

! TCE_CSL.CMD -- command file for TCE_BD.csl

PREPARE T, CInhPPM, CAIvPPM, CVTB, CLiv, CFat, CVen, CBldTCA, CLivTCA, &
& AUrnTCA, CTCOH, TotCTCOH, AUrnTCOGTCOH, AUrnTCTot, &
& AUrnTCTotMole, CDCA, AUrnNDCVC, AUrnNDCVCMole, MassBalTCE, &
& MassBalAbs, MassBalTCA, MassBalTCOH, MassBalTCOG, MassBalDCA, &
& MassBalDCVC, TotMassBal

SET NRWITG=.F., WESITG=.F.

PROCED ResetDoses

SET ZZXERR=39*1.0e-8, ZZMERR=39*1.0e-8
SET Conc=0.0, IVDose=0.0, PDose=0.0, Drink=0.0
SET CC=.FALSE., NRats=1.0, kLossC=0.0, VChC=1.0
SET Days=1.0, TMax=24.0
SET TStp=24.0, CINT=0.01

END

PROCED Human

SET BW=70.0
SET QCC=13.0, QPC=18.0
SET QFatC=0.052, QGutC=0.181, QLivC=0.046, QRapC=0.699
SET QSlwC=0.301, QTBC=0.025
SET VBldC=0.079, VBodC=0.2, VFatBldC=0.02, VFatC=0.214
SET VGutC=0.017, VKidC=0.004, VLivC=0.026, VRapC=0.192
SET VSlwC=0.651, VTBC=0.0008
SET VDDCAC=0.26, VDTCHC=0.65
SET PB=9.2, PFat=73.0, PGut=6.8, PLiv=6.8, PRap=6.8, PSlw=2.3, PTB=6.8
SET PAFatC1=10.0, PAFatC2=10.0
SET PBodTCA=1.9, PLivTCA=2.5
SET VMaxC=12.0, KM=1.5, kDCVCC=0.015, FracDCA=0.004, FractCE=0.08
SET VMaxClaraC=0.0045, KMClara=1.5, VMaxClearC=250.0, KMClear=250.0
SET kDissoc=174.6, NumSites=2.97, ProtConc=239.0
SET VMaxTCOHC=25.0, KMTCH=250.0, VMaxGlucC=5.0, KMGluc=25.0
SET kNATC=19.0, kKidCytoC=37.0
SET kAS=0.0, kTSD=10.0, kAD=1.0, kTD=0.0
SET kBileC=1.0, kEHRC=0.0
SET kClearDCAC=1.9, kUrnTCAC=0.2, kUrnTCOGC=3.0
SET FracPlas=0.58, TCAPlas=0.76

END

PROCED Mouse

SET BW=0.035
SET QCC=18.0, QPC=18.0
SET QFatC=0.07, QGutC=0.141, QLivC=0.02, QRapC=0.713, QSlwC=0.287
SET QTBC=0.005
SET VBldC=0.049, VBodC=0.2, VFatBldC=0.02, VFatC=0.07, VGutC=0.042
SET VKidC=0.017, VLivC=0.055, VRapC=0.217, VSlwC=0.619, VTBC=0.0007
SET VDDCAC=0.5, VDTCHC=0.65
SET PB=14.0, PFat=36.0, PGut=1.8, PLiv=1.8, PRap=1.8, PSlw=0.75
SET PTB=1.8
SET PAFatC1=10.0, PAFatC2=10.0
SET PBodTCA=0.76, PLivTCA=1.14
SET VMaxC=32.7, KM=0.25, kDCVCC=0.015, FracDCA=0.04, FractCE=0.035

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SET VMaxClaraC=3.0, KMClara=0.25, VMaxClearC=250.0, KMClear=250.0
SET kDissoc=46.1, NumSites=0.17, ProtConc=196.0
SET VMaxTCOHC=1.0, KMTCOH=0.25, VMaxGlucC=100.0, KMGluc=25.0
SET kNATC=0.5, kKidCytoC=0.4
SET kAS=0.0, kTSD=10.0, kAD=0.6, kTD=0.0
SET kBileC=1.0, kEHRC=0.0
SET kClearDCAC=1.0, kUrnTCAC=0.3, kUrnTCOGC=0.5
SET FracPlas=0.58, TCAPlas=0.76
END

```

PROCED Rat

```

SET BW=0.35
SET QCC=15.0, QPC=24.0
SET QFatC=0.07, QGutC=0.162, QLivC=0.021, QRapC=0.594, QSlwC=0.406
SET QTBC=0.021
SET VBldC=0.074, VBodC=0.2, VFatBldC=0.02, VFatC=0.07, VGutC=0.027
SET VKidC=0.007, VLivC=0.034, VRapC=0.213, VSlwC=0.664, VTBC=0.0005
SET VDDCAC=0.5, VDTCOHC=0.65
SET PB=18.5, PFat=27.5, PGut=1.3, PLiv=1.3, PRap=1.3, PSlw=0.5
SET PTB=1.3
SET PAFatC1=10.0, PAFatC2=10.0
SET PBodTCA=0.51, PLivTCA=0.76
SET VMaxC=11.2, KM=0.25, kDCVCC=0.015, FracDCA=0.04, FracTCE=0.04
SET VMaxClaraC=0.3, KMClara=0.25, VMaxClearC=250.0, KMClear=250.0
SET kDissoc=383.6, NumSites=1.49, ProtConc=190.0
SET VMaxTCOHC=0.12, KMTCOH=0.25, VMaxGlucC=100.0, KMGluc=25.0
SET kNATC=1.1, kKidCytoC=17.0
SET kAS=0.0, kTSD=10.0, kAD=0.3, kTD=0.0
SET kBileC=1.0, kEHRC=0.0
SET kClearDCAC=1.3, kUrnTCAC=0.3, kUrnTCOGC=0.5
SET FracPlas=0.58, TCAPlas=0.76
END

```

PROCED FisherMM

```

! Data from Fisher et al. (1991)
! From procedures FG3A and FG5A in TCENew.cmd
! 110 ppm TCE 4 hr -- Male Mouse
Mouse
ResetDoses
SET Conc=110.0, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=24.0
START /NC
PLOT /DATA=fishermm1 CVen
PLOT /DATA=fishermm2 CBldTCA
END

```

DATA FisherMM1 (T, CVen)

```

2.026 1.516
3.845 1.514
4.168 0.382
4.359 0.383
END

```

DATA FisherMM2 (T, CBldTCA)

```
1.976 18.519
3.869 47.996
4.23 49.273
4.267 38.833
5.065 69.449
5.994 53.35
8.015 40.811
20.974 7.224
END
```

```
PROCED FisherFMPParam
SET kUrntCAC=0.6
END
```

```
PROCED FisherFM
! Data from Fisher et al. (1991)
! From procedures FG4C and FG6C in TCENew.cmd
! 368 ppm TCE 4 hr -- Female Mouse
Mouse
ResetDoses
FisherFMPParam
SET Conc=368.0, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=30.0
START /NC
PLOT /DATA=fisherfm1 CVen
PLOT /DATA=fisherfm2 CBldTCA
END
```

```
DATA FisherFM1 (T, CVen)
2.013 5.964
3.831 6.427
4.32 1.076
4.688 0.839
5.012 0.226
END
```

```
DATA FisherFM2 (T, CBldTCA)
1.872 60.384
3.852 60.746
4.198 63.009
5.09 60.083
6.922 35.596
9.978 24.862
29.979 0.326
END
```

```
PROCED Fisher ! TCE in blood
! Data from Abbas R and Fisher JW. 1997. A physiologically based
! pharmacokinetic model for trichloroethylene and its metabolites,
! chloral hydrate, trichloroacetate, dichloroacetate, trichloroethanol,
! and trichloroethanol glucuronide in B6C3F1 mice. Toxicology and
! Applied Pharmacology 147:15-30.
!
! Sixteen male B6C3F1 mice (0.025-0.03 kg) (4 per dose group) were
! exposed by gavage to 300, 600, 1200, or 2000 mg/kg TCE in corn oil
! Abbas and Fisher. 1997. Mice - Gavage
```

```

!
! From procedure Fisher in TCENew.cmd
Mouse
ResetDoses
SET QPC=20.0, QCC=20.0
SET PDose=300.0, Days=1.0, TMax=48.0, TStp=250.0
START /NC

