat	Human
Reference	<b>16</b>	<b>130</b>	<b>53</b>	<b>53</b>
Partition coefficients				
Blood/air	34913	34913	32800	N/A
Liver/blood	1.02	1.02	1.0	1.1
Poorly perfused/blood	0.93	0.93	0.94	0.5
Richly perfused/blood	1.02		1.1	1.05
Fat/blood	0.05	0.05	0.04	0.034
Biochemical parameters				
V <sub>max</sub> <sub>MA</sub> (mmol/h/kg)	2.4	2.4		
K <sub>m</sub> <sub>MA</sub> (mmol/L)	0.15	0.15		
V <sub>max</sub> <sub>EG</sub> (mmol/h/kg)	0.16	0.16		
K <sub>m</sub> <sub>EG</sub> (mmol/L)	0.0083	0.0083		
K <sub>maac</sub> 2-ME to MAA (L/h/kg liver)			31	4.9
K <sub>egc</sub> 2-ME to EG (L/h/kg liver)			4.03	0.3
K <sub>a</sub> <sub>po</sub> Absorption from GI tract (h <sup>-1</sup> )	14.375			
Urinary excretion (L/h)			0.004	0.3

<b>Methyl ter-butyl ether</b>		
Species	Rat	Human
Reference	<b>12</b>	<b>91</b>
Partition coefficients		
Blood/air	11.5	17.7
Kidney/blood	3.11	0.72
Liver/blood	1.18	0.72
Richly perfused/blood	1.18	0.72
Fat/blood	10.05	4.79
Poorly perfused/blood	0.57	1.18
Biochemical parameters		
VmaxC pathway A ( $\mu\text{mol/h/kg}$ )	104.4	33.8
Km pathway A ( $\mu\text{M}$ )	264.3	61.7
VmaxC pathway B ( $\mu\text{mol/h/kg}$ )	8.3	6.2
Km pathway B ( $\mu\text{M}$ )	1.4	3.8

<b>Methylethylketone</b>		
Species	Rat	Human
Reference	<b>132</b>	<b>119</b>
Partition coefficients		
Blood/air	138	125
Lung/blood		0.82
GI Tract/blood		0.86
Liver/blood	1.10	0.86
Richly perfused/blood	1.10	0.86
Poorly perfused/blood	1.34	0.86
Fat/blood	0.73	1.30
Muscle/blood		0.82
Saline:air	143	
Biochemical parameters		
Vmax ( $\mu\text{mol}/\text{min}$ )		30.0
VmaxC (mg/h/kg)	5.44	
Km (mg/L)	0.63	0.144
<i>Kfo</i> First-order metabolic pathway constant ( $\text{h}^{-1}$ )	4.1	
<i>Ka</i> Absorption rate constant IP ( $\text{h}^{-1}$ )	0.91	
<i>Kas</i> Absorption rate constant oral ( $\text{h}^{-1}$ )	1.86	

<b>m-Xylene</b>									
Species	Rat	Rat	Rat	Human	Human	Human	Human	Human	Human
Reference	128	129	58	67	82	129	96	60	63
<b>Partition coefficients</b>									
Blood/air	46	46	46	26.4	26.4	26.4	19	26.4	34
Liver/blood	1.97	1.98	1.98	3.02	3.02	3.44	14.67	3.44	3.32
Slowly perfuseds/blood	0.91	0.91	0.91	2.01	2.01	1.59	2.79	1.59	
Richly perfused/blood	1.97	1.98	1.98	4.42	4.42	3.44	6.14	3.44	
Fat/blood	40.4	40.41	40.41	77.8	77.8	70.42	98.63	70.42	89.26
Lung /blood				4.09	4.09				
GI tract/blood				4.67	4.67				
Muscle + skin/blood				3.01	3.01				1.79
Muscle/blood							12.34		
Skin/blood							2.65		
Brain/blood									3.65
Kidneys/blood									1.82
Others/blood									2.32
<b>Biochemical parameters</b>									
VmaxC (mg/h/kg)	8.4	5.5	6.49	8.88 – 7.10		5.5	8.2	6.49	8.4
Km (mg/L)	0.2	0.20	0.45	3.5 – 35.04		0.20	0.1	0.45	0.2
Hepatic clearance (l/min)					2.16				
Kp Skin permeability constant (m/h)							0.005		
<b>Inhibition constants (mg/L)</b>									
Ki competitive (toluene)	0.6	0.77	0.328			0.77		0.33	
Ki competitive (benzene)			0.216					0.22	
Ki competitive (ethylbenzene)		1.5	1.667			1.5		1.67	0.23
Ki competitive (Dichloromethane)			0.322					0.32	
<b>Metabolite (MHA)</b>									
Urinary excretion rate MHA (h <sup>-1</sup> )				0.72	0.72				1.386
Fraction transformed in MHA							0.93		
K1 Removal of MHA from blood (h <sup>-1</sup> )							1.5		
K2 Appearance of MHA in urine (h <sup>-1</sup> )							0.9		

<b>Naphthalene</b>				
Species		Mouse	Rat	
Reference		<b>125</b>	<b>125</b>	
Coefficients partition				
	Fat/blood	796	796	
	Liver/blood	5.41	5.41	
	Lung/blood	0.627	0.627	
	Well-perfused tissues/blood	4	4	
	Muscle/blood	4.13	4,13	
	Kidney/blood	3.87	3.87	
Biochemical parameters				
	Lung RS			
		Vmax P450 (nmol/mg mp/min)	9	1.5
		Km N P450 ( $\mu$ M)	100	400
		Vmax EH (nmol/mg mp/min)	0.7	7
		Km NO EH ( $\mu$ M)	1	1
	Lung SR			
		Vmax P450 (nmol/mg mp/min)	1,1	3.4
		Km N P450 ( $\mu$ M)	400	1540
		Vmax EH (nmol/mg mp/min)	7	11.5
		Km NO EH ( $\mu$ M)	12	12
	Liver RS			
		Vmax P450 (nmol/mg mp/min)	7	1.8
		Km N P450 ( $\mu$ M)	310	400
		Vmax EH (nmol/mg mp/min)	2	3
		Km NO EH ( $\mu$ M)	1	1
	Liver SR			
		Vmax P450 (nmol/mg mp/min)	7	7.3
		Km N P450 ( $\mu$ M)	310	800
		Vmax EH (nmol/mg mp/min)	8	4.9
		Km NO EH ( $\mu$ M)	12	12

<b>Naphthalene Oxide</b>			
Species		Mouse	Rat
Reference		<b>125</b>	<b>125</b>
Coefficients partition			
	Fat/blood	796	796
	Liver/blood	5.41	5.41
	Lung/blood	0.627	0.627
	Well-perfused tissues/blood	4	4
	Muscle/blood	4.13	4.13
	Kidney/blood	3.87	3.87
Biochemical parameters			
	Lung		
		<i>V<sub>max</sub></i> GST (nmol/mg cp/min)	22.5      400
		<i>K<sub>m</sub><sup>NO</sup></i> GST (μM)	50      50
		<i>K<sub>m</sub><sup>GSH</sup></i> GST (μM)	3300      3300
		<i>K<sub>NOH</sub></i> (nmol/μM NO/min)	0.25      0.25
		<i>k<sub>b</sub></i> (nmol/mg tp/min)	2.00 x 10 <sup>-4</sup> 2.00 x 10 <sup>-4</sup>
		<i>C<sub>x</sub></i> GSHss (μM)	2200      1100
		<i>k<sub>x</sub></i> GD (L/min)	0.002      0.003
		<i>k<sub>x</sub></i> GSD <sub>1</sub> (L/min)	0.005      0.0025
		<i>k<sub>x</sub></i> GSS (nmol/mg mp/min)	5.80 x 10 <sup>-5</sup> 2.10 x 10 <sup>-5</sup>
		<i>K<sub>m</sub></i> GS (μM)	2000      2000
		Qty of microsomes (mg/g)	3.7      3.7
	Liver		
		<i>V<sub>max</sub></i> GST (nmol/mg cp/min)	150      500
		<i>K<sub>m</sub><sup>NO</sup></i> GST (μM)	50      50
		<i>K<sub>m</sub><sup>GSH</sup></i> GST (μM)	3300      3300
		<i>K<sub>NOH</sub></i> (nmol/μM NO/min)	0.25      0.25
		<i>k<sub>b</sub></i> (nmol/mg tp/min)	2.00 x 10 <sup>-4</sup> 2.00 x 10 <sup>-4</sup>
		<i>C<sub>x</sub></i> GSHss (μM)	6600      5500
		<i>k<sub>x</sub></i> GD (L/min)	0.006      0.003
		<i>k<sub>x</sub></i> GSD (L/min)	0.005      0.0025
		<i>k<sub>x</sub></i> GSS (nmol/mg mp/min)	2.40 <sup>E</sup> -04      3.70E-04
		<i>K<sub>m</sub></i> GS (μM)	2000      2000
		Qty of microsomes (mg/g)	16.4      16.4

