Table S1: Information for the 41 chemicals included in the model evaluation and PMIDs for the source of metabolism and concentration-time data

Chemical	DTXSID	CASRN	CAMEO Chemical Class	Molecular Weight (g/mol)	Log P	Solubility (mol/L)	Blood Air Partition Coefficient	Available Species Data	Vmax (µmol/h/kg BW)	K_M (µM)	Metabolism Data Source (PMID)
1,1-Dichloroethylene	DTXSID8021438	75-35-4	HOC	96.94	2.16	4.07E-02	16.63[a]	Rat	117.27	1.03	20685286
1,1,1-Trichloroethane	DTXSID0021381	71-55-6	HOC	133.40	2.43	1.39E-02	12.19[a]	Human	0.88	43.10	20685286
1,1,1,2-Tetrafluoroethane	DTXSID1021324	811-97-2	FOC	102.03	0.83	1.23E-03	0.61[a]	Human	0.08	4.90	17365028
1,1,2-Trichloro-1,2,2-trifluoroethane	DTXSID6021377	76-13-1	FOC	187.37	2.97	1.01E-03	2.20[a]	Human	0.23	5.34	17365028
1,2-Dichloroethane	DTXSID6020438	107-06-2	HOC	98.95	1.63	6.89E-02	25.11[a]	Rat	49.63	2.53	20685286
1,2-Dichloropropane	DTXSID0020448	78-87-5	HOC	112.98	1.99	1.86E-02	36.35[a]	Rat	77.22	5.11	14709629, 25072765
1,2,4-Trimethylbenzene	DTXSID6021402	95-63-6	ArH	120.20	3.62	5.05E-04	92.56[a]	Human	20.57	13.00	10079206
1,3-Butadiene	DTXSID3020203	106-99-0	Other (Conjugated diene)	54.09	1.92	1.80E-02	0.82[a]	Human|Rat	1582.09| 2462.40	390.00| 390.00	20122977
1,4-Dioxane	DTXSID4020533	123-91-1	Ether	88.11	-0.16	1.12E+01	1110.51[a]	Human	20.15	34.05	20685286
2-Butoxyethanol	DTXSID1024097	111-76-2	Alcohol	118.18	0.66	4.66E+00	2.69E+04	Human	145.98	200.00	21998005
2,2-Dichloro-1,1,1-trifluoroethane	DTXSID7020712	306-83-2	FOC	152.93	2.38	1.32E-02	2.61[a]	Rat	57.15	6.54	8516773
2H-Perfluoropropane	DTXSID4042048	431-89-0	FOC	170.03	1.85	3.16E-04	0.81[a]	Human	0.00	0.00	17365028
Acrylonitrile	DTXSID5020029	107-13-1	Other (Nitrile)	53.06	0.13	1.84E+00	386.88[a]	Rat	445.60	15.08	20685286
Benzene	DTXSID3039242	71-43-2	ArH	78.11	2.25	1.02E-02	22.51[a]	Human|Rat	2.54| 13.78	4.48| 4.48	20685286
Bromotrifluoromethane	DTXSID5026415	75-63-8	FOC	148.91	1.85	2.16E-03	0.11[a]	Human	0.00	0.00	17365028
Carbon tetrachloride	DTXSID8020250	56-23-5	HOC	153.81	2.73	8.19E-03	3.75[a]	Rat	6.41	1.63	20685286
Chlorobenzene	DTXSID4020298	108-90-7	Other (Aryl halide)	112.56	2.83	3.46E-03	68.70[a]	Human	53.04	0.36	15129550
Chloroform	DTXSID1020306	67-66-3	HOC	119.37	1.96	4.85E-02	24.10[a]	Rat	161.26	3.77	20685286
Decane	DTXSID6024913	124-18-5	AlH	142.29	5.24	4.95E-07	146.15[a]	Rat	7.51	10.54	17365028
Dichlorodifluoromethane	DTXSID6020436	75-71-8	FOC	120.91	2.10	3.49E-03	0.13[a]	Human	0.35	8.27	17365028
Dichloromethane	DTXSID0020868	75-09-2	HOC	84.93	1.43	1.22E-01	8.46[a]	Human	20.57	8.83	20685286
Ethanol	DTXSID9020584	64-17-5	Alcohol	46.07	-0.28	1.65E+01	4521.67	Human	3392.40	1000.00	21998005
Ethyl T-butyl ether	DTXSID0025604	637-92-3	Ether	102.18	1.52	5.28E-02	23.26	Human	25.70	50.00	21998005
Ethylbenzene	DTXSID3020596	100-41-4	ArH	106.17	3.18	1.64E-03	42.64[a]	Human|Rat	16.83| 91.23	9.80|9.80	20685286
Furan	DTXSID6020646	110-00-9	Ether	68.08	1.29	2.54E-01	276.57[a]	Rat	5.12	2.64	20685286
Isopropanol	DTXSID7020762	67-63-0	Alcohol	60.10	0.26	9.46E+00	3452.92[a]	Human|Rat	778.04| 4218.42	4160.01| 4160.01	17365028

Methanol	DTXSID2021731	67-56-1	Alcohol	32.04	-0.61	2.61E+01	4877.47[a]	Rat	689.63	1058.61	1440610
Methyl ethyl ketone	DTXSID3021516	78-93-3	Other (Ketones)	72.11	0.44	2.13E+00	405.97[a]	Human	75.44	8.74	12133235
Methyl tert-butyl ether	DTXSID3020833	1634-04-4	Ether	88.15	1.09	3.76E-01	28.42[a]	Human	3.93	4.99	20685286
n-Hexane	DTXSID0021917	110-54-3	AlH	86.18	3.94	1.52E-04	2.49[a]	Rat	3.93	4.64	20685286
N-Methyl-2-pyrrolidone	DTXSID6020856	872-50-4	Other (Amides/Imides)	99.13	-0.30	9.95E+00	2.74E+06	Human	23.74	2400.00	21998005
Nonane	DTXSID9025796	111-84-2	AlH	128.26	5.44	1.93E-06	211.67	Rat	84.81	6.93	21391144
Octane	DTXSID0026882	111-65-9	AlH	114.23	5.05	9.23E-06	39.83	Rat	4.63	10.42	21391144
Pyrene	DTXSID3024289	129-00-0	ArH	202.26	5.12	6.59E-07	1.58E+06	Rat	6.19	4.50	21998005
Styrene	DTXSID2021284	100-42-5	ArH	104.15	2.92	1.88E-03	82.51[a]	Human|Rat	25.23| 136.80	3.46| 3.46	20685286
tert-Amyl methyl ether	DTXSID8024521	994-05-8	Ether	102.18	1.74	8.57E-02	26.74[a]	Human	1800.00	1000.00	10367338
Tetrachloroethylene	DTXSID2021319	127-18-4	HOC	165.82	3.35	2.33E-03	21.42[a]	Human|Rat	0.70| 3.80	75.38| 75.38	20685286
Tetrahydrofuran	DTXSID1021328	109-99-9	Ether	72.11	0.60	2.96E+00	246.24[a]	Human	232618.59	138.68	20685286
Toluene	DTXSID7021360	108-88-3	ArH	92.14	2.62	4.61E-03	26.26[a]	Rat	97.05	5.97	20685286
Trichloroethylene	DTXSID0021383	79-01-6	HOC	131.38	2.29	1.13E-02	22.24[a]	Human|Rat	21.28| 115.37	11.42| 11.42	20685286
Vinyl chloride	DTXSID8021434	75-01-4	HOC	62.50	1.00	0.081502	2.89	Human	39.99	1.60	21391144

[a]Literature Blood:Air Partition Coefficient value available from Metabolism Data Source; CASRN, Chemical Abstracts Service Registry Number; DTXSID, DSSTox Substance Identifier, used in the EPA CompTox Dashboard; CAMEO, Computer-Aided Management of Emergency Operations, database of hazardous chemical datasheets that emergency responders and planners can use to get response recommendations and predict hazards; PMID, unique PubMed article ID number (for use on https://www.ncbi.nlm.nih.gov/pubmed/); HOC, halogenated organic compound; FOC, fluorinated organic compound; ArH, aromatic hydrocarbon; AlH, aliphatic hydrocarbon.

Table S2: List of all exposure scenarios included in the model evaluation

Chemical	Species	Matrix	Dose (ppm)	Exposure Length (hours)	Number of Data Points in Study	Source (PMID)
1,1-Dichloroethylene	Rat	EB	25	3	33	6845373
1,1-Dichloroethylene	Rat	EB	75	3	32	6845373
1,1-Dichloroethylene	Rat	EB	150	3	34	6845373
1,1-Dichloroethylene	Rat	EB	300	3	36	6845373
1,1-Dichloroethylene	Rat	VBL	25	3	24	6845373
1,1-Dichloroethylene	Rat	VBL	75	3	24	6845373
1,1-Dichloroethylene	Rat	VBL	150	3	24	6845373
1,1-Dichloroethylene	Rat	VBL	300	3	24	6845373
1,1,1-Trichloroethane	Human	EB	70	4	10	422270
1,1,1-Trichloroethane	Human	EB	145	4	10	422270
1,1,1-Trichloroethane	Human	BL	70	4	5	422270
1,1,1-Trichloroethane	Human	BL	145	4	5	422270
1,1,1-Trichloroethane	Human	BL (+W)	142	4	5	422270
1,1,1-Trichloroethane	Human	EB (+W)	142	4	9	422270
1,1,1,2-Tetrafluoroethane	Human	VBL	1000	1	17	17365028
1,1,1,2-Tetrafluoroethane	Human	VBL	2000	1	21	17365028
1,1,1,2-Tetrafluoroethane	Human	VBL	4000	1	22	17365028
1,1,1,2-Tetrafluoroethane	Human	VBL	8000	1	19	17365028
1,1,2-Trichloro-1,2,2-trifluoroethane	Human	VBL	250	4	14	17365028
1,2-Dichloroethane	Rat	BL	50	6	11	18579268
1,2-Dichloroethane	Rat	BL	150	6	12	18579268
1,2-Dichloroethane	Rat	BL	200	6	6	18579268
1,2-Dichloroethane	Rat	BL	250	6	15	18579268
1,2-Dichloropropane	Rat	BL	5	6	14	1897000
1,2-Dichloropropane	Rat	BL	50	6	15	1897000
1,2-Dichloropropane	Rat	BL	100	6	13	1897000
1,2,4-Trimethylbenzene	Human	EB	2	2	2	10079206
1,2,4-Trimethylbenzene	Human	EB	25	2	5	10079206