SET NRWITG=.T., PDose=600.0, QPC=15.0, QCC=15.0
START /NC

SET PDose=1200.0, QPC=12.0, QCC=12.0
START /NC

SET PDose=2000.0, QPC=6.0, QCC=6.0
START /NC

PLOT CVen/run=1, CVen/run=2, CVen/run=3, CVen/run=4, /DATA=fisher1 CVen
PLOT TotCTCOH/run=1, TotCTCOH/run=2, TotCTCOH/run=3, TotCTCOH/run=4,
/DATA=fisher2 TotCTCOH
PLOT CBldTCA/run=1, CBldTCA/run=2, CBldTCA/run=3, CBldTCA/run=4, /DATA=fisher3
CBldTCA
PLOT CDCA/run=1, CDCA/run=2, CDCA/run=3, CDCA/run=4, /DATA=fisher4 CDCA
PLOT AUrnTCOGTCOH/run=1, AUrnTCOGTCOH/run=2, AUrnTCOGTCOH/run=3,
AUrnTCOGTCOH/run=4, /DATA=fisher5 AUrnTCOGTCOH
PLOT AUrnTCA/run=1, AUrnTCA/run=2, AUrnTCA/run=3, AUrnTCA/run=4, /DATA=fisher6
AUrnTCA
SET NRWITG=.F.
END

```

DATA Fisher1 (T, CVen)

0.0	27.163
0.25	12.748
0.75	6.792
2.0	0.671
4.0	0.602
0.25	83.918
0.5	70.013
2.0	5.485
4.0	1.850
8.0	0.908
0.0	165.900
0.25	194.010
0.35	125.004
0.5	84.095
0.75	68.477
1.0	42.323
1.5	36.486
2.0	19.839
3.0	8.744
4.0	7.510
8.0	1.607
12.0	0.708
16.0	0.454
0.5	215.549
0.75	171.258

1.5	147.229
2.0	68.737
4.0	50.630
8.0	17.752
16.0	9.572
24.0	1.179

END

DATA Fisher2 (T, TotCTCOH)

0.25	14.951
0.5	19.507
1.0	38.154
2.0	9.823
4.0	4.857
8.0	2.260
16.0	1.493
0.0	18.211
0.25	26.209
2.0	23.683
4.0	8.231
8.0	2.157
12.0	1.006
0.25	19.170
0.35	28.340
0.5	31.025
1.0	36.238
1.5	28.637
2.0	42.998
3.0	22.019
4.0	24.938
6.0	4.559
12.0	4.293
0.25	21.512
0.5	33.544
1.0	42.775
2.0	37.136
4.0	29.707
16.0	4.323

END

DATA Fisher3 (T, CBldTCA)

0.0	21.153
0.25	28.602
2.0	44.260
4.0	55.510
8.0	49.842
16.0	45.073
24.0	37.740
30.0	26.349
0.0	11.742
0.25	15.416
2.0	29.059
4.0	34.313
8.0	34.148
16.0	31.568
24.0	26.453
40.0	22.201

0.0	5.114
0.1	11.547
0.25	16.582
0.5	22.928
0.75	28.620
1.0	35.192
1.5	41.618
2.0	59.699
3.0	62.719
4.0	68.996
6.0	93.311
8.0	89.934
16.0	65.678
24.0	43.161
30.0	40.748
40.0	9.223
0.25	11.747
0.5	21.259
1.0	31.250
2.0	45.460
4.0	66.279
16.0	136.826
24.0	52.348
30.0	57.359
48.0	9.197

END

DATA Fisher4 (T, CDCA)

0.25	0.040
2.0	0.181
4.0	0.195
8.0	0.108
16.0	0.060
24.0	0.051
0.25	0.047
2.0	0.166
4.0	0.467
8.0	0.897
16.0	0.127
24.0	0.087
0.0	0.074
0.5	0.214
1.0	0.149
1.5	0.184
2.0	0.232
3.0	0.409
4.0	0.378
6.0	0.455
8.0	0.920
16.0	0.589
24.0	0.501
30.0	0.406
40.0	0.177
0.5	0.099
4.0	2.046
8.0	2.861
24.0	1.869

40.0 0.186
END

DATA Fisher5 (T, AUrnTCOGTCOH)

24.0	1.935
48.0	3.537
72.0	3.732
96.0	3.792
120.0	3.806
144.0	3.819
24.0	6.844
48.0	9.000
72.0	9.522
96.0	9.646
120.0	9.738
144.0	9.807
24.0	8.248
48.0	11.220
72.0	12.043
96.0	12.257
120.0	12.460
144.0	12.478
24.0	15.291
48.0	21.270
72.0	23.935
96.0	24.801
120.0	25.488
144.0	26.000
168.0	26.047
192.0	26.075

END

DATA Fisher6 (T, AUrnTCA)

24.0	0.711
48.0	1.173
72.0	1.281
96.0	1.292
120.0	1.284
144.0	1.283
24.0	0.688
48.0	1.663
72.0	1.839
96.0	1.876
120.0	1.861
144.0	1.871
24.0	2.306
48.0	3.677
72.0	4.449
96.0	4.698
120.0	4.661
144.0	4.720
24.0	1.283
48.0	2.430
72.0	2.937
96.0	3.128
120.0	3.299
144.0	3.345

```
168.0    3.369
192.0    3.313
END
```

```
PROCED GargasMMParam
  SET VFatC=0.05
END
```

```
PROCED GargasMM
! Data from Abbas and Fisher (1997)
! Data from MICE_gasuptake_gargas.dat
! Male Mice Closed Chamber
  Mouse
  ResetDoses
  GargasMMParam
  SET BW=0.03, QPC=30.0
  SET Conc=1020.0, CC=.TRUE., NRats=14.0, kLossC=0.02, VChC=9.1
  SET TChng=6.0, Days=1.0, TMax=24.0, TStp=6.0
  START /NC
  SET NRWITG=.T.
  SET BW=0.026, Conc=1800.0, NRats=15.0
  START /NC
  SET BW=0.03, Conc=3800.0, NRats=14.0
  START /NC
  SET BW=0.028, Conc=5600.0, NRats=15.0
  START /NC
  SET BW=0.026, Conc=10000.0, NRats=15.0
  START /NC
  PLOT CInhPPM/run=1, CInhPPM/run=2, CInhPPM/run=3, CInhPPM/run=4,
CInhPPM/run=5, /DATA=gargasmm CInhPPM
  SET NRWITG=.F.
END
```

```
DATA GargasMM (T, CInhPPM)
  0.083    821.0
  0.167    620.0
  0.33     377.0
  0.5      226.0
  0.667    154.0
  0.83     98.0
  1.0      63.6
  1.167    41.8
  1.33     28.0
  1.5      18.5
  1.67     13.0
  1.83      8.99
  2.0       6.79
  2.167     5.27
  2.33      4.5
  0.167    1336.0
  0.25     1108.0
  0.33     940.0
  0.5      719.0
  0.67     600.0
  0.83     492.0
  1.0      400.0
```


1.167	310.0
1.33	246.0
1.5	186.0
1.67	131.0
1.83	92.9
2.0	63.7
2.167	41.4
2.33	27.4
2.5	17.4
2.67	12.1
2.83	8.65
0.167	2516.0
0.33	1846.0
0.5	1540.0
0.67	1351.0
0.83	1226.0
1.0	1128.0
1.167	1047.0
1.33	977.0
1.5	916.0
1.67	853.0
1.83	799.0
2.0	749.0
2.167	696.0
2.33	650.0
2.5	603.0
2.67	552.0
2.83	493.0
3.0	456.0
3.167	403.0
3.33	359.0
3.5	308.0
3.67	264.0
3.83	216.0
4.0	162.0
4.167	122.0
4.33	89.2
4.5	67.1
4.67	50.9
4.83	34.3
5.0	23.3
5.167	16.6
0.083	5143.0
0.167	4386.0
0.33	3255.0
0.5	2608.0
0.67	2209.0
0.83	1939.0
1.0	1786.0
1.167	1618.0
1.33	1513.0
1.5	1432.0
1.67	1360.0
1.83	1291.0
2.0	1232.0
2.167	1182.0
2.33	1128.0

2.5	1084.0
2.67	1046.0
2.75	1026.0
2.92	988.0
3.08	950.0
3.25	914.0
3.42	880.0
3.58	849.0
3.75	819.0
3.92	789.0
4.08	760.0
4.25	732.0
4.42	703.0
4.58	675.0
4.75	652.0
4.92	612.0
5.08	586.0
5.25	555.0
0.083	8218.0
0.167	7215.0
0.33	5804.0
0.5	5170.0
0.67	4752.0
0.83	4435.0
1.0	4101.0
1.167	3830.0
1.33	3623.0
1.5	3446.0
1.67	3305.0
1.83	3180.0
2.0	3114.0
2.167	3055.0
2.33	2948.0
2.5	2856.0
2.67	2790.0
2.83	2709.0
3.0	2637.0

END

```

PROCED GargasFMPParam
  SET VFatC=0.10, VMaxC=23.2
END

```

```

PROCED GargasFM
! Data from Abbas and Fisher (1997)
! Data from female_rat_mice_fisher.dat
! TCE - female B6C3F1 mice
! Female Mice Closed Chamber
Mouse
ResetDoses
GargasFMPParam
SET BW=0.024, QPC=30.0
SET Conc=300.0, CC=.TRUE., NRats=14.0, kLossC=0.02, VChC=9.1
SET TChng=7.0, Days=1.0, TMax=24.0, TStp=7.0
START /NC
SET NRWITG=.T.

```