<b>Nicotine</b>	
Species	Rat
Reference	<b>113</b>
Coefficients partition	
Muscle/blood	1.1
Skin/blood	1.1
Fat/blood	0.2
Liver/blood	7.0
Kidney/blood	24.8
Brain/blood	1.4
Heart/blood	0.6
Lung/blood	0.9
Poorly perfused/blood	6.4
Biochemical parameters	
<b>Metabolic constants</b>	
<i>V<sub>max</sub></i> Metabolism of nicotine to cotinine (μmol/h)	≥ 7.6
<i>K<sub>m</sub></i> Michaelis constnat of nicotine to cotinine (μM)	≥ 9
<i>K<sub>NC</sub></i> First-oder rate constant metabolism to cotinine (h <sup>-1</sup> )	75.8
<i>K<sub>NP</sub></i> First-oder rate constant metabolism to polar metabolites (h <sup>-1</sup> )	24.3
<i>K<sub>CP</sub></i> First-order rate transformation cotinine to polar metab. (h <sup>-1</sup> )	<0.001
<b>Nicotine binding constants</b>	
<i>B<sub>max</sub></i> Maximum binding capacity (nmol/heart)	0.039
<i>B<sub>max</sub></i> Maximum binding capacity (nmol/brain)	0.009
<i>B<sub>max</sub></i> Maximum binding capacity (nmol/lung)	0.039
<i>K<sub>D</sub></i> Dissociation constant (heart) nM	0.12
<i>K<sub>D</sub></i> Dissociation constant (brain) nM	0.12
<i>K<sub>D</sub></i> Dissociation constant (lung) nM	2.04

<b>Nitropyrene (1-)</b>		
Species		Rat
Reference		<b>104</b>
Coefficients partition		
	Kidney/blood	1
	Liver/blood	1
	Lung/blood	0.5
	Other tissues/blood	0.5
Biochemical parameters		
	Rate cst ( $h^{-1}$ )	
		GI absorption
		Metabolism
		Urinary excretion
		Biliary excretion
	Covalent Binding formation ( $h^{-1}$ )	
		Lung
		liver
		Kidney
		Other tissues
	Covalent Binding removal ( $h^{-1}$ )	
		Lung
		liver
		Kidney
		Other tissues



<b><i>n</i>-Hexane (2,5 Hexadione)</b>			
Species	Rat	Human	Human
Reference	<b>2</b>	<b>110</b>	<b>2</b>
Partition coefficients			
Blood/air	2.29	0.8	0.8
Liver/blood	2.27	6.5	6.5
Rapidly perfused/blood	2.27	5	6.5
Poorly perfused/blood	1.27	6.2	3.63
Fat/blood	69.43	130	198.75
Biochemical parameters			
V <sub>max</sub> C (mg/h/kg)	1.35		1.35
K <sub>m</sub> (mg/L)	0.4		0.4
<i>K<sub>i</sub></i> Competitive inhibition constant (toluene)	0.059		0.059
<i>K1</i> Rate of hexane disappearance (min <sup>-1</sup> )		0.3	
<i>K2</i> Rate of 2,5-hexanedione formation (min <sup>-1</sup> )		0.012	

<b>Parathion</b>		
Species		Mouse
Reference		<b>124</b>
Coefficients partition		
Liver/blood		6.56
Lung/blood		2.55
Brain/blood		3.51
Diaphragm/blood		1.37
Fat/blood		11.84
Rapidly perfused/blood		6.56
Slowly perfused/blood		4.51
Biochemical parameters		
Oxydative activation		
	Vmax (mg/hr)	2.07
	Km (mg/L)	7.21
Detoxification		
	Vmax (mg/hr)	1.78
	Km(mg/L)	7.22

<b>p-Chlorobenzotrifluoride (PCBTF)</b>		
Species	Rat	Human
Reference	<b>76</b>	<b>76</b>
Partition coefficients		
Parent compound (PCBTF)		
Blood/air	43.7	16.7
	1.17	
Liver/blood	(1.197)	3.07
Rapidly perfused/blood	0.86	2.26
Slowly perfused/blood	2.45	6.41
Fat/blood	22.4 (27.9)	58.6
Kidney/blood	0.86 (1.22)	2.26
Brain/blood	0.92 (1.33)	2.40
Metabolite (3-OH PCBTF)		
Liver/blood	1.11	1.11
Rapidly perfused/blood	1.09	1.09
Slowly perfused/blood	0.78	0.78
Fat/blood	20.0	20.0
Kidney/blood	1.31	1.31
Metabolite (2,3-diOH PCBTF)		
Liver/blood	1.0	1.0
Rapidly perfused/blood	1.0	1.0
Slowly perfused/blood	1.0	1.0
Fat/blood	20.0	20.0
Kidney/blood	1.0	1.0
Biochemical parameters		
PCBTF to 3-OH PCBTF		
Vmax1C ( $\mu\text{mol/h/kg}$ )	1.0	1.0
Km1 ( $\mu\text{M}$ )	65.7	65.7
PCBTF to 2,3-diOH PCBTF		
Vmax2C ( $\mu\text{mol/h/kg}$ )	1.0	1.0
Km2 ( $\mu\text{M}$ )	65.7	65.7
PCBTF glutathione conjugaison		
KCSC ( $\text{h}^{-1} \cdot \text{kg}^{-1}$ )	$5.0 \times 10^{-5}$	$5.0 \times 10^{-5}$
3-OH PCBTF glucuronic acid conjugaison		
Vmax4C ( $\mu\text{mol/h/kg}$ )	60	60
Km4 ( $\mu\text{M}$ )	12	12
2,3-diOH PCBTF glucuronic acid conjugaison		
Vmax5C ( $\mu\text{mol/h/kg}$ )	60	60
Km5 ( $\mu\text{M}$ )	12	12

<b>Pentachlorobiphenyl (2,2',4,5,5'-) (5-CB)</b>			
Species		Mouse	Rat
Reference		<b>136</b>	<b>136</b>
Coefficients partition			
Parent compound			
	Muscle/blood	5 (1)	1.0
	Skin/blood	20 (7)	7
	Fat/blood	200 (70)	70
	Liver/blood	14 (6)	6
	Gut lumen/blood		1
Metabolite			
	Muscle/blood	(0.1)	0.1
	Skin/blood	(0.1)	0.1
	Fat/blood	(0.4)	0.4
	Liver/blood	(2)	2
	Gut lumen/blood		1
Biochemical parameters			
	<i>km</i> Metabolic clearance DCB (ml/min)	(0.095)	0.39
	<i>kB</i> Biliary clearance of metabolite (ml/min)	0.0088 (0.01)	0.30
		0.00883	
	<i>kK</i> Kidney clearance of metabolite (ml/min)	(0.00817)	0.033
	<i>KG</i> Gut reabsorption of metabolite ( $h^{-1}$ )	(0.016)	0.010
	<i>kF</i> Fecal transport of metabolite ( $h^{-1}$ )	(0.08)	0.048