1,2,4-Trimethylbenzene	Human	ABL	2	2	17	10079206
1,2,4-Trimethylbenzene	Human	ABL	25	2	22	10079206
1,3-Butadiene	Rat	BL	63	6	9	26079054
1,3-Butadiene	Rat	BL	616	6	8	26079054
1,3-Butadiene	Rat	BL	1249	6	9	26079054
1,3-Butadiene	Human	EB	5	2	35	26079054
1,4-Dioxane	Human	PL	50	6	13	926203
2-Butoxyethanol	Human	BL	20	2	17	9878592
2,2-Dichloro-1,1,1-trifluoroethane	Rat	VBL	1000	4	11	17365028
2,2-Dichloro-1,1,1-trifluoroethane	Rat	VBL	10000	4	13	17365028
2H-Perfluoropropane	Human	VBL	1000	1	20	17365028
2H-Perfluoropropane	Human	VBL	2000	1	22	17365028
2H-Perfluoropropane	Human	VBL	4000	1	21	17365028
2H-Perfluoropropane	Human	VBL	8000	1	23	17365028
Acrylonitrile	Rat	BL	186	3	4	8887460
Acrylonitrile	Rat	BL	254	3	4	8887460
Acrylonitrile	Rat	BL	291	3	4	8887460
Benzene	Rat	BL	1000	2	28	1103957
Benzene	Human	EB	1.57	4	24	1439659
Benzene	Human	EB	9.39	4	33	1439659
Benzene	Human	EB	25	2	24	1103957
Benzene	Human	VBL	1.57	4	38	1439659
Benzene	Human	VBL	9.39	4	41	1439659
Benzene	Human	BL	25	2	20	1103957
Bromotrifluoromethane	Human	VBL	10000	24	60	17365028
Carbon tetrachloride	Rat	ABL	100	2	24	17365028
Carbon tetrachloride	Rat	ABL	1000	2	28	17365028
Chlorobenzene	Human	BL	10	8	27	11100949
Chloroform	Rat	BL	100	6	7	23143927
Decane	Rat	BL	1200	4	15	16036747
Dichlorodifluoromethane	Human	VBL	1000	1	31	17365028
Dichlorodifluoromethane	Human	VBL	4000	1	39	17365028

Dichloromethane	Human	EB	100	6	21	1900959
Dichloromethane	Human	EB	350	6	21	1900959
Dichloromethane	Human	VBL	100	6	7	1900959
Dichloromethane	Human	VBL	350	6	7	1900959
Ethanol	Human	BL	125	4	6	24495244
Ethanol	Human	BL	250	4	6	24495244
Ethanol	Human	BL	450	4	6	24495244
Ethanol	Human	BL	750	4	6	24495244
Ethanol	Human	BL	1000	4	6	24495244
Ethyl T-butyl ether	Human	BL	4.5	4	3	11504147
Ethyl T-butyl ether	Human	BL	40.6	4	8	11504147
Ethylbenzene	Rat	VBL	50	4	5	15777087
Ethylbenzene	Human	VBL	33	7	4	15777087
Furan	Rat	BL	52	4	3	8248934
Furan	Rat	BL	107	4	3	8248934
Furan	Rat	BL	208	4	3	8248934
Isopropanol	Rat	VBL	476	6	10	17365028
Isopropanol	Rat	VBL	4960	6	11	17365028
Isopropanol	Human	EEB	100	0.2	45	11568359
Isopropanol	Human	MEB	100	0.2	10	11568359
Methanol	Rat	BL	200	6	9	1440610
Methanol	Rat	BL	1200	6	9	1440610
Methanol	Rat	BL	2000	6	9	1440610
Methyl ethyl ketone	Human	VBL	25	4	27	2309238
Methyl ethyl ketone	Human	VBL	200	4	27	2309238
Methyl ethyl ketone	Human	VBL	400	4	30	2309238
Methyl tert-butyl ether	Human	BL	4.5	4	5	11504147
Methyl tert-butyl ether	Human	BL	25	4	11	17668360
Methyl tert-butyl ether	Human	BL	38.7	4	7	11504147
Methyl tert-butyl ether	Human	BL	75	4	10	17668360
n-Hexane	Rat	BL	3000	6	13	15793558
N-Methyl-2-pyrrolidone	Human	BL	2.47	8	7	19875680

N-Methyl-2-pyrrolidone	Human	BL	5.92	8	7	19875680
N-Methyl-2-pyrrolidone	Human	BL	13.07	8	7	19875680
N-Methyl-2-pyrrolidone	Human	PL	2.47	6.2	6	19875680
N-Methyl-2-pyrrolidone	Human	PL	9.87	6.2	6	19875680
N-Methyl-2-pyrrolidone	Human	PL	19.73	6.2	6	19875680
Nonane	Rat	BL	100	4	13	Source [a]
Nonane	Rat	BL	500	4	13	Source [a]
Nonane	Rat	BL	1000	4	13	Source [a]
Octane	Rat	BL	1000	2	4	22188408
Octane	Rat	BL	5000	2	1	22188408
Pyrene	Rat	BL	24.18	1.6	14	8078087
Pyrene	Rat	BL	60.44	1.6	15	8078087
Pyrene	Rat	BL	96.71	1.6	15	8078087
Styrene	Rat	BL	80	6	12	734422
Styrene	Rat	BL	80	24	8	734422
Styrene	Rat	BL	200	6	13	734422
Styrene	Rat	BL	200	24	8	734422
Styrene	Rat	BL	600	6	13	734422
Styrene	Rat	BL	600	24	8	734422
Styrene	Rat	BL	1200	6	12	734422
Styrene	Rat	BL	1200	24	9	734422
Styrene	Human	EB	80	6	11	7385239
Styrene	Human	BL	80	6	30	734422
tert-Amyl methyl ether	Human	BL	3.8	4	6	11504147
tert-Amyl methyl ether	Human	BL	15	4	10	17668360
tert-Amyl methyl ether	Human	BL	38.4	4	7	11504147
tert-Amyl methyl ether	Human	BL	50	4	9	17668360
Tetrachloroethylene	Rat	BL	600	6	10	538758
Tetrachloroethylene	Human	EB	72	4	10	422271
Tetrachloroethylene	Human	EB	144	4	8	422271
Tetrachloroethylene	Human	BL	72	4	8	422271
Tetrachloroethylene	Human	BL	144	4	8	422271

Tetrachloroethylene	Human	BL (+W)	142	4	8	422271
Tetrachloroethylene	Human	EB (+W)	142	4	6	422271
Tetrahydrofuran	Human	EB	150	4	16	10222575
Toluene	Rat	BL	100	2	7	629888
Trichloroethylene	Rat	EB	50	2	31	1891776
Trichloroethylene	Rat	EB	100	4	17	629888
Trichloroethylene	Rat	EB	500	2	31	1891776
Trichloroethylene	Rat	VBL	600	4	6	2315918
Trichloroethylene	Rat	VBL	600.4	4	6	2315918
Trichloroethylene	Rat	BL	100	4	11	629888
Trichloroethylene	Rat	BL	529	4	5	2068722
Trichloroethylene	Rat	BL	600	4	5	2068722
Trichloroethylene	Rat	BL	600.4	4	5	2749729
Trichloroethylene	Human	EB	100	4	41	9853003
Trichloroethylene	Human	BL	50	4	45	9853003
Trichloroethylene	Human	BL	100	4	28	9721257
Vinyl chloride	Human	EB	2.5	0.2	23	11453305
Vinyl chloride	Human	EB	2.5	0.5	24	11453305

[a]Source is a Defense Technical Information Center report, not indexed on PubMed; PMID, unique PubMed article ID number (for use on https://www.ncbi.nlm.nih.gov/pubmed/); EB, unspecified exhaled breath sample (assumed to be end-exhaled breath); VBL, venous blood; ABL, arterial blood; BL, unspecified blood sample (assumed to be venous blood); (+W), indicates there was also some light work or exercise during exposure.

Table S3: “Leave one out” sensitivity analysis. Table describes the goodness-of-fit parameters for log-transformed data detailed in the results if each of the 41 chemicals is individually left out of the regressions (compare to the top row with “None” left out).