```

SET BW=0.021, Conc=700.0
START /NC
SET BW=0.022, Conc=1100.0
START /NC
SET BW=0.022, Conc=3700.0
START /NC
SET BW=0.022, Conc=7000.0
START /NC
PLOT CInhPPM/run=1, CInhPPM/run=2, CInhPPM/run=3, CInhPPM/run=4,
CInhPPM/run=5, /DATA=gargasfm CInhPPM
SET NRWITG=.F.
END

```

DATA GargasFM (T, CInhPPM)

0.083	214.0
0.5	99.0
0.667	70.3
0.83	52.3
1.0	38.1
1.167	28.5
1.333	22.2
1.500	16.9
1.67	12.3
1.83	9.4
2.0	7.1
0.083	624.0
0.167	502.0
0.333	357.0
0.5	245.0
0.667	179.0
0.83	136.0
1.0	108.0
1.167	82.4
1.333	63.7
1.5	48.9
1.67	40.5
1.83	32.6
2.0	27.4
2.167	20.7
2.333	16.2
2.5	13.8
2.67	11.7
0.083	965.0
0.167	803.0
0.333	580.0
0.5	467.0
0.667	391.0
0.83	314.0
1.0	270.0
1.167	235.0
1.333	198.0
1.5	160.0
1.667	140.0
1.83	119.0
2.0	101.0
2.167	86.2
2.333	70.3

2.5	59.1
2.667	50.8
2.83	41.8
3.0	34.6
3.167	28.7
3.333	22.6
3.5	19.4
3.667	16.1
3.83	13.5
0.083	3611.0
0.167	2854.0
0.333	2269.0
0.5	1848.0
0.667	1569.0
0.83	1276.0
1.0	1244.0
1.167	1147.0
1.333	1080.0
1.5	982.0
1.667	940.0
1.83	935.0
2.0	897.0
2.167	869.0
2.333	840.0
2.5	816.0
2.667	792.0
3.0	742.0
3.167	719.0
3.333	699.0
3.5	676.0
3.667	656.0
3.83	621.0
4.0	602.0
4.167	578.0
4.333	553.0
4.5	530.0
4.667	505.0
4.83	480.0
5.0	451.0
5.167	429.0
5.333	402.0
5.5	374.0
5.667	350.0
6.0	297.0
0.083	6401.0
0.167	5475.0
0.333	4161.0
0.5	3303.0
0.667	2868.0
0.83	2702.0
1.0	2467.0
1.167	2290.0
1.333	2203.0
1.5	2122.0
1.667	2048.0
1.83	2004.0
2.0	1984.0

2.167	1951.0
2.333	1913.0
2.5	1885.0
2.667	1801.0
2.83	1776.0
3.0	1771.0
3.167	1753.0
3.333	1736.0
3.5	1711.0
3.667	1689.0
3.83	1667.0
4.0	1647.0
4.167	1622.0
4.333	1599.0
4.5	1574.0
5.0	1556.0
5.167	1531.0
5.333	1446.0
5.5	1418.0
5.667	1389.0
5.83	1369.0
6.0	1320.0

END

PROCED Greenberg ! TCE in blood

! Data from Greenberg MS, Burton GA, and Fisher JW. 1999.

! Physiologically based pharmacokinetic modeling of inhaled

! trichloroethylene and its oxidative metabolites in B6C3F mice.

! Toxicology and Applied Pharmacology 154:264-278.

!

! Male B6C3F1 mice (0.028-0.032 kg) were exposed by inhalation to

! 100 or 600 ppm for up to 4 hours

! Greenberg et al. 1999. Mice - Inhalation

!

! From procedure Greenberg in TCENew.cmd

Mouse

ResetDoses

SET ZZXERR=39*1.0e-9, ZXMERR=39*1.0e-9

SET Conc=100.0, CC=.FALSE., TChng=4.0, Days=1.0, TMax=48.0, TStp=48.0

START /NC

SET NRWITG=.T., Conc=600.0

SET ZZXERR=39*1.0e-8, ZXMERR=39*1.0e-8

START /NC

PLOT CVen/run=1, CVen/run=2, /DATA=greenberg1 CVen

PLOT CTCOH/run=1, CTCOH/run=2, /DATA=greenberg2 CTCOH

PLOT CBldTCA/run=1, CBldTCA/run=2, /DATA=greenberg3 CBldTCA

SET NRWITG=.F.

END

DATA Greenberg1 (T, CVen)

2.0 0.672

4.0 0.879

4.25 0.139

4.5 0.151

2.0	6.791
4.0	7.238
4.25	1.507
4.5	0.594
4.75	0.461
6.0	0.169

END

DATA Greenberg2 (T, CTCOH)

2.0	1.948
4.0	1.793
4.25	1.749
4.5	0.795
4.75	0.301
6.0	0.090
2.0	15.386
4.0	12.114
4.25	9.880
4.5	3.610
4.75	2.944
6.0	0.952

END

DATA Greenberg3 (T, CBldTCA)

2.0	17.771
4.25	29.296
4.5	25.167
4.75	30.500
6.0	26.292
12.0	6.945
18.0	3.922
28.0	1.965
2.0	55.636
4.25	71.795
4.5	94.831
4.75	93.010
6.0	103.233
12.0	24.451
18.0	13.390
28.0	7.196
48.0	0.790

END

PROCED ProutMParam

SET VMaxC=50.0, VMaxTCOHC=2.0, kAD=0.3

END

PROCED ProutM

! Data from Prout et al. (1985)

! From procedures P3M, P5M, and P6M in TCENew.cmd

! Mouse - 1000 mg/kg tce in oil

Mouse

ResetDoses

SET ZZXERR=39*1.0e-7, ZZMERR=39*1.0e-7

ProutMParam

SET BW=0.028, PDose=1000.0, Days=1.0, TMax=1.0, TStp=45.0

```
START /NC
PLOT /DATA=proutm1 CVen
PLOT /DATA=proutm2 CTCOH
PLOT /DATA=proutm3 CBldTCA
END
```

DATA ProutM1 (T, CVen)

0.09	9.81
0.415	17.719
0.753	13.021
1.028	7.965
1.638	10.105
2.035	6.004
2.717	5.831
3.097	1.154
3.571	1.329
4.161	1.679
4.714	2.17
5.302	2.485
5.766	2.554
6.285	3.529
6.766	3.864
7.233	1.735

END

DATA ProutM2 (T, CTCOH)

0.296	9.477
0.588	21.574
0.776	29.357
1.012	27.676
1.507	30.546
2.08	27.443
2.677	20.031
3.487	9.369
4.071	10.662
4.578	14.157
5.136	2.601
5.443	7.302
5.925	6.516
6.641	5.316
7.067	2.516
7.563	1.166
8.025	0.51

END

DATA ProutM3 (T, CBldTCA)

0.804	38.161
1.381	108.001
1.778	68.642
2.936	146.642
3.552	122.081
4.49	157.897
5.009	134.087
5.536	150.322
5.864	101.92
7.315	120.738

7.822	162.399
8.048	197.051
8.707	209.215
9.52	201.666
10.12	189.58
11.122	188.781
12.916	170.32
14.151	259.614
15.243	240.369
15.993	216.341
16.121	179.322
17.06	116.241
18.557	59.745
19.617	123.052
20.712	196.42
21.953	169.549
22.4	145.33
24.632	237.856
25.757	223.972
27.457	157.147
28.877	150.795
30.272	266.082
31.375	283.333
32.672	70.593
33.491	56.951
34.341	29.533
35.625	28.261
36.534	38.283
38.911	28.988
41.193	19.915
44.214	7.202

END

```

PROCED TemplinMParam
  SET VMaxC=60.0, VMaxTCOHC=0.5, kAD=1.0
END

```

```

PROCED TemplinM
! Data from Templin et al. (1993)
! From procedures T1TCE, T1TCA, T1TCOH, and T1DCA in TCENew.cmd
! Also from data block TCE500 in MouseB.cmd
! Mouse - 499.32 mg/kg TCE in 2% tween
  Mouse
  ResetDoses
  SET ZZXERR=39*1.0e-7, ZZMERR=39*1.0e-7
  TemplinMParam
  SET BW=0.02, PDose=500.0, Days=1.0, TMax=1.0, TStp=36.0
  START /NC
  PLOT /DATA=templinm1 CVen
  PLOT /DATA=templinm2 CBldTCA
  PLOT /DATA=templinm3 CTCOH
  PLOT /DATA=templinm4 CDCA
END

```

```

DATA TemplinM1 (T, CVen)
  0.267  27.871

```


0.489	24.25
0.756	21.428
0.976	11.727
1.479	3.827
1.964	1.709

END

DATA TemplinM2 (T, CBldTCA)

0.236	10.865
0.531	18.549
0.756	24.867
1.03	42.942
1.501	46.140
2.024	43.821
2.999	57.877
3.977	64.961
5.996	40.28
9.002	38.183
12.023	31.739
17.858	10.926
23.894	9.015
35.888	1.990

END

DATA TemplinM3 (T, CTCOH)

0.255	17.84
0.756	35.8
0.996	40.0
1.491	30.0
1.977	8.36
2.949	0.72

END

DATA TemplinM4 (T, CDCA)

0.229	0.787932
0.499	4.658448
0.756	4.728237
0.971	5.141037
1.469	5.768106
2.949	2.965452
5.965	1.68732
8.98	0.785094

END

PROCED MouseM

! Data from Abbas and Fisher (1997)
! From procedures Mouse300M, Mouse600M, Mouse1200M, Mouse2000M
! TCE300, TCE600, TCE1200 and TCE2000 in MouseB.cmd
! Data also in TCA_CTCV_CTCL.xls
! Mice data--April 1996, TCE oral gavage dosing in mice
! 300, 600, 1200, or 2000 mg/kg corn oil gavage
! Male
! Mouse
ResetDoses
SET PDose=300.0, Days=1.0, TMax=24.0, TStp=150.0
START

```
PLOT /DATA=mouse300m1 CVen
PLOT /DATA=mouse300m2 CLiv
PLOT /DATA=mouse300m3 CFat
PLOT /DATA=mouse300m4 CLivTCA
PLOT /DATA=mouse300m5 CBldTCA
PLOT /DATA=mouse300m6 AUrnTCA
```

```
SET PDose=600.0
SET ZZXERR=39*1.0e-10, ZZMERR=39*1.0e-10
START
PLOT /DATA=mouse600m1 CVen
PLOT /DATA=mouse600m2 CLiv
PLOT /DATA=mouse600m3 CFat
PLOT /DATA=mouse600m4 CLivTCA
PLOT /DATA=mouse600m5 CBldTCA
PLOT /DATA=mouse600m6 AUrnTCA
```

```
SET PDose=1200.0
START
PLOT /DATA=mouse1200m1 CVen
PLOT /DATA=mouse1200m2 CLiv
PLOT /DATA=mouse1200m3 CFat
PLOT /DATA=mouse1200m4 CLivTCA
PLOT /DATA=mouse1200m5 CBldTCA
PLOT /DATA=mouse1200m6 AUrnTCA
```