<b>Pentachloroethane</b>	
Species	Rat
Reference	<b>50</b>
Partition coefficients	
Blood/air	104
Liver/blood	2.5
Slowly perfused/blood	0.7
Fat/blood	39.6
Biochemical parameters	
VmaxC (mg/h/kg)	9.7
Km (mg/L)	0.9

<b>Pentafluoroethane (HFC-125)</b>	
Species	Human
Reference	<b>140</b>
Partition coefficients	
Blood/air	0.12
Liver/blood	2.17
Rapidly perfused/blood	2.17
Poorly perfused/blood	2.83
Fat/blood	3.75
Gut/blood	3.08
Biochemical parameters	
VmaxC (mg/h/kg)	0
Km (mg/L)	N/A

<b>Phthalate Di(2-ethylhexyl)</b>		
Species		Rat
Reference		<b>73</b>
Coefficients partition		
Parent compound (DEHP)		
	Liver/blood	21.8
	Fat/blood	351
	Muscle/blood	6.1
	Testes/blood	6.5
Metabolite (MEHP)		
	Liver/blood	1.7
	Fat/blood	0.12
	Muscle/blood	0.38
	Testes/blood	1.02
Biochemical parameters		
Parent compound (DEHP)		
	Vmax metabolism in small intestine (mg/h/kg)	100
	Km metabolism in small intestine (mg/L)	18
	Kl (L/h)	0.18
	Ka First-order absorption rate (oral) (L/h)	0.04
	kb First-order metabolism in blood ( $\text{h}^{-1} \cdot \text{kg}^{-1}$ )	$1.0 \times 10^{-6}$
	kl First order metabolism in liver ( $\text{h}^{-1} \cdot \text{kg}^{-1}$ )	0.44
Metabolite (MEHP)		
	Vmax metabolism in liver (mg/h/kg)	12
	Km metabolism in liver (mg/L)	0.5
	Ka First-order absorption rate (oral) (L/h)	7

<b>Polychlorotrifluoroethylene oligomer (Trimer)</b>	
Species	Rat
Reference	<b>138</b>
Partition coefficients	
Blood/air	33 *
Liver/blood	15
Kidney/blood	12.8
Rapidly perfused/blood	12
Slowly perfused/blood	2.25
Fat/blood	400
Perirenal fat/blood	400
Fat diffusion constant	0.33 x Qf 0.085 x
Perirenal fat diffusion constant	Qpr
Biochemical parameters	
<i>Kf</i> First order metabolism rate constant (h <sup>-1</sup> )	2
<i>KEX</i> First order excretion rate (h <sup>-1</sup> )	0.015
<b>Fluoride</b>	
<i>K0</i> First order fluoride from bone rate constant (h <sup>-1</sup> )	0.0016
<i>K1</i> First order fluoride to bone and urine rate constant (h <sup>-1</sup> )	0.82

\* Blood:air partition coefficient in subchronic exposures : 50-100



<b>Polychlorotrifluoroethylene oligomer (Tetramer)</b>	
Species	Rat
Reference	<b>138</b>
Partition coefficients	
Blood/air	35 *
Liver/blood	20
Kidney/blood	7.2
Rapidly perfused/blood	12
Slowly perfused/blood	2.25
Fat/blood	750
Perirenal fat/blood	750
Fat diffusion constant	0.5 x Qf 0.02 x
Perirenal fat diffusion constant	Qpr
Biochemical parameters	
<i>Kf</i> First order metabolism rate constant (h <sup>-1</sup> )	1
<i>KEX</i> First order excretion rate (h <sup>-1</sup> )	0.0006
<b>Fluoride</b>	
<i>K0</i> First order fluoride from bone rate constant (h <sup>-1</sup> )	0.0016
<i>K1</i> First order fluoride to bone and urine rate constant (h <sup>-1</sup> )	0.82

\* Blood:air partition coefficient in subchronic exposures : 175-200

<b>Pyrene</b>		
Species		Rat
Reference		<b>57</b>
Coefficients partition		
	Liver/plasma	2.37
	Lung/plasma	2.25
	Fat/plasma	11.84
	Richly perfused/plasma	1.71
	Slowly perfused/plasma	1.58
Biochemical parameters		
Metabolic constants		
	<i>V<sub>max</sub></i> Maximal velocity (mg/min/kg)	0.04
	<i>K<sub>m</sub></i> Michaelis affinity constant (mg/L)	5.61
Diffusion constants		
	<i>Flu</i> Lung	1.0
	<i>FR</i> Richly perfused	1.0
	<i>FS</i> Slowly perfused	0.01
	<i>FF</i> Fat	0.1
	<i>FL</i> Liver	1.0
Protein binding		
Maximal binding (mg/L)		
	<i>BML</i> Liver <i>Ah</i> receptors	7.90 x 10 <sup>-5</sup>
	<i>BMML</i> Liver proteins	70
	<i>BMMLu</i> Lung proteins	40
Binding association constants (mg/l) <sup>-1</sup>		
	<i>KBL</i> Liver <i>Ah</i> receptors	9.889
	<i>KBBL</i> Liver proteins	5
	<i>KBBLu</i> Lung proteins	5
Oral absorption rate constant (h <sup>-1</sup> )		
		0.035

<b>Styrene</b>				
Species	Mouse	Mouse	Mouse	Mouse
Reference	<b>114</b>	<b>24</b>	<b>84</b>	<b>120</b>
Partition coefficients				
Blood/air	40	110	40	40
Liver/blood	2.7	1.18	2.7	2
Rapidly perfused/blood	5.7	1.14	5.7	1.3
Muscle/blood	1	0.86	1	1.3
Fat/blood	50	40.9	50	87
Brain/blood				
Biochemical parameters				
<b>Cytochrome P-450</b>				
Vmax Liver (mg/h/g liver)		1.135		1.250
Vmax Liver (mg/h)	0.58		1.349	
Vmax Upper airways (nmol/min/ml tissue)				183
Vmax Transitional airways (nmol/min/ml tissue)				362
Km (mg/L)	0.36	1.35	0.364	1.04
ST/SO tissue-phase diffusivity (cm <sup>2</sup> /min)				2.0 x 10 <sup>-4</sup>
ST/SO air-phase diffusivity (cm <sup>2</sup> /min)				6
<i>K<sub>po</sub></i> Uptake p.o. (L/h)		0.8		
<i>K<sub>ip</sub></i> Uptake i.p. (L/h)		3		

<b>Styrene</b>				
Species	Rat	Rat	Rat	Rat
Reference	<b>114</b>	<b>4</b>	<b>24</b>	<b>120</b>
Partition coefficients				
Blood/air	40	40.2	110	40
Liver/blood	27	3.46	1.18	2
Rapidly perfused/blood	5.7		1.14	1.3
Muscle/blood	1	1.17	0.86	1.3
Fat/blood	50	86.47	40.9	87
Brain/blood				
Biochemical parameters				
<b>Cytochrome P-450</b>				
			0.583	0.312 – 0.937
Vmax Liver (mg/h/g liver)				
Vmax Liver (mg/h)	3.6	3.6		
Vmax Upper airways (nmol/min/ml tissue)				98
Vmax Transitional airways (nmol/min/ml tissue)				46.4
Km (mg/L)	0.36	0.4	1.56	1.04
ST/SO tissue-phase diffusivity (cm <sup>2</sup> /min)				2.0 x 10 <sup>-4</sup>
ST/SO air-phase diffusivity (cm <sup>2</sup> /min)				6
<i>K<sub>po</sub></i> Uptake p.o. (L/h)			0.5	
<i>K<sub>ip</sub></i> Uptake i.p. (L/h)			3	