Chemical Dropped	Overall Reg Slope	Overall Reg r^2	Overall Reg RMSE	Overall DC[a] RMSE	% Data Censored	Cmax Reg Slope	Cmax Reg r^2	Cmax DC[a] RMSE	AUC Reg Slope	AUC Reg r^2	AUC DC[a] RMSE
None	0.46	0.45	0.76	1.11	0.93	0.88	0.67	0.47	1.02	0.79	0.50
1,1-Dichloroethylene	0.44	0.43	0.76	1.17	1.05	0.86	0.67	0.48	1.02	0.79	0.51
1,1,1-Trichloroethane	0.47	0.43	0.76	1.06	0.95	0.87	0.68	0.48	1.02	0.79	0.50
1,1,1,2-Tetrafluoroethane	0.46	0.44	0.76	1.12	0.97	0.88	0.68	0.48	1.02	0.79	0.50
1,1,2-Trichloro-1,2,2-trifluoroethane	0.46	0.45	0.76	1.11	0.94	0.88	0.68	0.47	1.02	0.79	0.50
1,2-Dichloroethane	0.46	0.45	0.76	1.12	0.95	0.87	0.68	0.47	1.02	0.79	0.50
1,2-Dichloropropane	0.46	0.44	0.76	1.12	0.95	0.87	0.67	0.48	1.02	0.79	0.51
1,2,4-Trimethylbenzene	0.46	0.44	0.76	1.11	0.95	0.88	0.67	0.48	1.02	0.79	0.50
1,3-Butadiene	0.46	0.44	0.76	1.12	0.96	0.87	0.67	0.48	1.02	0.79	0.51
1,4-Dioxane	0.46	0.45	0.76	1.11	0.94	0.88	0.68	0.47	1.02	0.79	0.50
2-Butoxyethanol	0.46	0.45	0.76	1.11	0.94	0.88	0.68	0.48	1.02	0.79	0.50
2,2-Dichloro-1,1,1-trifluoroethane	0.48	0.46	0.76	1.07	0.94	0.87	0.66	0.48	1.02	0.79	0.50
2H-Perfluoropropane	0.48	0.49	0.76	1.09	0.97	0.91	0.74	0.43	1.02	0.79	0.45
Acrylonitrile	0.46	0.45	0.76	1.11	0.94	0.88	0.68	0.48	1.02	0.79	0.50
Benzene	0.41	0.41	0.76	1.14	0.98	0.86	0.64	0.49	1.02	0.79	0.51
Bromotrifluoromethane	0.47	0.45	0.76	1.11	0.91	0.88	0.68	0.48	1.02	0.79	0.50
Carbon tetrachloride	0.48	0.46	0.76	1.07	0.91	0.88	0.67	0.48	1.02	0.79	0.50
Chlorobenzene	0.46	0.44	0.76	1.12	0.95	0.88	0.67	0.48	1.02	0.79	0.50
Chloroform	0.46	0.45	0.76	1.11	0.94	0.88	0.68	0.48	1.02	0.79	0.50
Decane	0.47	0.45	0.76	1.11	0.94	0.88	0.68	0.47	1.02	0.79	0.49
Dichlorodifluoromethane	0.46	0.45	0.76	1.12	0.97	0.87	0.67	0.48	1.02	0.79	0.50
Dichloromethane	0.46	0.44	0.76	1.11	0.58	0.87	0.67	0.48	1.02	0.79	0.51
Ethanol	0.46	0.45	0.76	1.11	0.71	0.89	0.69	0.47	1.02	0.79	0.50
Ethyl T-butyl ether	0.46	0.45	0.76	1.11	0.94	0.88	0.67	0.48	1.02	0.79	0.50
Ethylbenzene	0.46	0.45	0.76	1.11	0.94	0.87	0.67	0.48	1.02	0.79	0.50
Furan	0.46	0.45	0.76	1.11	0.94	0.88	0.69	0.46	1.02	0.79	0.49
Isopropanol	0.46	0.45	0.76	1.11	0.97	0.84	0.66	0.47	1.02	0.79	0.50

Methanol	0.46	0.44	0.76	1.11	0.95	0.86	0.65	0.48	1.02	0.79	0.50
Methyl ethyl ketone	0.46	0.45	0.76	1.12	0.97	0.87	0.68	0.47	1.02	0.79	0.50
Methyl tert-butyl ether	0.46	0.44	0.76	1.11	0.85	0.88	0.67	0.48	1.02	0.79	0.51
n-Hexane	0.46	0.45	0.76	1.10	0.89	0.87	0.67	0.48	1.02	0.79	0.50
N-Methyl-2-pyrrolidone	0.46	0.45	0.76	1.12	0.95	0.89	0.67	0.48	1.02	0.79	0.51
Nonane	0.46	0.45	0.76	1.11	0.95	0.88	0.68	0.48	1.02	0.79	0.50
Octane	0.46	0.45	0.76	1.11	0.94	0.88	0.67	0.48	1.02	0.79	0.50
Pyrene	0.46	0.46	0.76	1.10	0.95	0.92	0.74	0.43	1.02	0.79	0.46
Styrene	0.47	0.44	0.76	1.06	0.99	0.85	0.67	0.48	1.02	0.79	0.51
tert-Amyl methyl ether	0.46	0.44	0.76	1.11	0.90	0.88	0.66	0.48	1.02	0.79	0.51
Tetrachloroethylene	0.46	0.44	0.76	1.11	0.96	0.88	0.68	0.48	1.02	0.79	0.50
Tetrahydrofuran	0.47	0.45	0.76	1.09	0.94	0.87	0.68	0.47	1.02	0.79	0.49
Toluene	0.46	0.45	0.76	1.11	0.94	0.88	0.68	0.48	1.02	0.79	0.50
Trichloroethylene	0.48	0.45	0.76	1.09	1.05	0.86	0.67	0.49	1.02	0.79	0.52
Vinyl chloride	0.46	0.44	0.76	1.12	0.95	0.87	0.67	0.48	1.02	0.79	0.50

[a]DC (Direct Comparison) indicates RMSE was calculated directly between log-transformed simulated and observed data (i.e. with the assumption y = x); Reg, Regression; RMSE, Root Mean Square Error; Cmax, Maximum concentration; AUC, area under the concentration time curve.

Table S4: Variability in fit slope and Root Mean Square Error (RMSE) vs. identity line with variable upper respiratory tract clearance constant (KurtC) value.

KurtC (L/hr/kg$^{0.75}$)	**Slope**	**RMSE**
1E-5	0.45	1.14
1E-4	0.47	1.09
1E-3	0.42	1.21
1E-2	0.40	1.24
1E-1	0.40	1.24
1	0.42	1.20
2	0.42	1.19
3	0.42	1.20
4	0.42	1.20
5	0.43	1.18
6	0.43	1.17
7	0.44	1.16
8	0.45	1.14
9	0.45	1.13
10	0.46	1.12
11	0.46	1.11
12	0.47	1.10
13	0.47	1.09
14	0.48	1.08
15	0.48	1.07
16	0.49	1.06
17	0.49	1.06
18	0.49	1.06
19	0.50	1.05
20	0.50	1.05

Table S5: List of concentration-time datapoints that had >2 orders of magnitude difference between simulated and observed concentrations

Chemical	CAMEO Chemical Class	Species	Sample Matrix	Time Quartile of Sample[a]	Log(SIM)	Log(OBS)	Log(SIM) - Log(OBS)
2,2-Dichloro-1,1,1-trifluoroethane	Fluorinated organic compound	Rat	VBL	4	-9.15	0.31	-9.47
2,2-Dichloro-1,1,1-trifluoroethane	Fluorinated organic compound	Rat	VBL	4	-8.15	0.76	-8.92
Carbon tetrachloride	Halogenated organic compound	Rat	ABL	4	-7.45	0.02	-7.46
Trichloroethylene	Halogenated organic compound	Rat	EB	4	-7.71	-0.41	-7.3
Trichloroethylene	Halogenated organic compound	Rat	BL	4	-7.43	-0.59	-6.85
Carbon tetrachloride	Halogenated organic compound	Rat	ABL	4	-6.53	0.19	-6.72
1,1,1-Trichloroethane	Halogenated organic compound	Human	EB	4	-8.79	-2.12	-6.67
1,1,1-Trichloroethane	Halogenated organic compound	Human	EB (+W)	4	-8.46	-1.86	-6.6
Trichloroethylene	Halogenated organic compound	Rat	EB	4	-6.84	-0.29	-6.55
1,1,1-Trichloroethane	Halogenated organic compound	Human	EB	4	-8.46	-1.92	-6.54
Styrene	Aromatic hydrocarbon	Rat	BL	4	-6.21	0.23	-6.44
Isopropanol	Alcohol	Rat	VBL	4	-3.64	2.31	-5.95
Styrene	Aromatic hydrocarbon	Rat	BL	4	-6.51	-0.72	-5.8
Carbon tetrachloride	Halogenated organic compound	Rat	ABL	4	-5.6	0.16	-5.75
Trichloroethylene	Halogenated organic compound	Rat	EB	4	-5.97	-0.29	-5.68
Styrene	Aromatic hydrocarbon	Rat	BL	4	-7.39	-1.72	-5.67
Styrene	Aromatic hydrocarbon	Rat	BL	4	-6.98	-1.54	-5.44
Dichloromethane	Halogenated organic compound	Human	VBL	4	-5.78	-0.37	-5.41
1,1,1-Trichloroethane	Halogenated organic compound	Human	EB (+W)	4	-7.02	-1.65	-5.37
1,1,1-Trichloroethane	Halogenated organic compound	Human	EB	4	-7.32	-1.99	-5.33
1,1,1-Trichloroethane	Halogenated organic compound	Human	EB	4	-7.01	-1.71	-5.31
Trichloroethylene	Halogenated organic compound	Rat	BL	4	-5.7	-0.41	-5.29
Styrene	Aromatic hydrocarbon	Rat	BL	4	-4.37	0.75	-5.12
Trichloroethylene	Halogenated organic compound	Rat	EB	4	-5.1	-0.18	-4.92
Carbon tetrachloride	Halogenated organic compound	Rat	ABL	4	-4.69	0.16	-4.85
n-Hexane	Aliphatic hydrocarbon	Rat	BL	4	-4.85	-0.16	-4.69
Styrene	Aromatic hydrocarbon	Rat	BL	4	-4.61	0.05	-4.66