```
SET PDose=2000.0, TStp=200.0
SET ZZXERR=39*1.0e-8, ZZMERR=39*1.0e-8
START
PLOT /DATA=mouse2000m1 CVen
PLOT /DATA=mouse2000m2 CLiv
PLOT /DATA=mouse2000m3 CFat
PLOT /DATA=mouse2000m4 CLivTCA
PLOT /DATA=mouse2000m5 CBldTCA
PLOT /DATA=mouse2000m6 AUrnTCA
```

END

DATA Mouse300M1 (T, CVen)

0.25	26.11
0.5	12.99
1.0	6.67
2.0	0.68
4.0	0.61

END

DATA Mouse300M2 (T, CLiv)

0.25	70.0
0.5	42.1
1.0	16.98
2.0	8.08
4.0	4.17
8.0	1.89
16.0	0.945
24.0	4.18
30.0	3.39
48.0	1.33

END

DATA Mouse300M3 (T, CFat)

0.25	60.13
0.5	125.4
1.0	189.9
2.0	72.58
4.0	40.32
8.0	18.12
16.0	31.3
24.0	0.65
30.0	0.778
48.0	0.32

END

DATA Mouse300M4 (T, CLivTCA)

0.25	18.9
2.0	35.8
4.0	45.6
8.0	48.0
16.0	35.3
24.0	8.16
30.0	10.4

END

DATA Mouse300M5 (T, CBldTCA)

0.25	26.7
0.5	20.4
2.0	42.6
4.0	53.4
8.0	47.6
16.0	43.2
24.0	35.9
30.0	25.0

END

DATA Mouse300M6 (T, AUrnTCA)

24.0	0.707
48.0	1.176
72.0	1.292
96.0	1.304
120.0	1.307
144.0	1.308

END

DATA Mouse600M1 (T, CVen)

0.25	81.9
0.5	71.3
2.0	5.71
4.0	1.94
8.0	0.965
24.0	1.72
30.0	0.72
40.0	0.71

END

DATA Mouse600M2 (T, CLiv)

0.25	213.5
------	-------

0.5	163.8
2.0	19.43
4.0	10.63
8.0	0.71
24.0	0.34
30.0	0.26
40.0	0.30

END

DATA Mouse600M3 (T, CFat)

0.25	278.50
0.5	659.0
2.0	468.91
4.0	46.76
8.0	9.48
24.0	0.13
30.0	0.15
40.0	0.12

END

DATA Mouse600M4 (T, CLivTCA)

0.25	11.2
0.5	22.9
2.0	33.5
4.0	39.9
8.0	54.99
16.0	39.06
24.0	28.2
30.0	15.3
40.0	7.6

END

DATA Mouse600M5 (T, CBldTCA)

0.25	11.18
0.5	14.26
2.0	26.98
4.0	31.73
8.0	31.87
16.0	29.48
24.0	24.81
40.0	21.1

END

DATA Mouse600M6 (T, AUrnTCA)

24.0	0.762
48.0	1.683
72.0	1.867
96.0	1.904
120.0	1.927
144.0	1.941

END

DATA Mouse1200M1 (T, CVen)

0.083	165.87
0.17	191.31
0.25	123.52
0.5	86.9

0.75	70.9
1.0	43.08
1.5	35.17
2.0	20.36
3.0	8.97
4.0	7.50
8.0	1.64
12.0	0.72
16.0	0.47
24.0	0.52
30.0	0.43
40.0	0.45

END

DATA Mouse1200M2 (T, CLiv)

0.083	522.6
0.17	585.3
0.25	499.4
0.5	408.0
0.75	289.8
1.0	228.8
1.5	63.04
2.0	38.97
3.0	59.74
4.0	26.5
6.0	15.37
8.0	14.97
16.0	12.86
24.0	1.79
30.0	1.27
40.0	1.42

END

DATA Mouse1200M4 (T, CFat)

0.083	61.53
0.17	156.7
0.25	567.2
0.5	826.0
0.75	865.3
1.5	1199.9
2.0	1050.5
3.0	550.2
4.0	485.0
6.0	219.2
8.0	293.7
16.0	4.400
24.0	1.446
30.0	1.121
40.0	1.507

END

DATA Mouse1200M4 (T, CLivTCA)

0.083	5.69
0.17	6.2
0.25	11.09
0.5	16.95
0.75	20.09

1.0	26.02
1.5	29.44
2.0	35.65
3.0	37.76
4.0	42.07
6.0	43.92
8.0	57.83
16.0	27.71
24.0	22.67
40.0	6.34

END

DATA Mouse1200M5(T, CBldTCA)

0.083	5.01
0.17	11.2
0.25	16.5
0.5	23.1
0.75	29.2
1.0	36.1
1.5	41.8
2.0	59.1
3.0	64.0
4.0	70.2
6.0	94.1
8.0	90.8
16.0	65.2
24.0	43.86
30.0	41.48
40.0	9.15

END

DATA Mouse1200M6(T, AUrnTCA)

24.0	2.294
48.0	3.731
72.0	4.579
96.0	4.796
120.0	4.848
144.0	4.878

END

DATA Mouse2000M1 (T, CVen)

0.25	208.3
0.5	162.01
1.0	140.1
2.0	64.8
4.0	48.6
8.0	17.48
16.0	9.4
24.0	1.15
40.0	0.78

END

DATA Mouse2000M2 (T, CLiv)

0.25	1498.0
0.5	335.0
1.0	379.7
2.0	116.2

16.0	9.2
24.0	2.0
30.0	1.2
40.0	0.3

END

DATA Mouse2000M3 (T, CFat)

0.25	1152.0
0.5	1993.0
1.0	4279.0
2.0	2015.0
4.0	1991.0
8.0	1503.0
16.0	75.5
24.0	7.4

END

DATA Mouse2000M4 (T, CLivTCA)

0.25	15.18
0.5	27.58
1.0	37.49
2.0	49.46
4.0	65.32
8.0	105.65
16.0	59.0
24.0	44.6
30.0	36.35
48.0	9.98

END

DATA Mouse2000M5 (T, CBldTCA)

0.25	11.22
0.5	20.57
1.0	30.34
2.0	43.51
4.0	63.43
16.0	131.85
24.0	51.38
30.0	54.57
48.0	8.74

END

DATA Mouse2000M6 (T, AUrnTCA)

24.0	1.423
48.0	2.486
72.0	3.122
96.0	3.294
120.0	3.395
144.0	3.426
168.0	3.438
192.0	3.450

END

PROCED BernRParam

SET KM=12.0

END

```

PROCED BernR
! Data from Bernauer et al. (1996) -- Rats
! From procedure BernR in TCENew.cmd
! Rats -- 40, 80, 160 ppm TCE for 6 hours
  Rat
  ResetDoses
  BernRParam
  SET BW=0.275
  SET Conc=40.0, CC=.FALSE., TChng=6.0, Days=1.0, TMax=6.0, TStp=50.0
  START /NC
  D AUrnTCTotMole, AUrnNDCVCMole, AUrnNDCVC

  SET NRWITG=.T., Conc=80.0
  START /NC
  D AUrnTCTotMole, AUrnNDCVCMole, AUrnNDCVC

  SET Conc=160.0
  START /NC
  D AUrnTCTotMole, AUrnNDCVCMole, AUrnNDCVC

  PLOT AUrnTCTotMole/run=1, AUrnTCTotMole/run=2, AUrnTCTotMole/run=3,
/DATA=bernr1 AUrnTCTotMole
  PLOT AUrnNDCVCMole/run=1, AUrnNDCVCMole/run=2, AUrnNDCVCMole/run=3,
/DATA=bernr2 AUrnNDCVCMole

  PLOT AUrnTCA/run=1, AUrnTCA/run=2, AUrnTCA/run=3, /DATA=bernr3 AUrnTCA
  PLOT AUrnTCOGTCOH/run=1, AUrnTCOGTCOH/run=2, AUrnTCOGTCOH/run=3, /DATA=bernr4
AUrnTCOGTCOH
  PLOT AUrnNDCVC/run=1, AUrnNDCVC/run=2, AUrnNDCVC/run=3, /DATA=bernr5 AUrnNDCVC
SET NRWITG=.F.
END

DATA BernR1 (T, AUrnTCTotMole)
  48.0    0.0069
  48.0    0.0130
  48.0    0.0333
END

DATA BernR2 (T, AUrnNDCVCMole)
  48.0    0.000007
  48.0    0.000010
  48.0    0.000013
END

DATA BernR3 (T, AUrnTCA)
  12.0    0.061
  24.0    0.061
  36.0    0.061
  48.0    0.061
  12.0    0.131
  24.0    0.210
  36.0    0.256
  48.0    0.281
  12.0    0.563
  24.0    0.858
  36.0    0.995

```


48.0 1.063
END

DATA BernR4 (T, AUrnTCOGTCOH)

12.0	1.166
24.0	1.234
36.0	1.309
48.0	1.345
12.0	2.338
24.0	2.827
36.0	3.100
48.0	3.294
12.0	3.850
24.0	4.320
36.0	4.666
48.0	4.937

END

DATA BernR5 (T, AUrnNDCVC)

12.0	5.41e-5
24.0	1.42e-4
36.0	1.95e-4
48.0	2.71e-4
12.0	1.23e-4
24.0	2.63e-4
36.0	4.05e-4
48.0	5.71e-4
12.0	2.13e-4
24.0	6.72e-4
36.0	1.24e-3
48.0	1.59e-3

END

PROCED FisherMR

! Data from Fisher et al. (1991)
! From procedures FG2B and FG2D in TCENew.cmd
! 505 ppm TCE 4 hr -- Male Rat
Rat
ResetDoses
SET Conc=505.0, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=33.0
START /NC
PLOT /DATA=fishermr1 CBldTCA

SET Conc=529.0, TStp=11.0
START /NC
PLOT /DATA=fishermr2 CVen

END

DATA FisherMR1 (T, CBldTCA)

1.97	6.445
3.915	11.179
5.986	22.381
7.982	21.866
10.099	20.455
12.099	17.526
26.216	6.232

```
32.139    4.561
END
```

```
DATA FisherMR2 (T, CVen)
```

```
1.976    21.091
3.981    34.209
6.031    6.027
8.031    1.662
10.054    0.986
```

```
END
```

```
PROCED FisherFRParam
```

```
SET QPC=15.0, VMaxC=20.0
```

```
END
```

```
PROCED FisherFR
```

```
! Data from Fisher et al. (1991)
```

```
! From procedures FG2A and FG2C in TCENew.cmd
```

```
! 600 ppm TCE 4 hr -- Female Rat
```

```
Rat
```

```
ResetDoses
```

```
FisherFRParam
```

```
SET Conc=600.0, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=50.0
```

```
START /NC
```

```
PLOT /DATA=fisherfr1 CVen
```

```
PLOT /DATA=fisherfr2 CBldTCA
```

```
END
```

```
DATA FisherFR1 (T, CVen)
```

```
0.498    9.448
3.556    25.889
4.215    19.272
5.033    6.865
6.009    3.341
```

```
END
```

```
DATA FisherFR2 (T, CBldTCA)
```

```
0.622    2.137
3.677    20.408
4.44     19.485
5.196    31.914
6.175    33.11
8.661    39.233
25.972   11.036
32.033    6.03
49.023    1.362
```