<b>Styrene</b>					
Species	Human	Human	Human	Human	Human
Reference	<b>114</b>	<b>4</b>	<b>24</b>	<b>111</b>	<b>120</b>
Partition coefficients					
Blood/air	52	51.9	48	52	48
Liver/blood	2.7	2.68	2.71	2.7	2
Rapidly perfused/blood	5.7		2.6	5.7	1.3
Muscle/blood	1	0.91	1.96	1	1.3
Fat/blood	50	86.47	93.8	106	50
Brain/blood				2.1	
Biochemical parameters					
<b>Cytochrome P-450</b>					
Vmax Liver (mg/h/g liver)			0.208		0.312
Vmax Liver (mg/h)	184	165		186	
Vmax Upper airways (nmol/min/ml tissue)					50
Vmax Transitional airways (nmol/min/ml tissue)					1.7
Km (mg/L)	0.36	0.4	1.04	0.36	1.04
ST/SO tissue-phase diffusivity (cm <sup>2</sup> /min)					2.0 x 10 <sup>-4</sup>
ST/SO air-phase diffusivity (cm <sup>2</sup> /min)					6
<i>K<sub>po</sub></i> Uptake p.o. (L/h)					
<i>K<sub>ip</sub></i> Uptake i.p. (L/h)					

<b>Styrene-7,8-oxide</b>		
Species	Mouse	Mouse
Reference	<b>24</b>	<b>120</b>
Partition coefficients		
Blood/air		2000
Liver/blood	2.6	1
Rapidly perfused/blood	2.6	0.6
Muscle/blood	1.5	0.6
Fat/blood	6.1	14
Biochemical parameters		
<b>Epoxide hydrolase</b>		
Vmax Liver (mmol/h/g tissue)	0.011	0.012
Kmih (mmol/L)	0.009	0.1
<b>GST</b>		
Vmax GST Liver (mmol/h/g tissue)	0.29	0.66
Vmax Upper airways (mmol/h/ml tissue)		0.06
Vmax Transitional airways (mmol/h/ml tissue)		0.06
Km GST (mmol/L)		2.5
Km SO (mmol/L)	2.5	0.7
Km GSH (mmol/L)	0.1	
Liver GSH basal conc (mmol/L)	5.5	8.3
Upper airways GSH basal conc (mmol/L)		1.0
Transitional airways GSH basal conc (mmol/L)		1.0
Kd First order elimination GSH (L/h)	0.1	
GSH production rate (h <sup>-1</sup> )		0.72
<i>Kpo</i> Uptake p.o. (L/h)	0.2	
<i>Khydr</i> Uptake p.o. (L/h)	6.9	
<i>Kip</i> Uptake i.p. (L/h)	5	

<b>Styrene-7,8-oxide</b>		
Species	Rat	Rat
Reference	<b>24</b>	<b>120</b>
Partition coefficients		
Blood/air		2000
Liver/blood	2.6	1
Rapidly perfused/blood	2.6	0.6
Muscle/blood	1.5	0.6
Fat/blood	6.1	14
Biochemical parameters		
<b>Epoxide hydrolase</b>		
Vmax Liver (mmol/h/g tissue)	0.011	0.015
Kmih (mmol/L)	0.013	0.1
<b>GST</b>		
Vmax GST Liver (mmol/h/g tissue)	0.37	0.378
Vmax Upper airways (mmol/h/ml tissue)		0.06
Vmax Transitional airways (mmol/h/ml tissue)		0.06
Km GST (mmol/L)		2.5
Km SO (mmol/L)	2.5	0.7
Km GSH (mmol/L)	0.1	
Liver GSH basal conc (mmol/L)	5.5	6.3
Upper airways GSH basal conc (mmol/L)		2.5
Transitional airways GSH basal conc (mmol/L)		1.0
<i>Kd</i> First order elimination GSH (L/h)	0.2	
GSH production rate (h <sup>-1</sup> )		0.72
<i>Kpo</i> Uptake p.o. (L/h)	0.6	
<i>Khydr</i> Uptake p.o. (L/h)	6.9	
<i>Kip</i> Uptake i.p. (L/h)	5	

<b>Styrene-7,8-oxide</b>			
Species		Human	Human
Reference		<b>24</b>	<b>120</b>
Partition coefficients			
	Blood/air		2000
	Liver/blood	2.6	1
	Rapidly perfused/blood	2.6	0.6
	Muscle/blood	1.5	0.6
	Fat/blood	6.1	14
Biochemical parametes			
	<b>Epoxide hydrolase</b>		
	Vmax Liver (mmol/h/g tissue)	0.0045	0.054
	Kmih (mmol/L)	0.001	0.1
	<b>GST</b>		
	Vmax GST Liver (mmol/h/g tissue)	0.028	0.084
	Vmax Upper airways (mmol/h/ml tissue)		0.018
	Vmax Transitional airways (mmol/h/ml tissue)		0.018
	Km GST (mmol/L)		2.5
	Km SO (mmol/L)	2.5	0.5
	Km GSH (mmol/L)	0.1	
	Liver GSH basal conc (mmol/L)	5.9	6
	Upper airways GSH basal conc (mmol/L)		1.0
	Transitional airways GSH basal conc (mmol/L)		1.0
	Kd First order elimination GSH (L/h)	0.2	
	GSH production rate (h <sup>-1</sup> )		0.72



Tetrabromodibenzo-p-dioxin (2,3,7,8-) (TBDD)		
Species		Rat
Reference		70
Partition coefficients		
Richly perfused/blood		10
Slowly perfused/blood		10
Fat/blood		1000
Skin/blood		100
Liver/blood		10
Biochemical parameters		
Diffusional Clearances (l/h)		
	<i>PAI</i> Liver	1.0 × Ql
	<i>PArp</i> Richly perfused	1.0 × Qrp
	<i>PAf</i> Fat	0.1 × Qf
	<i>PAsk</i> Skin	0.015 × Qsk
	<i>PAsp</i> Slowly perfused	0.05 × Qsp
KAB Blood binding constant		9,0
Dispositional rate constants		
	<i>KF</i> First-order metabolic rate constant (h <sup>-1</sup> · Kg <sup>-1</sup> )	2
	<i>Kp</i> Excretion rate of parent (h <sup>-1</sup> · kg <sup>-1</sup> )	0.015
	<i>KI</i> Excretion rate of impurity (h <sup>-1</sup> )	0.5
	<i>KEX</i> Fecal excretion rate (h <sup>-1</sup> )	0.075
	<i>KE</i> Excretion rate of unabsorbed oral dose (h <sup>-1</sup> )	0.1
	<i>KA</i> Oral absorption (h <sup>-1</sup> )	0.5
	<i>KDE</i> Dermal absorption (h <sup>-1</sup> )	0.2
<i>Ah</i> Receptor characteristics		
	<i>BM1</i> <i>Ah</i> receptor (pmol/liver)	3.75
	<i>KB1</i> <i>Ah</i> receptor affinity (pM)	35
CYP1A2		
	<i>BM2T</i> Basal amount (nmol)	12
	<i>K1A2</i> Degradation rate (h <sup>-1</sup> )	0.03
	<i>K0A2</i> Synthesis rate (nmol/h)	0.36
	<i>KOMAX2</i> Maximum synthesis increase (fold)	10
	<i>KB2</i> 1A2-dioxin binding constant (nM)	9
	<i>N2</i> Hill term	1.4
	<i>KD2</i> 1A2-DNA binding constant (pM)	0.03
CYP1A1		
	<i>IND</i> Basal amount (nmol)	0.1
	<i>K1A1</i> Degradation rate (h <sup>-1</sup> )	0.035
	<i>K0A1</i> Synthesis rate (nmol/h)	0.0035
	<i>KOMAX1</i> Maximum synthesis increase (fold)	500
	<i>N1</i> Hill term	1
	<i>KD1</i> 1A1-DNA binding constant (pM)	0.045

<b>Tetrachlorodibenzofuran (2,3,7,8-) (TCDF)</b>				
Species	Mouse C57	Mouse DBA	Rat	Monkey
Reference	<b>75</b>	<b>75</b>	<b>75</b>	<b>75</b>
Distribution ratio				
Liver/blood	130	100	30	30
Fat/blood	25	40	35	30
Skin/blood	8	12	4	7
Muscle/blood	2	4	2	2
Biochemical parameters				
Metabolic clearance (ml/min)	0.07	0.06	1	2.25
Metabolites excretion ratio (urinary/biliary)	0.14	0.27	0.03	0.19