Trichloroethylene	Halogenated organic compound	Rat	BL	4	-3.24	1.41	-4.65
2,2-Dichloro-1,1,1-trifluoroethane	Fluorinated organic compound	Rat	VBL	3	-3.58	0.65	-4.23
Carbon tetrachloride	Halogenated organic compound	Rat	ABL	3	-3.75	0.46	-4.21
Tetrahydrofuran	Ether	Human	EB	4	-3.76	0.42	-4.18
Trichloroethylene	Halogenated organic compound	Rat	EB	3	-4.23	-0.09	-4.14
Methanol	Alcohol	Rat	BL	4	-2.76	1.34	-4.1
Styrene	Aromatic hydrocarbon	Rat	BL	3	-2.47	1.63	-4.1
Tetrachloroethylene	Halogenated organic compound	Rat	BL	4	-3.9	0.11	-4.02
Styrene	Aromatic hydrocarbon	Rat	BL	4	-5.06	-1.19	-3.87
Carbon tetrachloride	Halogenated organic compound	Rat	ABL	4	-4.73	-0.89	-3.85
Styrene	Aromatic hydrocarbon	Human	EB	4	-5.39	-1.62	-3.77
Trichloroethylene	Halogenated organic compound	Rat	BL	3	-3.96	-0.23	-3.72
Styrene	Aromatic hydrocarbon	Human	BL	4	-4.7	-1.01	-3.69
Styrene	Aromatic hydrocarbon	Human	BL	4	-4.71	-1.02	-3.68
2,2-Dichloro-1,1,1-trifluoroethane	Fluorinated organic compound	Rat	VBL	3	-2.55	1.08	-3.63
Carbon tetrachloride	Halogenated organic compound	Rat	ABL	3	-2.8	0.66	-3.46
Tetrahydrofuran	Ether	Human	EB	4	-3.34	0.12	-3.46
Trichloroethylene	Halogenated organic compound	Rat	EB	3	-3.36	0.01	-3.37
Dichloromethane	Halogenated organic compound	Human	VBL	3	-3.35	-0.04	-3.3
Styrene	Aromatic hydrocarbon	Rat	BL	3	-1.54	1.67	-3.21
Trichloroethylene	Halogenated organic compound	Rat	BL	4	-1.5	1.72	-3.21
Dichloromethane	Halogenated organic compound	Human	EB	3	-3.08	0.11	-3.2
Carbon tetrachloride	Halogenated organic compound	Rat	ABL	4	-3.78	-0.58	-3.19
Isopropanol	Alcohol	Rat	VBL	3	-0.12	3.05	-3.17
Styrene	Aromatic hydrocarbon	Rat	BL	4	-4.56	-1.47	-3.09
Tetrahydrofuran	Ether	Human	EB	4	-2.93	0.12	-3.05
Dichloromethane	Halogenated organic compound	Human	VBL	3	-3.89	-0.85	-3.04
Styrene	Aromatic hydrocarbon	Rat	BL	3	-2.7	0.31	-3.02
Trichloroethylene	Halogenated organic compound	Rat	EB	3	-2.93	0.02	-2.95
Styrene	Aromatic hydrocarbon	Rat	BL	3	-0.6	2.26	-2.86
1,1,1-Trichloroethane	Halogenated organic compound	Human	EB	3	-4.05	-1.2	-2.85
n-Hexane	Aliphatic hydrocarbon	Rat	BL	4	-3.15	-0.31	-2.84

1,1,1-Trichloroethane	Halogenated organic compound	Human	EB	3	-4.38	-1.55	-2.83
1,1,1-Trichloroethane	Halogenated organic compound	Human	EB (+W)	3	-4.06	-1.25	-2.81
Bromotrifluoromethane	Fluorinated organic compound	Human	VBL	4	-2.27	0.5	-2.76
Tetrahydrofuran	Ether	Human	EB	4	-2.51	0.22	-2.73
Bromotrifluoromethane	Fluorinated organic compound	Human	VBL	4	-2.2	0.5	-2.7
Methanol	Alcohol	Rat	BL	4	-1.33	1.34	-2.67
Styrene	Aromatic hydrocarbon	Rat	BL	3	-3.17	-0.58	-2.59
Trichloroethylene	Halogenated organic compound	Rat	EB	3	-2.49	0.08	-2.57
Carbon tetrachloride	Halogenated organic compound	Rat	ABL	2	-1.87	0.69	-2.56
Methanol	Alcohol	Rat	BL	3	0.15	2.72	-2.56
Styrene	Aromatic hydrocarbon	Rat	BL	3	-1.73	0.82	-2.55
Bromotrifluoromethane	Fluorinated organic compound	Human	VBL	4	-2.11	0.43	-2.54
tert-Amyl methyl ether	Ether	Human	BL	4	-3.03	-0.49	-2.54
Isopropanol	Alcohol	Rat	VBL	4	-1.12	1.41	-2.53
Benzene	Aromatic hydrocarbon	Rat	BL	4	-2.02	0.49	-2.51
tert-Amyl methyl ether	Ether	Human	BL	4	-3.55	-1.06	-2.49
Benzene	Aromatic hydrocarbon	Rat	BL	4	-1.94	0.46	-2.4
Tetrachloroethylene	Halogenated organic compound	Rat	BL	3	-1.86	0.54	-2.4
Benzene	Aromatic hydrocarbon	Rat	BL	4	-2.17	0.22	-2.39
Tetrachloroethylene	Halogenated organic compound	Human	EB (+W)	4	-3.04	-0.65	-2.39
Tetrachloroethylene	Halogenated organic compound	Human	EB	4	-3.35	-1.03	-2.31
Benzene	Aromatic hydrocarbon	Human	EB	4	-4.07	-1.79	-2.28
Tetrachloroethylene	Halogenated organic compound	Human	BL (+W)	4	-2.91	-0.64	-2.28
Carbon tetrachloride	Halogenated organic compound	Rat	ABL	3	-2.86	-0.58	-2.27
Tetrachloroethylene	Halogenated organic compound	Human	EB	4	-3.04	-0.78	-2.26
Bromotrifluoromethane	Fluorinated organic compound	Human	VBL	4	-2.15	0.08	-2.24
Methyl tert-butyl ether	Ether	Human	BL	4	-2.81	-0.57	-2.24
Benzene	Aromatic hydrocarbon	Rat	BL	4	-2.1	0.12	-2.22
Methyl tert-butyl ether	Ether	Human	BL	4	-3.6	-1.4	-2.21
Bromotrifluoromethane	Fluorinated organic compound	Human	VBL	4	-1.6	0.6	-2.2
Trichloroethylene	Halogenated organic compound	Rat	EB	3	-2.06	0.12	-2.18
Tetrachloroethylene	Halogenated organic compound	Human	BL	4	-2.91	-0.75	-2.16

Trichloroethylene	Halogenated organic compound	Rat	BL	3	-2.22	-0.06	-2.16
Tetrachloroethylene	Halogenated organic compound	Human	BL	4	-3.23	-1.1	-2.13
Tetrahydrofuran	Ether	Human	EB	3	-1.7	0.42	-2.12
Styrene	Aromatic hydrocarbon	Rat	BL	3	-0.88	1.18	-2.06
Benzene	Aromatic hydrocarbon	Rat	BL	4	-1.41	0.63	-2.04
Ethyl T-butyl ether	Ether	Human	BL	4	-2.8	-0.77	-2.04
Isopropanol	Alcohol	Rat	VBL	3	1.57	3.6	-2.03
Styrene	Aromatic hydrocarbon	Rat	BL	2	0.39	2.41	-2.02
Decane	Aliphatic hydrocarbon	Rat	BL	3	2.22	0.21	2.01
2H-Perfluoropropane	Fluorinated organic compound	Human	VBL	3	1.96	-0.1	2.06

[a]Time quartile of the concentration-time curve from which sample was taken, 1 being the first time quartile of the curve, 4 being the final quartile of the curve; CAMEO, Computer-Aided Management of Emergency Operations, database of hazardous chemical datasheets that emergency responders and planners can use to get response recommendations and predict hazards; SIM, simulated concentration; OBS, observed concentration; EB, unspecified exhaled breath sample (assumed to be end-exhaled breath); VBL, venous blood; ABL, arterial blood; BL, unspecified blood sample (assumed to be venous blood); (+W), indicates there was also some light work or exercise during exposure.