```
END
```

```
PROCED GargasR
```

```
! Data from Andersen et al. (1987)
```

```
! Data from CC.dat from Mike Gargas
```

```
! Rat Closed Chamber
```

```
Rat
```

```
ResetDoses
```

```
SET BW=0.256
```

```

SET Conc=100.0, CC=.TRUE., NRats=3.0, kLossC=0.01, VChC=9.1
SET TChng=6.0, Days=1.0, TMax=24.0, TStp=6.0
START /NC
SET NRWITG=.T.
SET BW=0.249, Conc=450.0
START /NC
SET BW=0.274, Conc=1000.0
START /NC
SET BW=0.269, Conc=2000.0
START /NC
SET BW=0.272, Conc=4640.0
START /NC
PLOT CInhPPM/run=1, CInhPPM/run=2, CInhPPM/run=3, CInhPPM/run=4,
CInhPPM/run=5, /DATA=gargasr CInhPPM
SET NRWITG=.F.
END

```

DATA GargasR (T, CInhPPM)

0.083	92.30
0.167	76.10
0.333	54.90
0.500	41.00
0.667	31.30
0.833	21.70
1.000	16.30
1.167	13.00
1.333	10.00
1.500	7.90
1.667	6.30
1.833	5.40
2.000	4.80
2.167	4.30
2.333	3.20
0.083	435.00
0.167	375.00
0.333	270.00
0.500	206.00
0.667	153.00
0.833	116.00
1.000	89.20
1.167	69.10
1.333	50.30
1.500	37.40
1.667	28.50
1.833	22.00
2.000	18.20
2.167	15.00
2.333	11.20
2.500	9.52
2.667	7.82
0.083	884.00
0.167	738.00
0.333	519.00
0.500	406.00
0.667	312.00
0.833	259.00
1.000	215.00

1.167	184.00
1.333	152.00
1.500	128.00
1.667	111.00
1.833	94.00
2.000	82.00
2.167	70.00
2.333	58.00
2.500	50.00
2.667	45.00
2.833	38.00
3.000	32.00
3.167	26.00
3.333	23.00
3.500	19.00
3.667	17.00
3.833	15.00
4.000	14.00
4.167	13.00
4.333	11.00
0.083	1741.00
0.167	1460.00
0.333	1076.00
0.500	887.00
0.667	697.00
0.833	580.00
1.000	501.00
1.167	427.00
1.333	369.00
1.500	324.00
1.667	276.00
1.833	259.00
2.000	240.00
2.167	236.00
2.333	218.00
2.500	198.00
2.667	195.00
2.833	181.00
3.000	165.00
3.167	162.00
3.333	152.00
3.500	145.00
3.667	138.00
3.833	132.00
4.000	122.00
4.167	113.00
4.333	104.00
4.500	95.10
4.667	88.10
4.833	82.30
5.000	74.10
5.167	62.10
5.333	61.90
5.500	55.40
5.667	52.90
5.833	48.30
6.000	45.00

0.083	3986.00
0.167	3333.00
0.333	2443.00
0.500	1904.00
0.667	1553.00
0.833	1298.00
1.000	1128.00
1.167	1004.00
1.333	902.00
1.500	825.00
1.667	775.00
1.833	724.00
2.000	675.00
2.167	661.00
2.333	631.00
2.500	612.00
2.667	591.00
2.833	570.00
3.000	556.00
3.167	538.00
3.333	535.00
3.500	522.00
3.667	512.00
3.833	500.00
4.000	498.00
4.167	486.00
4.333	474.00
4.500	472.00
4.667	465.00
4.833	455.00
5.000	445.00
5.167	439.00
5.333	436.00
5.583	428.00
5.667	418.00
5.833	409.00
6.000	403.00

END

```

PROCED LarsonRParam
  SET FractTCE=0.02, VMaxGlucC=20.0
END

```

```

PROCED LarsonR
! Data from Larson and Bull (1992)
! From procedures LarTCE1-LarTCE3, LarTCA1-LarTCA3, and LarTOH1-LarTOH3
! in TCENew.cmd
! Rat - 200 mg/kg TCE in 1% tween
Rat
ResetDoses
LarsonRParam
SET PDose=200.0, Days=1.0, TMax=24.0, TStp=48.0
START /NC
PLOT /DATA=larsonr1a CVen
PLOT /DATA=larsonr1b CBldTCA
PLOT /DATA=larsonr1c CTCOH

```

```

! Rat - 600 mg/kg TCE in 1% tween
SET PDose=600.0
START /NC
PLOT /DATA=larsonr2a CVen
PLOT /DATA=larsonr2b CBldTCA
PLOT /DATA=larsonr2c CTCOH

! Rat - 2996 mg/kg TCE in 1% tween
SET PDose=2996.0, TStp=73.0
SET ZZXERR=39*1.0e-7, ZZMERR=39*1.0e-7
START /NC
PLOT /DATA=larsonr3a CVen
PLOT /DATA=larsonr3b CBldTCA
PLOT /DATA=larsonr3c CTCOH
END

```

DATA LarsonR1a (T, CVen)

1.0	9.745938
2.0	5.031306
4.0	2.116854
8.0	1.069596
12.0	0.36135

END

DATA LarsonR1b (T, CBldTCA)

1.0	5.36769
2.0	7.650388
4.0	11.841598
8.0	12.996836
12.0	10.447796
24.0	1.516352
48.0	0.047386

END

DATA LarsonR1c (T, CTCOH)

1.0	13.27261
2.0	22.883965
4.0	23.739105
8.0	6.07269
12.0	2.17373
24.0	0.399165

END

DATA LarsonR2a (T, CVen)

1.0	26.530974
2.0	34.693542
4.0	20.953044
8.0	6.132438
12.0	2.934162
24.0	0.674082

END

DATA LarsonR2b (T, CBldTCA)

1.0	2.828454
2.0	6.370966
4.0	9.233734

8.0	20.766506
12.0	24.740394
24.0	17.43478
48.0	0.042484

END

DATA LarsonR2c (T, CTCOH)

1.0	13.47294
2.0	16.94134
4.0	27.195545
8.0	44.252
12.0	32.46542
24.0	4.75111
48.0	0.145015

END

DATA LarsonR3a (T, CVen)

1.0	69.226776
2.0	185.690538
4.0	120.072006
8.0	98.804916
12.0	55.408752
24.0	7.852464
48.0	0.237834

END

DATA LarsonR3b (T, CBldTCA)

1.0	4.058856
2.0	10.104656
4.0	11.207606
8.0	23.965878
12.0	28.884218
24.0	61.918796
48.0	5.496776
72.0	0.165034

END

DATA LarsonR3c (T, CTCOH)

1.0	17.48851
2.0	29.883555
4.0	29.961295
8.0	33.76906
12.0	51.827165
24.0	34.89928
48.0	0.86411

END

PROCED ProutR

! Data from Prout et al. (1985)

! From procedures P3R, P5R, and P6R in TCENew.cmd

! Rat - 1000 mg/kg TCE in corn oil

Rat

ResetDoses

SET BW=0.19, PDose=1000.0, Days=1.0, TMax=1.0, TStp=40.0

START /NC

PLOT /DATA=proutr1 CVen

```
PLOT /DATA=proutr2 CTCOH
PLOT /DATA=proutr3 CBldTCA
END
```

```
DATA ProutR1 (T, CVen)
```

0.058	5.227
0.201	14.055
0.431	19.529
0.616	24.837
1.358	19.794
1.742	23.578
2.301	42.371
3.015	62.47
4.06	43.553
4.507	40.977
5.121	29.243
5.707	28.869
6.148	28.964
7.105	21.193
8.092	18.967
9.33	13.418
10.354	11.543
11.279	8.631

```
END
```

```
DATA ProutR2 (T, CTCOH)
```

1.042	0.802
1.531	0.989
2.105	0.889
2.597	0.778
3.091	0.773
3.48	0.767
4.06	1.092
4.513	1.256
5.182	0.774
5.55	1.126
6.068	0.933
6.663	1.229
7.149	0.655
8.118	0.918
9.113	1.455
10.001	7.222
11.14	2.062
12.033	2.214
13.026	1.278
13.955	0.592
14.975	1.994
16.041	0.772
17.016	0.92
18.071	0.71

```
END
```

```
DATA ProutR3 (T, CBldTCA)
```

2.153	3.391
3.815	4.492
4.723	10.821
6.058	10.155

6.918	14.629
8.071	14.598
9.365	25.456
10.354	18.378
11.496	45.88
12.31	38.522
13.248	49.159
15.695	28.235
17.43	34.252
19.366	44.523
20.272	40.253
21.761	24.383
22.843	18.858
24.838	14.865
25.888	14.386
28.323	22.531
29.447	32.197
30.457	38.11
31.603	32.229
33.151	19.265
34.613	20.718
36.365	20.975
39.99	6.918

END

```

PROCED TemplinRParam
  SET FractTCE=0.01, VMaxTCOHC=0.06, VMaxGlucC=150.0, kEHRC=0.3, kAD=0.6
END

```

```

PROCED TemplinR
! Data from Templin et al. (1995)
! From procedures TT, TC, and TS in TCENew.cmd
! Rat - 100 mg/kg TCE in 2% tween
Rat
ResetDoses
TemplinRParam
SET BW=0.2, PDose=100.0, Days=1.0, TMax=24.0, TStp=48.0
START /NC
PLOT /DATA=templinr1 CVen
PLOT /DATA=templinr2 CBldTCA
PLOT /DATA=templinr3 CTCOH
END

```

```

DATA TemplinR1 (T, CVen)
  0.252    5.627367
  0.494    8.889005
  0.736   10.184595
  0.993    6.760255
  1.49     2.313853
  1.972    1.55759
  2.475    0.922502
END

```

```

DATA TemplinR2 (T, CBldTCA)
  0.252    0.951757

```

0.494	1.410765
0.728	1.923237
0.984	1.645322
1.958	4.274023
2.475	3.862448
2.984	4.968566
3.987	6.032467
4.97	6.719023
5.97	6.954884
8.979	7.540054
11.98	7.226116
23.963	4.362369
47.986	1.516552

END

DATA TemplinR3 (T, CTCOH)

0.233	0.8934
0.482	1.5903
0.728	1.97115
0.961	2.0589
1.463	2.0523
1.962	2.7261
2.455	3.28275
2.958	2.7078
3.972	2.52705
5.017	2.24115
5.984	2.06565
8.964	1.02

END

PROCED BernH

! Data from Bernauer et al. (1996) -- Human

! From procedure BernH in TCENew.cmd

! Human -- 40, 80, 160 ppm TCE for 6 hours

Human

ResetDoses

SET Conc=40.0, CC=.FALSE., TChng=6.0, Days=1.0, TMax=6.0, TStp=54.0

START /NC

D AUrnTCTotMole, AUrnNDCVCMole, AUrnNDCVC

SET NRWITG=.T., Conc=80.0

START /NC

D AUrnTCTotMole, AUrnNDCVCMole, AUrnNDCVC

SET Conc=160.0

START /NC

D AUrnTCTotMole, AUrnNDCVCMole, AUrnNDCVC

PLOT AUrnTCTotMole/run=1, AUrnTCTotMole/run=2, AUrnTCTotMole/run=3,
/DATA=bernh1 AUrnTCTotMole

PLOT AUrnNDCVCMole/run=1, AUrnNDCVCMole/run=2, AUrnNDCVCMole/run=3,
/DATA=bernh2 AUrnNDCVCMole

PLOT AUrnTCA/run=1, AUrnTCA/run=2, AUrnTCA/run=3, /DATA=bernh3 AUrnTCA

PLOT AUrnTCOGTCOH/run=1, AUrnTCOGTCOH/run=2, AUrnTCOGTCOH/run=3, /DATA=bernh4
AUrnTCOGTCOH