**Tetrachlorodibenzo-*p*-dioxin (2,3,7,8-) (TCDD)**

Species		Mouse	Mouse
Reference		C57BL/6J	DBA/2J
Parameters		<b>87</b>	<b>87</b>
Coefficients partition			
	Liver/blood (free??)	20	20
	GI/blood (free??)		
	Fat/blood (free??)	350	350
	Viscera/blood (free??)		
	Richly perfused/blood (free??)	20	20
	Slowly perfused/blood (free??)	250	250
	Muscle/blood (free??)		
	Skin/blood (free??)		
	Liver/total blood		
	Fat/total blood		
	Skin/total blood		
	Kidney/total blood		
	Spleen/total blood		
	Lung/total blood		
	Rest of the body/total blood		
	<b>Membrane transfer/ Transport factor /Diffusional clearance</b>		
		Liver	
		Fat	
		Viscera	
		Richly perfused tissues	
		GI	
		Slowly perfused tissues	
		Muscle	
		Kidney	
		Skin	
		Rest of the body	

Biochemical parameters

	k absorption ( $\text{kg}^{0.75}/\text{day}$ )		
	K proteolysis ( $\text{day}^{-1}$ )		
	K endocytosis ( $\text{day}^{-1}$ )		
	Excretion rate urine ( $\text{day}^{-1}$ )		
	Excretion rate bile ( $\text{day}^{-1}$ )		
	Excretion rate feces ( $\text{day}^{-1}$ )		
	K conjugation ( $\text{day}^{-1}$ )		
	K lysis ( $\text{day}^{-1}$ )		
KA	GI absorption cst ( $\text{h}^{-1}$ )	0.02	0.02
KFC	Metabolism constant ( $\text{h}^{-1}$ )	3.25	1.75
KFC	First order metabolic rate cst ( $\text{h}^{-1} \cdot \text{Kg}^{-1}$ liver)		
Fold	Induction cst (fold over basal)		
BASAL	AHH activity non-induced (nmol/min/g)		
MAXIND	AHH activity maximally-induced (nmol/min/g)		
KE	Excretion rate constant urine ( $\text{h}^{-1}$ )		
<b>Ah Receptor characteristics</b>			
BM1	Ah maximum/ Binding capacity to cytosolic protein in liver (pmol/liver)	4.2	4.2
KB1	Ah affinity/ Binding dissociation to cytosolic protein in liver (pmol/L)	290	2000
	TCDD-Ah-DNA interaction constant (nM)		
	Ah Receptor level in kidney (nM)		
	Ah Receptor level in skin (nM)		
	Ah Receptor level in liver(nM)		
	Ah Receptor level in lung (nM)		
	Ah Receptor level in spleen (nM)		
<b>CYP1A2</b>			
	Basal level in liver (nmol/g)		
	Max (nmol/liver)		
BM2-1			
BM2-0	Binding capacity to microsomal prot. non-induced (nmol/liver)	20	20

BM21		Binding capacity to microsomal prot. induced (nmol/liver)		
KB2		Affinity (nM)		
KB2		Binding dissociation to microsomal protein (nmol/L)	20	75
n		Hill term		
Kd		Hill binding constant (pM)		
		Basal induction rate for CYP1A2 synthesis (nM/h)		
		Maximum fold of synthesis rate over basal rate		
		Degradation rate cst (L/h)		
		Hill coefficient (h)		
		Holding time (h)		
Binding of TCDD to hepatic induced protein (CYP1A2)		TCDD-CYP1A2 dissociation constant (nM)		
	<b>CYP1A1</b>			
		Hill term		
Kd1		Hill binding cst (pM)		
k1		Degradation rate cst ( $h^{-1}$ )		
K0		Synthesis-basal rate cst (units/h)		
K0max		Maximum induction (fold)		
	<b>Protein binding</b>			
		Blood binding protein (nmol/L)		
KAB		Binding to blood ( $h^{-1}$ )	2.5	2.5
BM1R		Binding capacity to cytosolic protein (pmol/richly perfused)		
BM1S		Binding capacity to cytosolic protein (pmol/slowly perfused)		

**Tetrachlorodibenzo-*p*-dioxin (2,3,7,8-) (TCDD)**

Species	Mouse C57BL/6J	Rat
Reference	<b>87</b>	<b>87</b>
Coefficients partition		
Liver/blood (free??)	10	20
GI/blood (free??)		
Fat/blood (free??)	300	350
Viscera/blood (free??)		
Richly perfused/blood (free??)	10	20
Slowly perfused/blood (free??)	3	40
Muscle/blood (free??)		
Skin/blood (free??)	200	
Liver/total blood		
Fat/total blood		
Skin/total blood		
Kidney/total blood		
Spleen/total blood		
Lung/total blood		
Rest of the body/total blood		
<b>Membrane transfer/ Transport factor /Diffusional clearance</b>		
	Liver	
	Fat	
	Viscera	
	Richly perfused tissues	
	GI	
	Slowly perfused tissues	
	Muscle	
	Kidney	
	Skin	
	Rest of the body	

Biochemical parameters

	k absorption ( $\text{kg}^{0.75}/\text{day}$ )		
	K proteolysis ( $\text{day}^{-1}$ )		
	K endocytosis ( $\text{day}^{-1}$ )		
	Excretion rate urine ( $\text{day}^{-1}$ )		
	Excretion rate bile ( $\text{day}^{-1}$ )		
	Excretion rate feces ( $\text{day}^{-1}$ )		
	K conjugation ( $\text{day}^{-1}$ )		
	K lysis ( $\text{day}^{-1}$ )		
KA	GI absorption cst ( $\text{h}^{-1}$ )	0.04	0.2
KFC	Metabolism constant ( $\text{h}^{-1}$ )	1.0	
KFC	First order metabolic rate cst ( $\text{h}^{-1} \cdot \text{Kg}^{-1}$ liver)		2
Fold	Induction cst (fold over basal)		
BASAL	AHH activity non-induced (nmol/min/g)		0.7
MAXIND	AHH activity maximally-induced (nmol/min/g)		27.5
KE	Excretion rate constant urine ( $\text{h}^{-1}$ )	0.02	
	<b>Ah Receptor characteristics</b>		
BM1	Ah maximum/ Binding capacity to cytosolic protein in liver (pmol/liver)	4.2	54
KB1	Ah affinity/ Binding dissociation to cytosolic protein in liver (pmol/L)	290	15
	TCDD-Ah-DNA interaction constant (nM)		
	Ah Receptor level in kidney (nM)		
	Ah Receptor level in skin (nM)		
	Ah Receptor level in liver(nM)		
	Ah Receptor level in lung (nM)		
	Ah Receptor level in spleen (nM)		
	<b>CYP1A2</b>		
	Basal level in liver (nmol/g)		
BM2-1	Max (nmol/liver)		
BM2-0	Binding capacity to microsomal prot. non-induced (nmol/liver)	1.75	25

BM21	Binding capacity to microsomal prot. induced (nmol/liver)		175
KB2	Affinity (nM)		
KB2	Binding dissociation to microsomal protein (nmol/L)	20	7
n	Hill term		
Kd	Hill binding constant (pM)		
	Basal induction rate for CYP1A2 synthesis (nM/h)		
	Maximum fold of synthesis rate over basal rate		
	Degradation rate cst (L/h)		
	Hill coefficient (h)		
	Holding time (h)		
Binding of TCDD to hepatic induced protein (CYP1A2)	TCDD-CYP1A2 dissociation constant (nM)		
	<b>CYP1A1</b>		
	Hill term		
Kd1	Hill binding cst (pM)		
k1	Degradation rate cst ( $h^{-1}$ )		
K0	Synthesis-basal rate cst (units/h)		
K0max	Maximum induction (fold)		
	<b>Protein binding</b>		
	Blood binding protein (nmol/L)		
KAB	Binding to blood ( $h^{-1}$ )	1.0	2.5
BM1R	Binding capacity to cytosolic protein (pmol/richly perfused)	1.1	
BM1S	Binding capacity to cytosolic protein (pmol/slowly perfused)	12.6	