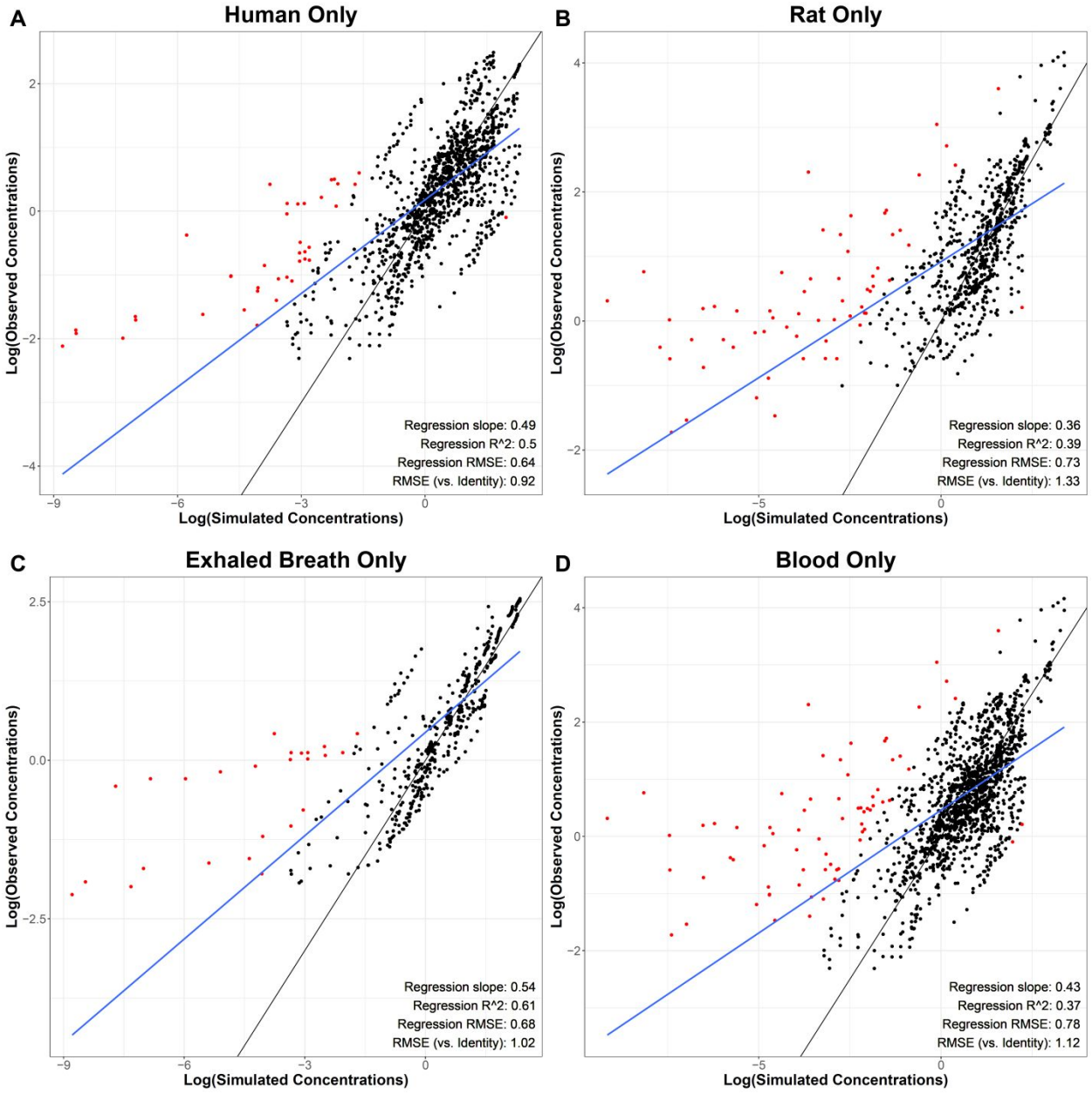

Figure S1: Log-transformed observed (y-axis) vs. simulated (x-axis) concentrations subsetted by species (A: Human, B: Rat) or sampling matrix (C: Aggregated Exhaled Breath [ppm], D: Aggregated Blood [µM]). Aggregated Exhaled Breath includes all unspecified exhaled breath, end exhaled breath, and mixed exhaled breath samples. Aggregated Blood includes all unspecified blood, venous blood, arterial blood, and plasma samples. Blue line is the regression line of best fit. Black line is the line of identity (x = y). Red points are >2 log-orders different between observed and simulated values.

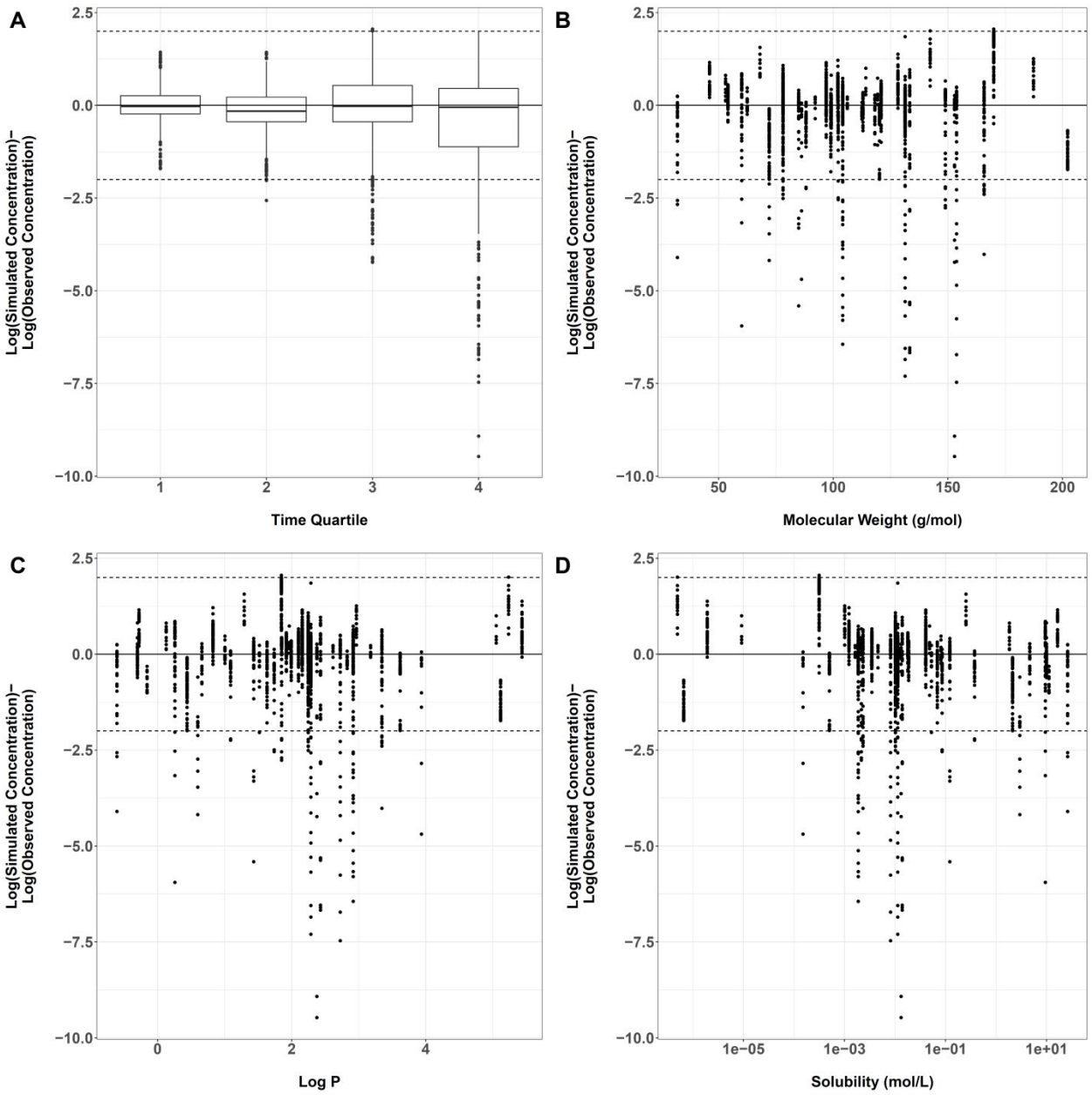

Figure S2 A-D: Log difference between observed and simulated concentrations grouped by time quartile of the concentration-time curve (A), molecular weight (B), log P (C), and solubility (D). Labeled points in S1A are >2 log-orders different between observed and simulated values.

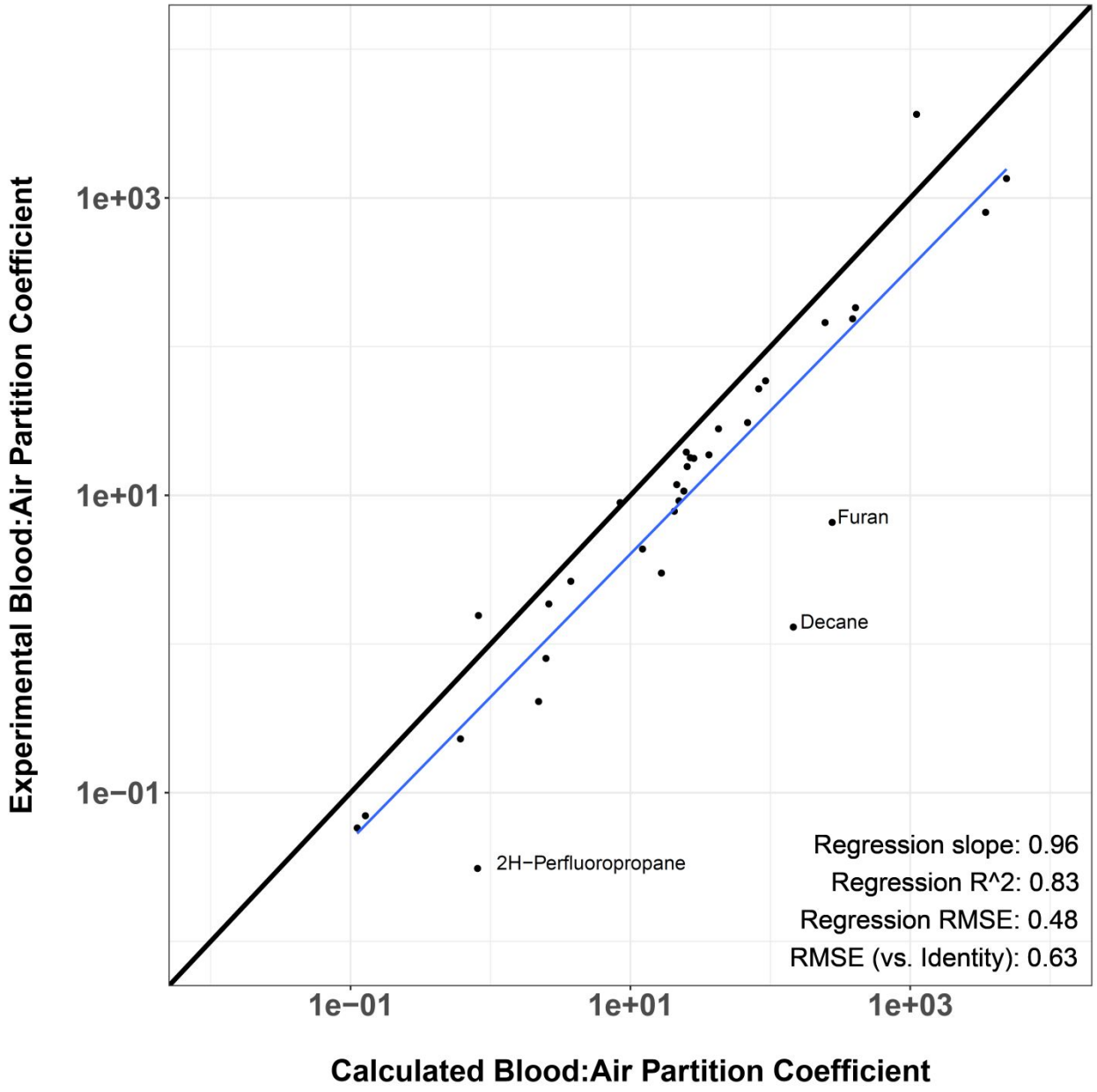

Figure S3: Comparison of experimentally-derived (from literature) and calculated blood:air partition coefficients. Labeled points were > 1 log-order different between experimental and calculated values. Blue line is regression line of best fit with the slope and r^2 value noted in the bottom. Black line is the line of identity (x = y). RMSE is compared to line of identity.