```
PLOT AUrnNDCVC/run=1, AUrnNDCVC/run=2, AUrnNDCVC/run=3, /DATA=bernh5 AUrnNDCVC
SET NRWITG=.F.
END
```

```
DATA BernH1 (T, AUrnTCTotMole)
```

```
54.0 0.823
```

```
54.0 1.775
```

```
54.0 3.080
```

```
END
```

```
DATA BernH2 (T, AUrnNDCVCMole)
```

```
54.0 0.00025
```

```
54.0 0.00037
```

```
54.0 0.00043
```

```
END
```

```
DATA BernH3 (T, AUrnTCA)
```

```
6.0 0.84
```

```
11.0 1.56
```

```
16.0 3.37
```

```
23.0 6.19
```

```
30.0 9.73
```

```
35.0 11.49
```

```
40.0 13.20
```

```
47.0 15.14
```

```
54.0 16.46
```

```
6.0 2.06
```

```
11.0 4.27
```

```
16.0 6.52
```

```
23.0 10.49
```

```
30.0 17.08
```

```
35.0 21.57
```

```
40.0 26.87
```

```
47.0 31.84
```

```
54.0 37.96
```

```
6.0 2.29
```

```
11.0 5.71
```

```
16.0 10.74
```

```
23.0 18.57
```

```
30.0 28.08
```

```
35.0 34.58
```

```
40.0 41.75
```

```
47.0 49.31
```

```
54.0 57.51
```

```
END
```

```
DATA BernH4 (T, AUrnTCOGTCOH)
```

```
6.0 12.65
```

```
11.0 28.58
```

```
16.0 43.41
```

```
23.0 53.72
```

```
30.0 65.12
```

```
35.0 73.70
```

```
40.0 81.61
```

```
47.0 88.40
```

```
54.0 93.21
```

```
6.0 37.44
```

11.0	79.43
16.0	112.69
23.0	145.30
30.0	173.21
35.0	188.35
40.0	201.73
47.0	217.09
54.0	230.08
6.0	52.50
11.0	113.78
16.0	168.73
23.0	222.17
30.0	243.14
35.0	263.43
40.0	280.17
47.0	294.98
54.0	311.45

END

DATA BernH5 (T, AUrnNDCVC)

6.0	0.0015
11.0	0.0028
16.0	0.0049
23.0	0.0068
30.0	0.0124
35.0	0.0144
40.0	0.0163
47.0	0.0180
54.0	0.0193
6.0	0.0035
11.0	0.0055
16.0	0.0113
23.0	0.0152
30.0	0.0262
35.0	0.0306
40.0	0.0347
47.0	0.0384
54.0	0.0416
6.0	0.0051
11.0	0.0118
16.0	0.0225
23.0	0.0301
30.0	0.0368
35.0	0.0382
40.0	0.0447
47.0	0.0531
54.0	0.0577

END

PROCED MonsterParam

SET VBodC=0.12, VMaxc=18.0, VMaxTCOHC=12.0, kUrnTCAC=0.15

END

PROCED Monster

! Data from Monster et al. (1979)

! From procedures AF5A-AF5D in TCENew.cmd

```

! 70 ppm TCE -- Human
Human
ResetDoses
MonsterParam
SET Conc=70.0, CC=.FALSE., TChng=4.0, Days=5.0, TMax=150.0, TStp=340.0
START /NC
PLOT /DATA=monster1 CVen
PLOT /DATA=monster2 CBldTCA
PLOT /DATA=monster3 AUrnTCA
PLOT /DATA=monster4 AUrnTCOGTCOH
END

```

DATA Monster1 (T, CVen)

4.0	2.2
5.4	0.33
22.0	0.014
28.0	2.2
29.4	0.3
46.0	0.02
52.0	2.2
53.4	0.33
70.0	0.027
76.0	2.2
77.4	0.365
94.0	0.027
100.0	2.209
101.4	0.361
118.0	0.03

END

DATA Monster2 (T, CBldTCA)

2.807	4.484
3.899	7.958
22.0	13.177
27.956	21.134
45.658	24.953
48.779	33.159
52.451	33.057
69.989	36.207
75.3	38.465
75.772	43.948
94.43	48.398
98.451	50.838
100.291	51.825
118.458	50.265
165.324	38.583
237.579	21.545
334.247	9.462

END

DATA Monster3 (T, AUrnTCA)

2.277	1.607
10.14	5.542
17.883	9.98
26.19	16.14
33.796	27.248
41.501	35.067

49.78	48.356
57.61	65.827
66.042	77.979
74.02	96.759
81.924	121.256
90.081	141.155
98.153	167.439
106.014	198.695
114.175	218.116
122.134	246.406
129.989	273.143
138.0	289.619
146.006	308.377
153.675	328.452
161.622	342.279
169.804	348.791
177.792	357.064
185.706	362.083

END

DATA Monster4 (T, AUrnTCOGTCOH)

3.912	51.482
11.904	106.747
20.184	138.360
27.984	202.971
36.072	284.271
44.064	320.665
52.128	393.523
60.312	471.060
68.232	512.698
76.368	591.433
84.552	671.339
92.736	717.257
100.704	795.718
108.696	884.483
116.472	928.646
124.656	959.874
132.672	976.041
140.760	986.787
148.344	998.355
156.192	1006.748
163.992	1012.067
243.912	1014.424
251.976	1016.263
259.968	1017.808

END

PROCED Monster2
! Data from Monster et al. (1979)
! From procedure Monster in HumanB.cmd
! Male
Human
ResetDoses
SET BW=69.7
SET Conc=70.0, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=220.0
START /NC

```
PLOT /DATA=mon70a CBldTCA
PLOT /DATA=mon70b AUrnTCOGTCOH
PLOT /DATA=mon70c AUrnTCA
PLOT /DATA=mon70d CTCOH
```

```
SET Conc=140.0
START /NC
PLOT /DATA=mon140a CBldTCA
PLOT /DATA=mon140b AUrnTCOGTCOH
PLOT /DATA=mon140c AUrnTCA
PLOT /DATA=mon140d CTCOH
```

END

DATA Mon70a (T, CBldTCA)

4.0	3.5
6.0	5.1
24.0	8.19
48.0	8.97
72.0	8.58
144.0	5.07
216.0	2.73

END

DATA Mon70b (T, AUrnTCOGTCOH)

6.0	35.3
14.0	86.4
22.0	113.4
30.0	133.7
38.0	143.5
46.0	149.2
54.0	153.4
62.0	158.1
70.0	160.7

END

DATA Mon70c (T, AUrnTCA)

22.0	7.0
46.0	18.7
70.0	26.5

END

DATA Mon70d (T, CTCOH)

4.0	4.4
6.0	4.1
24.0	0.91

END

DATA Mon140a (T, CBldTCA)

4.0	3.8
6.0	6.0
24.0	11.3
48.0	12.8
72.0	11.3
144.0	7.55
216.0	4.5

END

DATA Mon140b (T, AUrnTCOGTCOH)

6.0	55.1
14.0	153.9
22.0	206.8
30.0	243.3
38.0	265.3
46.0	276.4
54.0	284.0
62.0	290.0

END

DATA Mon140c (T, AUrnTCA)

22.0	7.6
46.0	24.1
70.0	42.3

END

DATA Mon140d (T, CTCOH)

4.0	6.4
6.0	7.2
24.0	2.5
48.0	0.6

END

PROCED MullerSingleParam

SET VBodC=0.12, kUrnTCAC=0.15

END

PROCED MullerSingle

! Data from Muller et al. (1974, 1975)

! From procedures AF3A-AF3F in TCENew.cmd

! 100 ppm TCE -- Human

Human

ResetDoses

MullerSingleParam

SET Conc=100.0, CC=.FALSE., TChng=6.0, Days=1.0, TMax=24.0, TStp=75.0

START /NC

PLOT /DATA=mullersingle1 CVen

PLOT /DATA=mullersingle2 CBldTCA

PLOT /DATA=mullersingle3 AUrnTCA

PLOT /DATA=mullersingle4 TotCTCOH

PLOT /DATA=mullersingle5 AUrnTCOGTCOH

PLOT /DATA=mullersingle6 CALvPPM

END

DATA MullerSingle1 (T, CVen)

0.965	0.67
1.879	1.105
2.9	0.961
3.876	0.859
4.8	0.994
5.992	1.093
6.396	0.756
6.736	0.539
7.851	0.323
8.86	0.217

9.915	0.179
11.853	0.14
13.741	0.11
23.769	0.072
35.864	0.034
47.915	0.031
59.823	0.023
1.021	0.804
2.954	1.014
3.944	1.407
4.921	1.1
5.898	1.318
6.195	0.93
6.369	0.617
6.749	0.732
7.362	0.561
7.887	0.441
8.891	0.381
9.897	0.289
13.864	0.16
23.731	0.073

END

DATA MullerSingle2 (T, CBldTCA)

0.974	2.553
2.032	8.048
3.965	12.369
5.913	19.65
7.946	26.426
9.915	31.304
11.92	36.274
13.897	39.523
13.902	39.419
23.873	47.577
35.93	43.756
48.006	40.306
59.891	38.657
1.996	4.038
4.0	8.087
6.011	13.162
8.011	17.286
10.006	19.154
13.985	20.938
23.887	28.444

END

DATA MullerSingle3 (T, AUrnTCA)

23.826	41.585
47.946	86.675
72.156	122.458
2.970	0.484
6.457	3.771
8.533	6.289
10.468	10.26
23.859	25.593

END

DATA MullerSingle4 (T, TotCTCOH)

0.984	0.775
2.032	1.807
3.006	2.638
4.009	3.490
5.044	4.332
6.007	5.941
6.216	4.647
6.646	4.943
7.008	5.030
8.017	4.589
9.008	3.715
9.994	3.719
12.005	3.129
14.007	2.771
24.546	1.265
35.566	0.829
49.399	0.336
59.480	0.245
0.027	0.024
1.006	1.010
3.025	2.419
4.058	3.367
5.082	3.675
6.051	4.477
6.396	4.525
6.523	4.477
6.798	4.444
7.040	4.401
7.597	4.031
8.101	4.006
9.099	3.623
10.090	3.082
14.034	2.399
23.997	1.069

END

DATA MullerSingle5 (T, AUrnTCOGTCOH)

24.0	245.244
48.0	301.207
72.0	316.49
3.158	18.6
6.573	71.2
8.634	107.2
10.627	142.3
24.47	233.1

END

DATA MullerSingle6 (T, CALvPPM)

1.041	8.909
1.959	8.914
2.942	13.337
3.965	14.060
4.949	18.097
5.968	13.956
6.368	5.407
7.008	2.765

7.032	4.025
8.017	2.589
9.026	1.549
9.994	0.770
11.987	0.388
13.978	0.393
24.586	0.199
35.520	0.103
48.493	0.065
59.576	0.061
0.027	1.280
1.006	6.968
2.018	8.344
2.970	10.207
3.989	11.057
4.966	13.605
5.924	11.602
6.077	6.861
6.269	5.581
6.434	3.635
6.919	2.997
7.426	2.488
7.895	2.396
8.891	1.532
9.913	1.342
13.902	0.681
23.997	0.420

END