**Tetrachlorodibenzo-*p*-dioxin (2,3,7,8-) (TCDD)**

Species	Rat Wistar	Rat	Rat S D (female)
Reference	<b>87</b>	<b>87</b>	
Coefficients partition			
Liver/blood (free??)	20	20	
GI/blood (free??)		20	
Fat/blood (free??)	375	425	
Viscera/blood (free??)		20	
Richly perfused/blood (free??)	20		
Slowly perfused/blood (free??)	30		
Muscle/blood (free??)		30	
Skin/blood (free??)			
Liver/total blood			6
Fat/total blood			100
Skin/total blood			10
Kidney/total blood			6
Spleen/total blood			5
Lung/total blood			6
Rest of the body/total blood			1.5
<b>Membrane transfer/ Transport factor /Diffusional clearance</b>			
Liver	0.5 × Ql	0.6 × Ql	0.35 × Ql
Fat	0.2 × Qf	0.06 × Qf	0.08 × Qf
Viscera		0.3 × Qvs	
Richly perfused tissues	0.5 × Qrp		
GI		0.3 × Qgi	
Slowly perfused tissues	0.5 × Qsp		
Muscle		0.1 × Qm	
Kidney			0.01 × Qk
Skin			0.09 × Qsk
Rest of the body			0.03 × Qre

Biochemical	k absorption ( $\text{kg}^{0.75}/\text{day}$ )		4.8	
	K proteolysis ( $\text{day}^{-1}$ )		0.693	
	K endocytosis ( $\text{day}^{-1}$ )		0.271	
	Excretion rate urine ( $\text{day}^{-1}$ )		5.36	
	Excretion rate bile ( $\text{day}^{-1}$ )		3.81	
	Excretion rate feces ( $\text{day}^{-1}$ )		1.152	
	K conjugation ( $\text{day}^{-1}$ )		56.693	
	K lysis ( $\text{day}^{-1}$ )		200	
KA	GI absorption cst ( $\text{h}^{-1}$ )		0.071	
KFC	Metabolism constant ( $\text{h}^{-1}$ )	1.65		
KFC	First order metabolic rate cst ( $\text{h}^{-1} \cdot \text{Kg}^{-1}$ liver)			
Fold	Induction cst (fold over basal)	1.0		
BASAL	AHH activity non-induced (nmol/min/g)			
MAXIND	AHH activity maximally-induced (nmol/min/g)			
KE	Excretion rate constant urine ( $\text{h}^{-1}$ )		0.223	
	<b>Ah Receptor characteristics</b>			
BM1	Ah maximum/ Binding capacity to cytosolic protein in liver (pmol/liver)	3.75		
KB1	Ah affinity/ Binding dissociation to cytosolic protein in liver (pmol/L)	35	270	100
	TCDD-Ah-DNA interaction constant (nM)			130
	Ah Receptor level in kidney (nM)			0.25
	Ah Receptor level in skin (nM)			0.05
	Ah Receptor level in liver(nM)			0.35
	Ah Receptor level in lung (nM)			0.35
	Ah Receptor level in spleen (nM)			0.1
	<b>CYP1A2</b>			
BM2-1	Basal level in liver (nmol/g)	1.24		1.6
BM2-0	Max (nmol/liver)	85		
	Binding capacity to microsomal prot. non-induced (nmol/liver)			

BM21	Binding capacity to microsomal prot. induced (nmol/liver)		
KB2	Affinity (nM)	6.5	
KB2	Binding dissociation to microsomal protein (nmol/L)		
n	Hill term	1.0	
Kd	Hill binding constant (pM)	50	
	Basal induction rate for CYP1A2 synthesis (nM/h)		160
	Maximum fold of synthesis rate over basal rate		600
	Degradation rate cst (L/h)		0.1
	Hill coefficient (h)		0.6
	Holding time (h)		0.25
Binding of TCDD to hepatic induced protein (CYP1A2)	TCDD-CYP1A2 dissociation constant (nM)		30
	<b>CYP1A1</b>		
	Hill term	2.3	
Kd1	Hill binding cst (pM)	180	
k1	Degradation rate cst (h <sup>-1</sup> )	0.035	
K0	Synthesis-basal rate cst (units/h)	0.7	
K0max	Maximum induction (fold)	50	
	<b>Protein binding</b>		
	Blood binding protein (nmol/L)		1.0
KAB	Binding to blood (h <sup>-1</sup> )		
BM1R	Binding capacity to cytosolic protein (pmol/richly perfused)		
BM1S	Binding capacity to cytosolic protein (pmol/slowly perfused)		

<b>Tetrachloroethane (1,1,1,2-)</b>	
Species	Rat
Reference	<b>50</b>
Partition coefficients	
Blood/air	41.7
Liver/blood	2.12
Slowly perfused/blood	0.95
Fat/blood	51.5
Biochemical parameters	
VmaxC (mg/h/kg)	6.39
Km (mg/L)	0.9

<b>Tetrachloroethane (1,1,2,2-)</b>	
Species	Rat
Reference	<b>50</b>
Partition coefficients	
Blood/air	142
Liver/blood	1.38
Slowly perfused/blood	0.71
Fat/blood	26.5
Biochemical parameters	
VmaxC (mg/h/kg)	12.9
Km (mg/L)	0.8

<b>Tetrachloroethylene</b>								
Species	Mouse	Mouse	Rat	Rat	Rat	Rat	Rat	Rat
Reference	<b>144</b>	<b>118</b>	<b>144</b>	<b>79</b>	<b>51</b>	<b>14</b>	<b>30</b>	<b>118</b>
Partition coefficients								
Blood/air	16.9	16.9	18.9	12.9	18.9	33.5	19.6	18.85
Liver/blood	4.16	3.01	3.72	3.54	3.72	1.9	5.2	3.73
Rapidly perfused/blood	4.16	3.01	3.72		3.72	1.67		2.69
Muscle/blood	1.18		1.06		1.06		3	
Slowly perfused/blood		2.59		1.53		0.93		1.06
Fat/blood	121.9	48.28	121.7	100.9	86.67	42.35	152.5	86.84
Lung/blood							2.5	
Brain/blood							4.4	
Heart/blood							2.7	
Kidney/blood							4.4	
Rest of body/blood							3	
Milk/blood						12		
Biochemical parameters								
V <sub>maxC</sub> (mg/h/kg)	1.80		0.19	0.528		0.03		
V <sub>max</sub> (mg/h)		0.355					0.009	0.325
K <sub>m</sub> (mg/L)	0.4	3.69	0.3	1.0		0.32	0.019	5.62
K <sub>f</sub> (h <sup>-1</sup> )	1.84		2.73					
K <sub>f</sub> (h <sup>-1</sup> · kg <sup>-1</sup> )					0.3			
K <sub>a</sub> Oral absorption in oil vehicle (min <sup>-1</sup> )	0.010							
K <sub>a</sub> Oral absorption in polyethylene glycol vehicle (min <sup>-1</sup> )							0.025	

<b>Tetrahydrofuran</b>	
Species	Human
Reference	<b>34</b>
Partition coefficients	
Blood/air	145.3
Lungs/blood	1.0
Liver/blood	1.0
Kidneys/blood	1.0
Muscle and skin/blood	1.0
Brain/blood	1.0
Fat/blood	1.4
Others/blood	1.0
Urine/blood	1.1
Biochemical parameters	
Metabolic clearance (L/min)	100