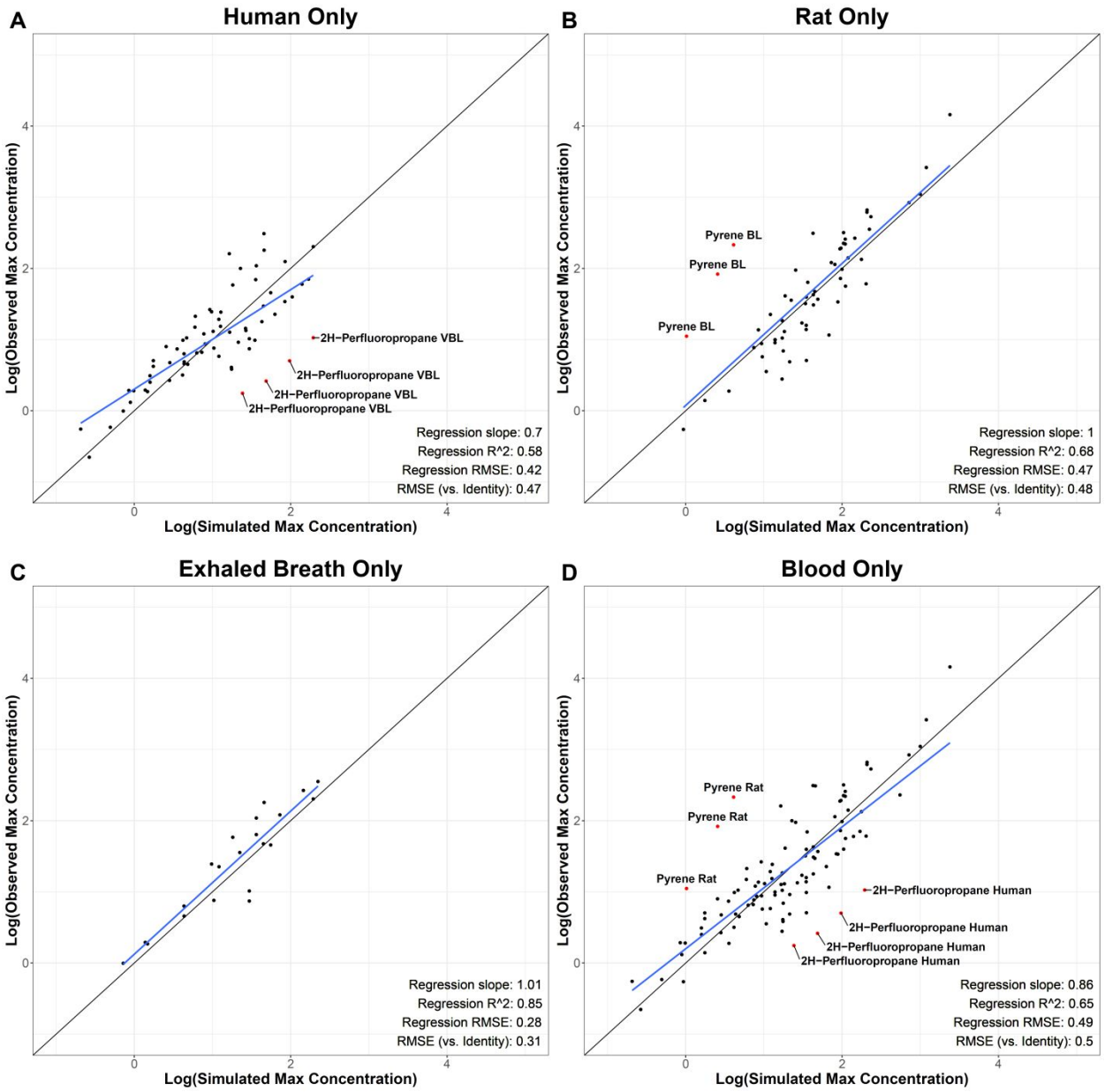

Figure S4: Log-transformed observed (y-axis) vs. simulated (x-axis) max concentrations subsetted by species (A: Human, B: Rat) or sampling matrix (C: Aggregated Exhaled Breath [ppm], D: Aggregated Blood [µM]). Aggregated Exhaled Breath includes all unspecified exhaled breath, end exhaled breath, and mixed exhaled breath samples. Aggregated Blood includes all unspecified blood, venous blood, arterial blood, and plasma samples. Blue line is the regression line of best fit. Black line is the line of identity (x = y). Labeled red points are >1 log-order different between observed and simulated values.

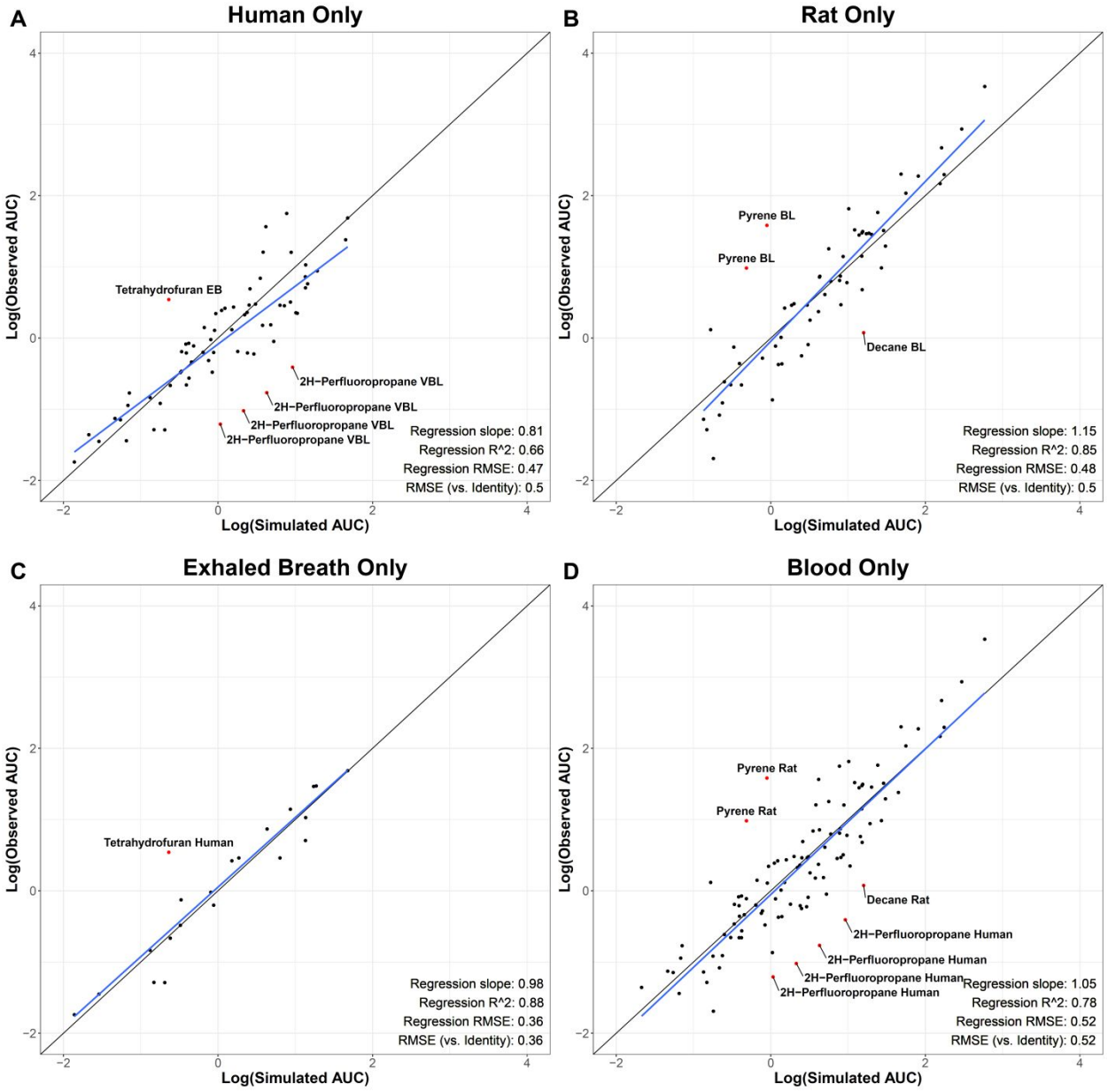

Figure S5: Log-transformed observed (y-axis) vs. simulated (x-axis) area under the concentration-time curve (AUC) subsetted by species (A: Human, B: Rat) or sampling matrix (C: Aggregated Exhaled Breath [ppm], D: Aggregated Blood [µM]). Aggregated Exhaled Breath includes all unspecified exhaled breath, end exhaled breath, and mixed exhaled breath samples. Aggregated Blood includes all unspecified blood, venous blood, arterial blood, and plasma samples. Blue line is the regression line of best fit. Black line is the line of identity (x = y). Labeled red points are >1 log-order different between observed and simulated values.