```

PROCED MullerMultiParam
  SET VMaxC=8.0, VMaxTCOHC=30.0
END

```

```

PROCED MullerMulti
! Data from Muller et al. (1974, 1975)
! From procedures AF7A-AF7D in TCENew.cmd
! 50 ppm TCE -- Human
  Human
  ResetDoses
  MullerMultiParam
  SET Conc=50.0, CC=.FALSE., TChng=6.0, Days=5.0, TMax=150.0, TStp=430.0
  START /NC
  PLOT /DATA=mullermulti1 CBldTCA
  PLOT /DATA=mullermulti2 AUrnTCA
  PLOT /DATA=mullermulti3 TotCTCOH
  PLOT /DATA=mullermulti4 AUrnTCOGTCOH
END

```

```

DATA MullerMulti1 (T, CBldTCA)
  0.338    5.501
  7.905   13.882
  9.745   17.048
 23.744   17.932
 29.249   27.023
 32.948   29.95
 46.87    27.981

```

52.887	36.986
57.38	38.724
71.086	35.964
76.223	42.944
80.282	43.978
94.18	41.804
100.307	49.053
104.611	51.055
118.7	49.005
142.839	42.958
201.431	29.181
249.517	19.104
287.758	15.022
345.641	11.051
419.058	5.815

END

DATA MullerMulti2 (T, AUrnTCA)

22.913	19.094
46.855	57.6
69.715	124.243
93.319	198.682
117.8	297.932
141.622	386.56

END

DATA MullerMulti3 (T, TotCTCOH)

13.800	1.703
18.312	1.318
32.520	0.428
38.616	2.079
42.480	1.318
56.088	0.606
62.880	2.197
67.176	1.513
80.424	0.710
86.736	2.257
90.720	1.519
104.184	0.649
110.784	2.270
115.080	1.640
129.672	0.665
155.304	0.202
212.664	0.075

END

DATA MullerMulti4 (T, AUrnTCOGTCOH)

24.0	102.573
48.0	236.288
72.0	380.370
96.0	529.931
120.0	687.668
144.0	721.680
192.0	725.865
240.0	728.355

END

```

PROCED Muller72
! Data from Muller et al. (1972)
! From procedure Muller72 in HumanB.cmd
! Male
  Human
  ResetDoses
  SET Conc=50.0, CC=.FALSE., TChng=6.0, Days=1.0, TMax=24.0, TStp=25.0
  START /NC
  PLOT /DATA=muller72a CBldTCA
  PLOT /DATA=muller72b CTCOH
  PLOT /DATA=muller72c AUrnTCOGTCOH
  PLOT /DATA=muller72d AUrnTCA
END

```

```

! CBldTCA, TCA data divided by 2, plasma to whole blood conversion
DATA Muller72a (T, CBldTCA)
  7.0    2.9
  13.0   7.1
  17.0   8.9
END

```

```

DATA Muller72b (T, CTCOH)
  16.0    1.7
  20.0    1.3
END

```

```

DATA Muller72c (T, AUrnTCOGTCOH)
  24.0   100.8
END

```

```

DATA Muller72d (T, AUrnTCA)
  24.0   18.4
END

```

```

PROCED Muller74
! Data from Muller et al. (1974)
! From procedure Muller74 in HumanB.cmd
! Male
  Human
  ResetDoses
  SET Conc=100.0, CC=.FALSE., TChng=6.0, Days=1.0, TMax=24.0, TStp=75.0
  START /NC
  PLOT /DATA=muller74a CVen
  PLOT /DATA=muller74b CTCOH
  PLOT /DATA=muller74c CBldTCA
  PLOT /DATA=muller74d CALvPPM
  PLOT /DATA=muller74e AUrnTCOGTCOH
  PLOT /DATA=muller74f AUrnTCA
END

```