<b>Toluene</b>									
Species	Rat	Rat	Rat	Rat	Rat	Human	Human	Human	Human
Reference	<b>128</b>	<b>32</b>	<b>128</b>	<b>2</b>	<b>58</b> <b>59</b>	<b>82</b>	<b>128</b>	<b>2</b>	<b>60</b>
Partition coefficients									
Blood/air	18	18	18	18	18	15.6	15.6	15.6	15.6
Liver/blood	4.64	4.6	4.64	4.64	4.64	3.08	5.36	5.36	5.36
Slowly perfuseds/blood	1.54	1.5	1.54	1.54	1.54	1.67	1.78	1.78	1.78
Richly perfused/blood	4.64	4.6	4.64	4.64	4.64	2.2	5.36	5.36	5.36
Fat/blood	56.7	56.7	56.72	56.72	56.72	69	65.45	65.45	65.45
Brain/blood		2.0							
Lung /blood						1.4			
GI tract/blood						3.08			
Muscle + skin/blood						2.2			
Biochemical parameters									
VmaxC (mg/h/kg)	4.8	*	4.8	4.8	3.44	4.8	4.8	4,8	3.44
Km (mg/L)	0.55	*	0.55	0.55	0.13	0.55	0.55	0,55	0.13
<b>Inhibition constants (mg/L)</b>									
<i>Ki</i> competitive (dichloromethane)					0.155				0.16
<i>Ki</i> competitive (m-xylene)	0.35		0.17		0.357		0.17		0.36
<i>Ki</i> competitive (benzene)					0.144				0.14
<i>Ki</i> competitive (ethylbenzene)			0.79		0.948		0.79		0.95
<i>Ki</i> competitive (n-Hexane)				1.11				1.11	

\* Values reported from 8 studies published in the litterature. VmaxC: 3.69-7.5 mg/h/kg; Km : 0.3-11.96 mg/L



<b>Trichlorobromomethane</b>	
Species	Rat
Reference	<b>131</b>
Partition coefficients	
Blood/air	18.2
Liver/blood	2.3
Muscle/blood	1.5
Fat/blood	60
Biochemical parameters	
Control	
VmaxC (mg/h/kg)	3.55
Km (mg/L)	0.5
Kfc (h <sup>-1</sup> . kg <sup>-1</sup> )	15
Chlordecone pretreated	
VmaxC (mg/h/kg)	3.92
Km (mg/L)	0.5
Kfc (h <sup>-1</sup> . kg <sup>-1</sup> )	15.5
Phenobarbital pretreated	
VmaxC (mg/h/kg)	8.52
Km (mg/L)	0.5
Kfc (h <sup>-1</sup> . kg <sup>-1</sup> )	12.9
Mirex pretreated	
VmaxC (mg/h/kg)	5.06
Km (mg/L)	0.5
Kfc (h <sup>-1</sup> . kg <sup>-1</sup> )	17.6

<b>Trichloroethane (1,1,2-)</b>	
Species	Rat
Reference	<b>50</b>
Partition coefficients	
Blood/air	58
Liver/blood	1.26
Slowly perfused/blood	0.39
Fat/blood	24.8
Biochemical parameters	
VmaxC (mg/h/kg)	7.69
Km (mg/L)	0.75

<b>Trichloroethane (1,1,1-)</b>						
Species	Mouse	Rat	Rat	Rat	Human	Human
Reference	<b>116</b>	<b>116</b>	<b>28</b>	<b>51</b>	<b>116</b>	<b>83</b>
Partition coefficients						
Blood/air	10.8	5.76	8.6	5.76	2.53	4.35
Lung/blood			1.49			1.08
Liver/blood	0.80	1.49	1.49	1.49	3.40	3.68
GI Tract/blood						3.68
Fat/blood	24.35	45.66	47.7	45.66	103.95	57.70
Rapidly perfused /blood	0.80	1.49	1.49		3.40	1.91
Poorly perfused/Blood	0.29	0.55		0.55	1.25	1.54
Muscle + skin /blood			0.55			1.54
Biochemical parameters						
VmaxC (mg/h/kg)	0.419	0.419			0.419	0.42
Km (mg/L)	5.75	5.75			5.75	5.75
<i>K<sub>f</sub></i> Metabolic rate constant (min <sup>-1</sup> )			0.115	0.083		
Lu:alveolar mass transfer coeff. (ml/min)			500			
<i>K<sub>a</sub></i> Oral absorption in water vehicle (h <sup>-1</sup> )					1.25	
<b>Metabolites</b>						
Excretion rate of trichloroethanol (urine) (h <sup>-1</sup> )						0.0066
Excretion rate of TCA (urine) (h <sup>-1</sup> )						0.0082
Excretion rate of trichloroethanol (other pathways) (h <sup>-1</sup> )						0.0102
Excretion rate of TCA (other pathways) (h <sup>-1</sup> )						0.0055
Conversion rate of trichloroethanol to TCA (h <sup>-1</sup> )						0.0362

<b>Trichloroethylene</b>					
Species	Mouse Male	Mouse Female	Mouse	Mouse	Mouse
Reference	<b>43</b>	<b>43</b>	<b>1</b>	<b>56</b>	<b>17</b>
Partition coefficients					
Blood/air	13.4	14.3	15.91	15.91	14
Lung/blood			2.61	2.61	
Liver/blood	2.03	1.62	1.73	1.73	1.8
GI Tract/blood					
Fat/blood	41.3	31.3	36.38	36.38	36
Kidney/blood			2.07	2.07	
Rapidly perfused/blood	2.03	1.62	1.73	1.73	1.8
Slowly perfused/blood	1	0.48		2.36	0.75
Muscle+skin/blood			2.36	2.36	
Gut/blood					1.8
Tracheobronchial/blood					1.8
Biochemical parameters					
VmaxC (mg/h/kg)	32.7	23.2	32.7	32.7	39.0
Km (mg/L)	0.25	0.25	4.61	0.25	0.25
Kf (h <sup>-1</sup> )					
Ka Oral absorption in water vehicle (h <sup>-1</sup> )					

<b>Trichloroethylene</b>										
Species	Rat	Rat	Rat	Rat	Rat	Rat	Rat	Rat	Rat	Rat
	Female		Lacting Dam			Male	Female		Male	
Reference	<b>41</b>	<b>79</b>	<b>42</b>	<b>51</b>	<b>29</b>	<b>43</b>	<b>43</b>	<b>10</b>	<b>123</b>	<b>17</b>
Partition coefficients										
Blood/air	15	25.8	13.1	21.9	21.9	21.9	15.0	20.5	21.9	18.5
Lung/blood										
Liver/blood	1.46	2.43	1.67	1.24	1.24	1.2	1.46	1.3	1.2	1.3
GI Tract/blood									1	
Fat/blood	29.83	23.8	34.2	25.30	25.3	25.3	29.82	26	25.3	27.5
Kidney/blood								1		
Rapidly perfused/blood	1.46	2.43	1.67	1.24	1.24	1.2	1.46		1.2	1.3
Slowly perfused/blood	0.46	0.84	0.53		0.46	0.46	0.46		0.46	0.5
Muscle+skin/blood				0.46				0.6		
Gut/blood										1.3
Tracheobronchial/blood										1.3
Biochemical parameters										
V <sub>max</sub> C (mg/h/kg)	10.98	10	9.26	11.0	10.0	11.0	11.0	11.4	11.0	12.0
K <sub>m</sub> (mg/L)	0.25	2.5	0.25	0.25	0.25	0.25	0.25	0.09	0.25	0.25
K <sub>f</sub> (h <sup>-1</sup> )	7.08						6.96			
K <sub>a</sub> Oral absorption in water vehicle (h <sup>-1</sup> )	5.4									

<b>Trichloroethylene</b>						
Species	Human	Human	Human	Human Male	Human Female	Human
Reference	<b>43</b>	<b>80</b>	<b>84</b>	<b>44</b>	<b>44</b>	<b>18</b>
Partition coefficients						
Blood/air	9	9.77	9.1	11.15	9.13	9.2
Lung/blood			1.54	0.42	0.39	
Liver/blood	2.2	6.42	3.19	5.92	4.85	6.8
GI Tract/blood			3.19			
Fat/blood	66.7	62.85	72.42	63.88	52.34	73
Kidney/blood				1.32	1.08	
Rapidly perfused/blood	2.2	6.42	2.31			6.8
Slowly perfused/blood	2.1	2.21	2.09			2.3
Muscle+skin/blood			2.09	1.68	1.38	
Gut/blood						6.8
Tracheobronchial/blood						6.8
Biochemical parameters						
VmaxC (mg/h/kg)	*	10	11	4.0	5.0	10
Km (mg/L)		2.5	0.25	1.66	1.8	1.5
Kf (h <sup>-1</sup> )						
Ka Oral absorption in water vehicle (h <sup>-1</sup> )						