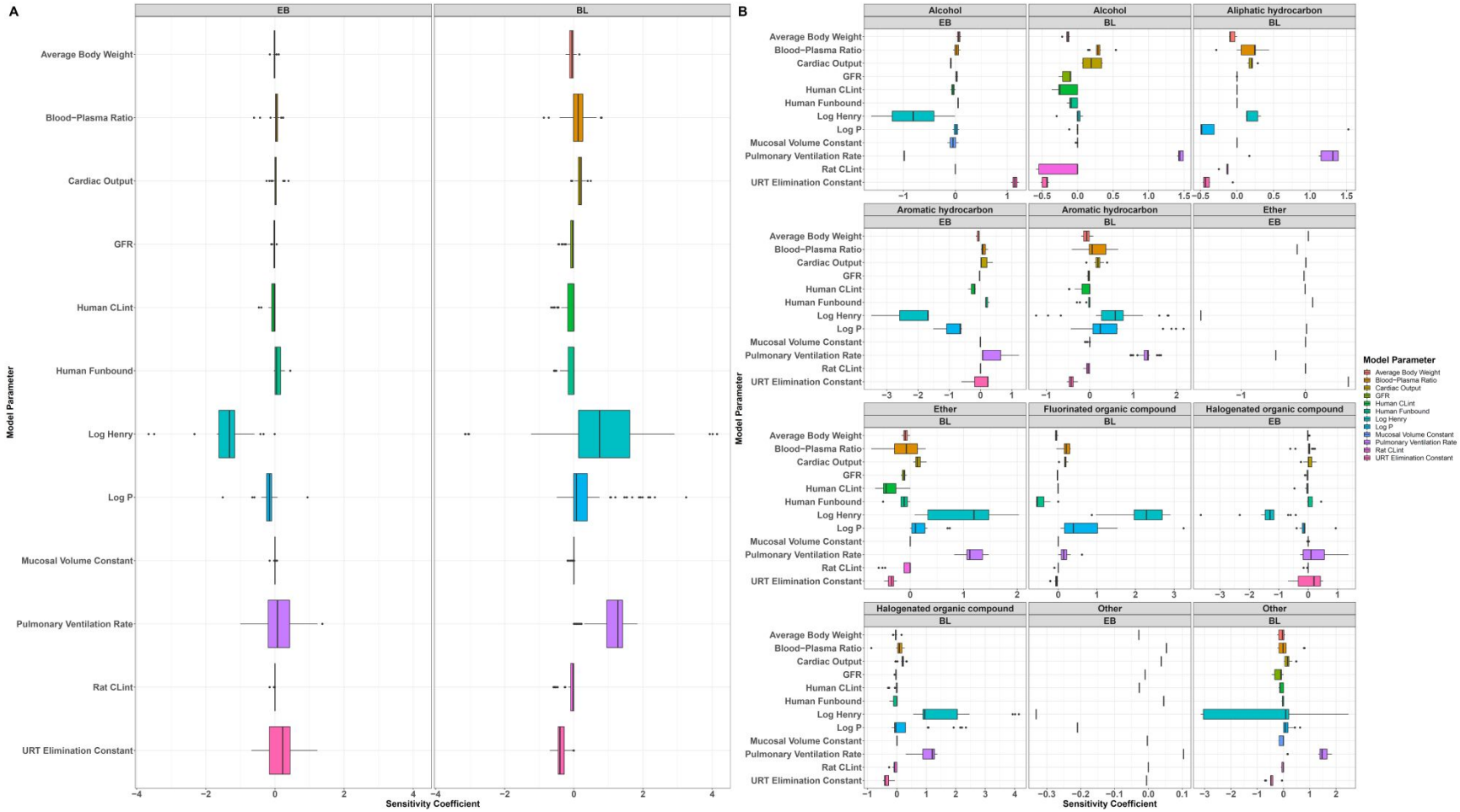

Figure S6 A-B: Sensitivity analysis for input quantities used to calculated model-relevant inhalation values (e.g. Qalv, Kblood2air, Kmuc2air) grouped by **A)** sampling matrix alone (EB, exhaled breath, end exhaled breath, mixed exhaled breath; BL, blood, arterial blood, venous blood, plasma) or **B**) sampling matrix and chemical class. GFR, glomerular filtration rate; CLint, intrinsic clearance; Funbound, fraction unbound in plasma; URT, upper respiratory tract

Model Code Supplement:

```
/* inhalation.c for R deSolve package
   _____________________________________________________

   Model File:  inhalation.model

   Date:

   Created by:
    -- a model preprocessor by Don Maszle
   _____________________________________________________

   Copyright (c) 1993-2015 Free Software Foundation, Inc.
```

The following section is entirely a commented list of states, inputs, outputs, and parameters and their default values (where applicable).

```
   Model calculations for compartmental model:

   14 States (user input units):
     Agutlumen = 0.0,          //Amount in the gut lumen
     Agut = 0.0,               //Amount in the gut
     Aliver = 0.0,             //Amount in the liver
     Aven = 0.0,               //Amount in venous circulation
     Alung = 0.0,              //Amount in the lung tissue
     Aart = 0.0,               //Amount in arterial circulation
     Arest = 0.0,              //Amount in the “rest-of-body” compartment
     Akidney = 0.0,            //Amount in the kidney
     Atubules = 0.0,           //Amount in the tubules
     Ametabolized = 0.0,       //Amount metabolized (cumulative)
     AUC = 0.0,                //Area under concentration-time curve
     Ainh = 0.0,               //Amount inhaled
     Aexh = 0.0,               //Amount exhaled
     Amuc = 0.0,               //Amount in mucus

   13 Outputs (user input  units):
    "Cgut",                    //Concentration in the gut
    "Cliver",                  //Concentration in the liver
    "Cven",                    //Concentration in venous circulation
    "Clung",                   //Concentration in the lung tissue
    "Cart",                    //Concentration in arterial circulation
    "Crest",                   //Concentration in the “rest-of-body” compartment
    "Ckidney",                 //Concentration in the kidney
    "Cplasma",                 //Concentration in the plasma
    "Aplasma",                 //Amount in the plasma
    "Calv",                    //Concentration in the alveolar space
    "Cendexh",                 //Concentration in end-exhaled breath
    "Cmixexh",                 //Concentration in mix-exhaled breath
    "Cmuc",                    //Concentration in the mucus

   1 Input (user input units):
     Cinh (forcing function)   //Inhalation (exposure) concentration
```

```
53 Parameters:
  BW = 70,                          //Body weight (kg)
  Clmetabolismc = 0.203,            //Unscaled metabolism parameter (L/d/kg^0.75)
  vmax = 0,                         //Unscaled Vmax (mg/h/kg^0.75)
  hematocrit = 0.44,                //Hematocrit concentration (units)
  kgutabs = 1,                      //Gut absorption coefficient (%)
  Kkidney2pu = 0,                   //Kidney-Unbound Plasma partition coefficient
  Kliver2pu = 0,                    //Liver-Unbound Plasma partition coefficient
  Krest2pu = 0,                     //Rest-Unbound Plasma partition coefficient
  Kgut2pu = 0,                      //Gut-Unbound Plasma partition coefficient
  Klung2pu = 0,                     //Lung-Unbound Plasma partition coefficient
  Qcardiacc = 4.8,                  //Unscaled cardiac output (CO, L/d)
  Qgfrc = 0.108,                    //Unscaled glomerular filtration rate (units)
  Qgutf = 0.205,                    //Gut blood flow (fraction of CO)
  Qkidneyf = 0.221,                 //Kidney blood flow (fraction of CO)
  Qliverf = 0.0536,                 //Liver blood flow (fraction of CO)
  Qlungf = 0,                       //Lung blood flow (fraction of CO)
  Vartc = 0.0487,                   //Unscaled arterial volume (L/kg)
  Vgutc = 0.0158,                   //Unscaled gut volume (L/kg)
  Vkidneyc = 0.00119,               //Unscaled kidney volume (L/kg)
  Vliverc = 0.02448,                //Unscaled liver volume (L/kg)
  Vlungc = 0.00723,                 //Unscaled lung volume (L/kg)
  Vrestc = 0.77654,                 //Unscaled “rest-of-body” volume (L/kg)
  Vvenc = 0.0487,                   //Unscaled venous volume (L/kg)
  Fraction_unbound_plasma = 0.0682,
  Rblood2plasma = 0.0,              //Blood-to-plasma ratio
  Clmetabolism = 0.0,               //Hepatic metabolic clearance (L/d)
  Qcardiac = 0.0,                   //Cardiac output (L/d)
  Qgfr = 0.0,                       //Glomerular filtration (L/d)
  Qgut = 0.0,                       //Gut blood flow (L/d)
  Qkidney = 0.0,                    //Kidney blood flow (L/d)
  Qliver = 0.0,                     //Liver blood flow (L/d)
  Qlung = 0.0,                      //Lung blood flow (L/d)
  Qrest = 0.0,                      //”Rest-of-body” blood flow (L/d)
  Vart = 0.0,                       //Arterial volume (L)
  Vgut = 0.0,                       //Gut volume (L)
  Vkidney = 0.0,                    //Kidney volume (L)
  Vliver = 0.0,                     //Liver volume (L)
  Vlung = 0.0,                      //Lung volume (L)
  Vrest = 0.0,                      //”Rest-of-body” volume (L)
  Vven = 0.0,                       //Venous volume (L)
  Qalv = 0,                         //Alveolar ventilation (L/d)
  Kblood2air = 0,                   //Blood-air partition coefficient
  InhMag = 0,                       //Unused parameter
  Period = 0,                       //Time between exposure events (h)
  Exposure = 0,                     //External chemical exposure (user input units)
  kUrtc = 11.0,                     //Unscaled upper respiratory tract uptake parameter (L/h/kg^0.75)
  kUrt = 0,                         //Upper respiratory tract uptake parameter (L/h)
  Kmuc2air = 0,                     //Mucus to air partition coefficient
  Vmucc = 0.0001,                   //Unscaled mucosal volume (L)
  Vmuc = 0.0,                       //Mucosal volume (L)
```

```
     Vmax = 0,                    //Maximum metabolism rate (mg/h)
     Km = 1,                      //Michaelis-Menten Coefficient (mg/L)
*/

#include <R.h>
```