### Trichloroethylene (Metabolites)

#### Données partielles à compléter avec les sous-compartiments

Species	Mouse Male	Mouse Female	Mouse	Mouse	Mouse
Reference	<b>43</b>	<b>43</b>	<b>2</b>	<b>56</b>	<b>17</b>
Fraction of CH transformed to trichloroethanol					
Fraction of CH transformed to TCA (PO)	0.06 - 0.13	0.07 - 0.23			0.035
Conversion rate of trichloroethanol to TCA (h <sup>-1</sup> )					
Excretion rate of trichloroethanol (urine) (h <sup>-1</sup> )					
Excretion rate of TCA (urine) (h <sup>-1</sup> )					
Excretion rate of trichloroethanol (other pathways) (h <sup>-1</sup> )					
Excretion rate of TCA (other pathways) (h <sup>-1</sup> )					
Excretion rate of trichloroethanol (urine) (mg/h/kg)					
Excretion rate of trichloroethanol (urine) (mg/L)					

**Trichloroethylene (Metabolites)**

**Données partielles à compléter avec les sous-compartiments**

Species	Rat	Rat	Rat	Rat	Rat	Rat	Rat	Rat	Rat	Human
	Female		Lacting Dam		Male	Female		Male		
Reference	<b>41</b>	<b>79</b>	<b>42</b>	<b>29</b>	<b>43</b>	<b>43</b>	<b>10</b>	<b>123</b>	<b>18</b>	<b>39</b>
Fraction of CH transformed to trichloroethanol			0.83 0.73	or				0.83		0.78
Fraction of CH transformed to TCA (PO)			0.17 0.27	or	0.06	0.18		0.15	0.02	0.22
Conversion rate of trichloroethanol to TCA (h <sup>-1</sup> )										0.019
Excretion rate of trichloroethanol (urine) (h <sup>-1</sup> )										0.026
Excretion rate of TCA (urine) (h <sup>-1</sup> )										0.007
Excretion rate of trichloroethanol (other pathways) (h <sup>-1</sup> )										0.008
Excretion rate of TCA (other pathways) (h <sup>-1</sup> )										0.007
Excretion rate of trichloroethanol (urine) (mg/h/kg)										
Excretion rate of trichloroethanol (urine) (mg/L)										



<b>Trichloropropane (1,2,3-)</b>	
Species	Rat
Reference	<b>141</b>
Partition coefficients	
Liver/blood	3.8
Muscle/blood	2
Fat/blood	15
Muscle/blood	0.6
Skin/blood	1.3
Biochemical parameters	
Metabolism constant (ml/min)	20

<b>CHLOROFLUOROHYDROCARBONS</b>	
<b>1,1,2-Trichloro-1,2,2-trifluoroethane</b>	
Species	Human
Reference	<b>9</b>
Partition coefficients	
Blood/air	0.41
Liver/blood	2.07
Rapidly perfused/blood	2.07
Slowly perfused/blood	9.2
Fat/blood	146
Biochemical parameters	
Total metabolic clearance (Cl/Qc)	0.46

<b>Trifluoroethane (1,1,1-)</b>	
Species	Rat
Reference	<b>95</b>
Partition coefficients	
Blood/air	0.91
Liver/blood	1.43
Fat/blood	13.9
Rapidly perfused /blood	1.43
Lean tissue/blood	0.50
Biochemical parameters	
<i>K<sub>f</sub></i> First order metabolism rate constant (h <sup>-1</sup> . kg <sup>-1</sup> )	1.17

<b>Trifluoriodiomethane</b>	
Species	Human
Reference	<b>139</b>
Partition coefficients	
Blood/air	0.97
Liver/blood	1.26
Rapidly perfused/blood	1.26
Poorly perfused/blood	1.31
Fat/blood	11.59
Gut/blood	1.62
Biochemical parameters	
VmaxC (mg/h/kg)	0.38
Km (mg/L)	0.1

<b>Trihaloethane (1,1,1-)</b>	
Species	Rat
Reference	<b>95</b>
Partition coefficients	
Blood/air	5.55
Liver/blood	1.42
Fat/blood	40.54
Rapidly perfused /blood	1.42
Lean tissue/blood	0.50
Biochemical parameters	
<i>K<sub>f</sub></i> First order metabolism rate constant (h <sup>-1</sup> . kg <sup>-1</sup> )	3.78

<b>Trimethylbenzene (1,2,4-)</b>	
Species	Human
Reference	<b>64</b>
Partition coefficients	
Blood/air	59
Liver/blood	5
Fat/blood	125
Rapidly perfused /blood	5
Slowly perfused/blood	5
Biochemical parameters	
Pathway1	
Vmax ( $\mu\text{mol}/\text{min}$ )	24
Km ( $\mu\text{M}$ )	13
Pathway2 (3,4-DMHA)	
Clearance rate (L/min)	0.6
ke Excretion rate ( $\text{min}^{-1}$ )	0.016

<b>2,4,4-Trimethyl-2-pentanol</b>	
Species	Rat
Reference	<b>11</b>
Partition coefficients	
Blood/air	214
Liver/blood	2.5
Fat/blood	10.3
Rapidly perfused /blood	4,8
Slowly perfused/blood	1.1
Biochemical parameters	
Vmax oxidation ( $\mu\text{mol/h/kg}$ )	330
Km ( $\mu\text{M}$ )	23
Diffusional clearance in fat (L/h)	0.34* QF
Kd Diss. constant of binding to alpha2u ( $\mu\text{M}$ )	0.2

<b>Vinyl chloride</b>		
Species	Rat	Rat
Reference	<b>51</b>	<b>10</b>
Partition coefficients		
Blood/air	1.68	2.4
Liver/blood	0.95	0.7
Fat/blood	11.90	10
Muscle/blood	1.25	0.4
Kidney/blood		0.7
Rapidly perfused/blood	0.95	
Biochemical parameters		
VmaxC (mg/h/kg)	2.8	3.0
Km (mg/L)	0.1	0.01
Kfc (h <sup>-1</sup> .kg <sup>-1</sup> )	1.0	



<b>Vinyl fluoride</b>		
Species	Mouse	Rat
Reference	<b>15</b>	<b>15</b>
Partition coefficients		
Blood/air	0.75	0.75
Liver/blood	1.11	1.11
Rapidly perfused/blood	1.11	1.11
Poorly perfused/blood	0.72	0.72
Fat/blood	2.43	2.43
Biochemical paremeters		
VmaxC (mg/h/kg)	0.3	0.1
Km (mg/L)	< 0.02	< 0.02

<b>Vinylidene Fluoride (1,1-difluoroethylene)</b>	
Species	Rat
Reference	<b>102</b>
Partition coefficients	
Blood/air	0.18
Liver/blood	4.4
Rapidly perfused/blood	4.4
Poorly perfused/blood	1.6
Fat/blood	5.6
Biochemical parameters	
VmaxC (mg/h/kg)	0.07
Km (mg/L)	0.13

<b>Zinc</b>		
Species	Rat	
Reference	<b>62</b>	<b>62</b>
Parameters	Linear binding constants	Diffusion constants (h <sup>-1</sup> )
Skin and fur/plasma	6.50	0.0339
Muscle/plasma	11.04	0.0171
Liver/plasma	28.00	0.4076
Intestine/plasma	14.75	0.3132
Stomach/plasma	18.00	0.1181
Fat/plasma	0.70	0.0037
Thyroid/plasma	11.35	0.1815
Bone and marrow/plasma	25.00	0.0799
Heart/plasma	13.00	0.1216
Bladder/plasma	17.00	0.0739
Prostate/plasma	6.00	0.0633
Spleen/plasma	15.00	0.2083
Pancreas/plasma	20.00	0.1884
Kidneys/plasma	20.00	0.3278
Brain/plasma	11.43	0.0191
Gonads/plasma	15.00	0.0500
Sex organs/plasma	8.00	0.0399
Gut lumen/plasma	16.08	0.1274
Red blood cells/plasma	5.53	

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