/*These next sections define the States, Outputs, and Parameters for the model, see definitions above*/

```
/* Model variables: States */
#define ID_Agutlumen 0x00000
#define ID_Agut 0x00001
#define ID_Aliver 0x00002
#define ID_Aven 0x00003
#define ID_Alung 0x00004
#define ID_Aart 0x00005
#define ID_Arest 0x00006
#define ID_Akidney 0x00007
#define ID_Atubules 0x00008
#define ID_Ametabolized 0x00009
#define ID_AUC 0x0000a
#define ID_Ainh 0x0000b
#define ID_Aexh 0x0000c
#define ID_Amuc 0x0000d

/* Model variables: Outputs */
#define ID_Cgut 0x00000
#define ID_Cliver 0x00001
#define ID_Cven 0x00002
#define ID_Clung 0x00003
#define ID_Cart 0x00004
#define ID_Crest 0x00005
#define ID_Ckidney 0x00006
#define ID_Cplasma 0x00007
#define ID_Aplasma 0x00008
#define ID_Calv 0x00009
#define ID_Cendexh 0x0000a
#define ID_Cmixexh 0x0000b
#define ID_Cmuc 0x0000c

/* Parameters */
static double parms[53];

#define BW parms[0]
#define Clmetabolismc parms[1]
#define vmax parms[2]
#define km parms[3]
#define hematocrit parms[4]
#define kgutabs parms[5]
#define Kkidney2pu parms[6]
#define Kliver2pu parms[7]
#define Krest2pu parms[8]
#define Kgut2pu parms[9]
#define Klung2pu parms[10]
#define Qcardiacc parms[11]
#define Qgfrc parms[12]
```

```
#define Qgutf parms[13]
#define Qkidneyf parms[14]
#define Qliverf parms[15]
#define Qlungf parms[16]
#define Vartc parms[17]
#define Vgutc parms[18]
#define Vkidneyc parms[19]
#define Vliverc parms[20]
#define Vlungc parms[21]
#define Vrestc parms[22]
#define Vvenc parms[23]
#define Fraction_unbound_plasma parms[24]
#define Rblood2plasma parms[25]
#define Clmetabolism parms[26]
#define Qcardiac parms[27]
#define Qgfr parms[28]
#define Qgut parms[29]
#define Qkidney parms[30]
#define Qliver parms[31]
#define Qlung parms[32]
#define Qrest parms[33]
#define Vart parms[34]
#define Vgut parms[35]
#define Vkidney parms[36]
#define Vliver parms[37]
#define Vlung parms[38]
#define Vrest parms[39]
#define Vven parms[40]
#define Qalv parms[41]
#define Kblood2air parms[42]
#define InhMag parms[43]
#define Period parms[44]
#define Exposure parms[45]
#define kUrtc parms[46]
#define kUrt parms[47]
#define Kmuc2air parms[48]
#define Vmucc parms[49]
#define Vmuc parms[50]
#define Vmax parms[51]
#define Km parms[52]

/* Forcing (Input) functions */
static double forc[1];

#define Cinh forc[0]

/*----- Initializers */
void initmod_inh (void (* odeparms)(int *, double *))
{
  int N=53;
  odeparms(&N, parms);
}

void initforc_inh (void (* odeforcs)(int *, double *))
{
  int N=1;
  odeforcs(&N, forc);
```

```
}


void getParms_inh (double *inParms, double *out, int *nout) {
/*----- Model scaling */

  int i;

  for (i = 0; i < *nout; i++) {
    parms[i] = inParms[i];
  }
```

/* Unit conversion, hours (*24), kg (*BW or *BW$^{0.75}$ for allometric scaling)*/

```
  kgutabs = kgutabs * 24 ;
  Clmetabolism = Clmetabolismc * 24 * BW ;
  Qcardiac = Qcardiacc * 24 * pow ( BW , 0.75 ) ;
  Qgfr = Qgfrc * pow ( BW , 0.75 ) * 24 ;
  Qgut = Qcardiac * Qgutf ;
  Qkidney = Qcardiac * Qkidneyf ;
  Qliver = Qcardiac * Qliverf ;
  Qlung = Qcardiac * Qlungf ;
  Qrest = Qcardiac - ( Qgut + Qkidney + Qliver + Qlung ) ;
  Vart = Vartc * BW ;
  Vgut = Vgutc * BW ;
  Vkidney = Vkidneyc * BW ;
  Vliver = Vliverc * BW ;
  Vlung = Vlungc * BW ;
  Vrest = Vrestc * BW ;
  Vven = Vvenc * BW ;
  Qalv = Qalv * 24 * pow ( BW , 0.75 ) ;
  kUrt = fmin ( kUrtc , Qalv /24/pow( BW , 0.75)) * pow( BW , 0.75 ) * 24 ;
  Vmuc = Vmucc * BW ;
  Vmax = vmax * 60 * 24 ;
  Km = km ;

  for (i = 0; i < *nout; i++) {
    out[i] = parms[i];
  }
  }
/*----- Dynamics section */

void derivs_inh (int *neq, double *pdTime, double *y, double *ydot, double
*yout, int *ip)
{

  yout[ID_Cgut] = y[ID_Agut] / Vgut ;          //Calculate gut concentration

  yout[ID_Cliver] = y[ID_Aliver] / Vliver ;    //Calculate liver concentration

  yout[ID_Cven] = y[ID_Aven] / Vven ;          //Calculate venous concentration

  yout[ID_Clung] = y[ID_Alung] / Vlung ;       //Calculate lung concentration

  yout[ID_Cart] = y[ID_Aart] / Vart ;          //Calculate arterial concentration

  yout[ID_Crest] = y[ID_Arest] / Vrest ;       //Calculate "rest-of-body" concentration
```

```
yout[ID_Ckidney] = y[ID_Akidney] / Vkidney ;//Calculate kidney concentration

yout[ID_Cplasma] = y[ID_Aven] / Vven
      / Rblood2plasma ;                        //Calculate plasma concentration

yout[ID_Aplasma] = y[ID_Aven]
      / Rblood2plasma * ( 1 - hematocrit ) ;//Calculate amount in the plasma

yout[ID_Calv] = yout[ID_Cart] / Kblood2air ;//Calculate alveolar concentration

yout[ID_Cendexh] = ((Qalv * yout[ID_Calv])
       + kUrt * ((yout[ID_Cmuc] / Kmuc2air)
       - yout[ID_Calv] ) ) / Qalv ;          //Calculate end-exhaled breath concentration

yout[ID_Cmixexh] = 0.7 * yout[ID_Cendexh]
       + 0.3 * Cinh ;                         //Calculate mix-exhaled breath concentration

yout[ID_Cmuc] = y[ID_Amuc] / Vmuc ;          //Calculate mucosal/URT concentration

ydot[ID_Agutlumen] = - kgutabs
       * y[ID_Agutlumen] ;                    // Rate of absorption from the gut lumen

ydot[ID_Agut] = kgutabs * y[ID_Agutlumen]
       + Qgut * ( yout[ID_Cart]
      - yout[ID_Cgut] * Rblood2plasma
       / Kgut2pu
      / Fraction_unbound_plasma ) ;          //Gut rate

ydot[ID_Aliver] = Qliver * yout[ID_Cart]
      + Qgut * yout[ID_Cgut] * Rblood2plasma
      / Kgut2pu / Fraction_unbound_plasma
      - ( Qliver + Qgut ) * yout[ID_Cliver]
      / Kliver2pu / Fraction_unbound_plasma
      * Rblood2plasma - Clmetabolism
      * yout[ID_Cliver] / Kliver2pu
      / Fraction_unbound_plasma
      * Rblood2plasma - Vmax * yout[ID_Cliver]
      / Kliver2pu / ( Km + yout[ID_Cliver]
      / Kliver2pu ) ;                        //Liver rate

ydot[ID_Aven] = ( ( Qliver + Qgut )
      * yout[ID_Cliver] / Kliver2pu
      + Qkidney * yout[ID_Ckidney]
      / Kkidney2pu + Qrest * yout[ID_Crest]
      / Krest2pu + Qlung * yout[ID_Clung]
      / Klung2pu ) * Rblood2plasma
      / Fraction_unbound_plasma - Qcardiac
      * yout[ID_Cven] ;                      //Venous rate

ydot[ID_Alung] = Qlung * ( yout[ID_Cart]
      - yout[ID_Clung] * Rblood2plasma
      / Klung2pu / Fraction_unbound_plasma) ;//Lung tissue rate

ydot[ID_Aart] = ( Qcardiac * ( yout[ID_Cven]
```

```
        - yout[ID_Cart] ) ) + ( Qalv * ( Cinh
        - yout[ID_Calv] ) ) - ( kUrt * ( Cinh
        - ( yout[ID_Cmuc] / Kmuc2air ) ) ) ;   //Arterial rate

  ydot[ID_Arest] = Qrest * ( yout[ID_Cart]
        - yout[ID_Crest] * Rblood2plasma
        / Krest2pu / Fraction_unbound_plasma) ;//"Rest-of-body" rate

  ydot[ID_Akidney] = Qkidney * yout[ID_Cart]
        - Qkidney * yout[ID_Ckidney]
        / Kkidney2pu * Rblood2plasma
        / Fraction_unbound_plasma - Qgfr
        * yout[ID_Ckidney] / Kkidney2pu ;      //Kidney rate

  ydot[ID_Atubules] = Qgfr * yout[ID_Ckidney]
        / Kkidney2pu ;                         //Kidney tubules rate

  ydot[ID_Ametabolized] = Clmetabolism
        * yout[ID_Cliver] / Kliver2pu
        / Fraction_unbound_plasma
        * Rblood2plasma + Vmax * yout[ID_Cliver]
        / Kliver2pu / ( Km + yout[ID_Cliver]
        / Kliver2pu ) ;                        //Hepatic metabolism rate

  ydot[ID_AUC] = yout[ID_Cven]/Rblood2plasma; //Area under the curve calc

  ydot[ID_Ainh] = ( Qalv * ( yout[ID_Calv]
        - Cinh ) ) + kUrt * ( ( yout[ID_Cmuc]
        / Kmuc2air ) - yout[ID_Calv] ) ;       //Rate of chemical inhalation

  ydot[ID_Aexh] = ( Qalv * yout[ID_Calv] )
        + kUrt * ( ( yout[ID_Cmuc] / Kmuc2air )
        - yout[ID_Calv] ) ;                    //Rate of chemical exhalation

  ydot[ID_Amuc] = ( kUrt * ( Cinh
        - ( yout[ID_Cmuc] / Kmuc2air ) ) )
        - ( kUrt * ( ( yout[ID_Cmuc]
        / Kmuc2air ) - yout[ID_Calv] ) ) ;     //Mucosal/URT rate

} /* derivs */


/*----- Jacobian calculations: */
void jac_inh (int *neq, double *t, double *y, int *ml, int *mu, double *pd,
int *nrowpd, double *yout, int *ip)
{

} /* jac */


/*----- Events calculations: */
void event_inh (int *n, double *t, double *y)
{

} /* event */
```

```
/*----- Roots calculations: */
void root_inh (int *neq, double *t, double *y, int *ng, double *gout, double
*out, int *ip)
{

} /* root */
```

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Manuscript Number: JESEE-19-3138.R1

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