```

! TCA data divided by 2 to account for plasma
DATA Muller74a (T, CVen)
  0.97    0.67
  1.92    1.05
  3.0     0.93

```

3.97	0.83
5.00	1.02
5.95	1.02
6.38	0.72
6.53	0.52
7.98	0.31
8.99	0.21
10.0	0.18

END

DATA Muller74b (T, CTCOH)

0.97	0.76
1.92	1.74
3.0	2.51
3.97	3.43
5.00	4.18
5.95	5.75
6.38	5.02
6.53	4.47
7.98	4.42
8.99	3.54
10.0	3.59
12.0	3.03
14.0	2.61
24.5	1.24
35.59	0.8
48.5	0.33

END

DATA Muller74c (T, CBldTCA)

0.97	1.2
1.92	3.8
3.97	5.9
5.95	9.4
7.98	13.1
10.0	14.3
12.0	16.7
14.0	19.1
24.5	23.3
35.59	21.8
48.5	19.7
59.5	18.7

END

DATA Muller74d (T, CALvPPM)

0.97	9.0
1.92	9.0
3.0	13.44
3.97	14.27
5.00	18.34
5.95	14.06
6.38	5.37
6.53	3.94
7.98	2.52
8.99	1.5
10.0	0.76
12.0	0.37

END

DATA Muller74e (T, AUrnTCOGTCOH)

24.5	244.8
48.5	300.8
72.0	315.9

END

DATA Muller74f (T, AUrnTCA)

24.5	43.2
48.5	88.1
72.0	133.5

END

PROCED StewartParam

SET VMaxC=5.0

END

PROCED Stewart

! Data from Stewart et al. (1970)

! From procedures AF6A, AF6B, and AF6C in TCENew.cmd

! 200 ppm TCE -- Human

Human

ResetDoses

SET ZZERR=39*1.0e-7, ZZMERR=39*1.0e-7

StewartParam

SET Conc=200.0, CC=.FALSE., TChng=7.0, Days=5.0, TMax=150.0, ...

TStp=410.0

START /NC

PLOT /DATA=stewart1 CALvPPM

PLOT /DATA=stewart2 AUrnTCA

PLOT /DATA=stewart3 AUrnTCOGTCOH

END

DATA Stewart1 (T, CALvPPM)

3.399	10.264
3.135	75.053
8.505	10.84
9.198	8.306
11.141	5.108
14.287	3.315
23.69	1.207
27.506	10.935
32.604	11.376
32.965	9.629
34.996	4.435
38.121	2.753
47.419	1.602
51.096	75.077
51.43	11.628
56.358	12.144
56.589	8.984
59.26	3.528
61.543	2.448
71.645	1.616
75.282	8.477

79.185	8.686
81.269	7.745
82.919	3.548
86.226	2.931
95.579	1.648
99.343	8.523
103.74	8.834
105.49	8.082
107.159	3.686
110.124	2.926

END

DATA Stewart2 (T, AUrnTCA)

23.928	51.208
47.574	225.786
71.475	455.927
95.852	761.268
119.615	1154.375
143.872	1402.376
168.119	1594.802
191.701	1713.81
215.25	1813.51
239.152	1858.527
263.597	1927.884

END

DATA Stewart3 (T, AUrnTCOGTCOH)

24.0	308.0
48.0	667.0
72.0	1066.0
96.0	1604.0
120.0	2009.0
144.0	2154.0
168.0	2303.0
192.0	2355.0
216.0	2395.0
240.0	2410.0
264.0	2414.0
336.0	2428.0
408.0	2442.0

END

PROCED Triebig

! Data from Triebig et al. (1976)

! From procedure Triebig in HumanB.cmd

! Male

Human

ResetDoses

SET Conc=136.0, CC=.FALSE., TChng=6.0, Days=1.0, TMax=24.0, TStp=25.0

START /NC

PLOT /DATA=trieb1g1 CVen

PLOT /DATA=trieb1g2 CTCOH

PLOT /DATA=trieb1g3 CBldTCA

PLOT /DATA=trieb1g4 CALvPPM

END

DATA Triebig1 (T, CVen)

6.0 1.3

END

DATA Triebig2 (T, CTCOH)

6.0 6.2

24.0 3.8

END

DATA Triebig3 (T, CBldTCA)

6.0 12.1

24.0 32.8

END

DATA Triebig4 (T, CALvPPM)

6.0 31.9

24.0 4.6

END

PROCED M60

! Data from Fisher et al. (1998)

! Data from procedure M60 (in Bld50_M and Urin50_M) in HumanB.cmd

! Male 50 ppm exposure, n=3

Human

ResetDoses

SET BW=71.1, VFatC=0.14

SET Conc=55.2, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=100.0

START /NC

PLOT /DATA=m60a CVen

PLOT /DATA=m60b CTCOH

PLOT /DATA=m60c CBldTCA

PLOT /DATA=m60d AUrnTCA

PLOT /DATA=m60e AUrnTCOGTCOH

END

DATA M60a (T, CVen)

0.58 1.89

0.98 1.36

2.02 2.68

3.02 2.67

4.02 2.79

4.25 2.42

4.44 1.52

5.02 0.82

5.83 0.37

8.0 0.29

END

DATA M60b (T, CTCOH)

0.58 0.63

0.98 1.07

2.02 1.57

3.02 1.90

4.02 1.94

4.25 2.02

4.44 2.26

5.02	1.02
5.83	0.96
8.0	1.65
10.0	1.38
12.0	1.26
14.17	1.13
16.02	1.03
18.02	1.05
20.0	0.90

END

DATA M60c (T, CbldTCA)

0.58	0.43
0.98	0.55
2.02	1.07
3.02	1.57
4.02	1.96
4.25	2.01
4.44	2.19
5.02	2.28
5.83	2.52
8.0	2.92
10.0	3.20
12.0	3.56
14.17	4.19
16.02	3.90
18.02	4.95
20.0	5.04
22.0	5.08
44.83	5.51
68.72	9.45
93.12	4.27

END

DATA M60d (T, AUrnTCA)

0.5	0.002
3.12	0.082
4.63	0.184
5.45	0.249
6.45	0.307
8.13	0.539
10.17	0.852
12.15	1.35
14.27	1.78
16.13	2.12
18.15	2.48
20.2	2.89
22.22	3.48
24.22	4.28
32.85	5.35
34.22	5.66
39.85	6.72
44.25	7.42
47.25	8.14
52.13	8.93
58.59	10.17
67.75	11.19

72.37	12.56
77.15	13.78
82.92	14.44
91.83	15.63

END

DATA M60e (T, AUrnTCOGTCOH)

0.5	0.0
3.12	8.24
4.63	11.60
5.45	13.64
6.45	15.64
8.13	19.73
10.17	23.26
12.15	28.95
14.27	28.95
16.13	29.79
18.15	32.07
20.2	34.21
22.22	38.49
24.22	43.06
32.85	47.48
34.22	48.60
39.85	52.15
44.25	53.88
47.25	55.21
52.13	57.21
58.59	59.15
67.75	60.89
72.37	61.46
77.15	61.84
82.92	62.20
91.83	62.56

END

PROCED M50_1

! Data from Fisher et al. (1998)

! Data from procedure M50_1 (in Bld50_M and Urin50_M) in HumanB.cmd

! Male 50 ppm exposure, n=3

Human

ResetDoses

SET BW=52.3, VFatC=0.1

SET Conc=53.1, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=110.0

START /NC

PLOT /DATA=m50_1a CVen

PLOT /DATA=m50_1b CTCOH

PLOT /DATA=m50_1c CBldTCA

PLOT /DATA=m50_1d AUrnTCA

PLOT /DATA=m50_1e AUrnTCOGTCOH

END

DATA M50_1a (T, CVen)

0.5	0.67
1.0	1.37
2.03	1.96
3.0	1.92

4.02	2.08
4.25	1.13
4.5	0.76
5.02	0.42
6.02	0.30
8.08	0.21
10.0	0.15

END

DATA M50_1b (T, CTCOH)

1.0	0.43
2.03	1.20
3.0	1.26
4.02	1.69
4.25	1.66
4.5	1.60
5.02	1.58
6.02	1.51
8.08	1.44
10.0	1.52
12.0	1.14
14.0	1.05
16.0	1.04
18.0	1.06
20.0	0.45
22.0	0.75

END

DATA M50_1c (T, CBldTCA)

1.0	0.29
2.03	0.77
3.0	1.33
4.02	1.84
4.25	1.93
4.5	2.07
5.02	2.27
6.02	2.94
8.08	3.58
10.0	3.72
12.0	3.98
14.0	4.40
16.0	4.58
18.0	4.86
20.0	5.73
22.0	4.22
44.78	5.00
68.72	4.72
100.4	4.47

END

DATA M50_1d (T, AUrnTCA)

5.25	1.00
5.97	1.53
8.0	3.34
10.17	6.01
12.17	7.60
14.17	13.02

16.17	14.83
18.17	16.67
20.17	18.69
22.17	21.30
25.0	21.95
29.83	26.24
37.83	31.79
44.83	40.44
45.67	40.86
49.67	42.64
53.33	42.94
61.23	43.80
62.83	44.54
79.1	48.73

END

DATA M50_1e (T, AUrnTCOGTCOH)

5.25	5.26
5.97	8.23
8.0	13.05
10.17	16.30
12.17	19.05
14.17	24.62
16.17	26.97
18.17	29.06
20.17	30.62
22.17	32.53
25.0	33.35
29.83	35.43
37.83	37.99
44.83	38.21
45.67	39.06
49.67	39.63
53.33	39.70
61.23	39.90
62.83	40.23
79.1	40.67

END

PROCED M50_2

! Data from Fisher et al. (1998)

! Data from procedure M50_2 (in Bld50_M and Urin50_M) in HumanB.cmd

! Male 50 ppm exposure, n=3

Human

ResetDoses

SET BW=69.3, VFatC=0.27

SET Conc=49.3, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=100.0

START /NC

PLOT /DATA=m50_2a CVen

PLOT /DATA=m50_2b CTCOH

PLOT /DATA=m50_2c CBldTCA

PLOT /DATA=m50_2d AUrnTCA

PLOT /DATA=m50_2e AUrnTCOGTCOH

END

DATA M50_2a (T, CVen)

0.5	0.61
1.0	0.74
2.0	1.11
3.0	1.01
4.0	1.05
4.25	0.81
4.5	0.46

END

DATA M50_2b (T, CTCOH)

0.5	0.44
1.0	0.55
2.0	0.83
3.0	1.08
4.0	1.35
4.25	1.26
4.5	1.34
5.0	1.11
6.0	1.01
8.0	0.9
10.0	0.76
14.0	0.66
16.0	0.63
18.0	0.56
20.0	0.51

END

DATA M50_2c (T, CBldTCA)

0.5	0.29
1.0	0.65
2.0	1.47
3.0	2.27
4.0	2.91
4.25	2.99
4.5	3.12
5.0	3.49
6.0	3.66
8.0	4.29
10.0	4.69
12.0	5.11
14.0	5.17
16.0	5.26
18.0	5.66
20.0	5.18
22.0	5.69
49.08	6.67
71.72	6.49
97.47	6.01

END

DATA M50_2d (T, AUrnTCA)

4.55	0.041
5.08	0.062
6.06	0.15
8.08	0.26
10.06	0.41
12.08	0.53

14.08	0.65
16.08	0.80
18.08	0.92
20.08	1.05
22.17	1.18
31.33	1.46
49.0	2.20
64.33	3.61
77.0	4.36
86.25	5.03

END

DATA M50_2e (T, AUrnTCOGTCOH)

4.55	8.45
5.08	15.20
6.06	21.60
8.08	28.09
10.06	35.67
12.08	39.98
14.08	43.78
16.08	47.68
18.08	50.54
20.08	53.03
22.17	55.30
31.33	60.62
49.0	69.80
64.33	73.15
77.0	74.82
86.25	76.02

END

PROCED F50_1

! Data from Fisher et al. (1998)

! Data from procedure F50_1 (in Bld50_F and Urin50_F) in HumanB.cmd

! Female 50 ppm exposure, n=2

Human

ResetDoses

SET BW=62.3, VFatC=0.24

SET Conc=53.0, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=110.0

START /NC

PLOT /DATA=f50_1a CVen

PLOT /DATA=f50_1b CTCOH

PLOT /DATA=f50_1c CBldTCA

PLOT /DATA=f50_1d AUrnTCA

PLOT /DATA=f50_1e AUrnTCOGTCOH

END

DATA F50_1a (T, CVen)

0.5	0.93
1.0	1.33
2.0	1.65
3.0	1.85
4.0	1.45
4.27	0.94
4.55	0.63
5.10	0.32

6.0 0.18
END

DATA F50_1b (T, CTCOH)

1.0	0.33
2.0	0.63
3.0	0.79
4.0	0.98
4.27	0.83
4.55	0.83
5.10	0.90
6.0	0.89
8.0	0.76
10.0	0.66
12.0	0.67
14.0	0.54
16.05	0.48
18.0	0.47
22.0	0.35

END

DATA F50_1c (T, CBldTCA)

1.0	0.38
2.0	1.23
3.0	1.96
4.0	2.80
4.27	2.81
4.55	3.23
5.10	3.34
6.0	3.72
8.0	4.88
10.0	4.93
12.0	5.28
14.0	5.18
16.05	5.37
18.0	6.03
20.02	4.87
22.0	6.66
44.92	6.66
68.86	5.27
100.44	2.27

END

DATA F50_1d (T, AUrnTCA)

5.25	1.35
5.97	4.49
8.0	7.17
10.17	9.38
12.17	10.36
14.17	11.91
16.17	13.46
18.17	14.70
20.17	15.64
22.17	16.49
25.0	22.11
29.83	23.27
37.83	26.03

44.83	27.35
49.67	33.94
53.33	35.83
61.23	42.58
62.83	43.36
67.92	50.68
75.75	52.36
79.63	53.79
96.67	54.16
96.92	55.93

END

DATA F50_1e (T, AUrnTCOGTCOH)

5.25	4.42
5.97	6.71
8.0	12.00
10.17	15.40
12.17	16.73
14.17	20.35
16.17	23.49
18.17	25.44
20.17	25.44
22.17	26.96
25.0	30.55
29.83	32.71
37.83	34.38
44.83	34.88
49.67	37.25
53.33	38.53
61.23	41.16
62.83	41.38
67.92	43.01
75.75	43.29
79.63	43.53
96.67	43.66
96.92	43.85

END

PROCED F60_1

! Data from Fisher et al. (1998)

! Data from procedure F60_1 (in Bld50_F and Urin50_F) in HumanB.cmd

! Female 50 ppm exposure, n=2

Human

ResetDoses

SET BW=66.5, VFatC=0.32

SET Conc=55.1, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=100.0

START /NC

PLOT /DATA=f60_1a CVen

PLOT /DATA=f60_1b CTCOH

PLOT /DATA=f60_1c CBldTCA

PLOT /DATA=f60_1d AUrnTCA

PLOT /DATA=f60_1e AUrnTCOGTCOH

END

DATA F60_1a (T, CVen)

0.58	1.00
------	------

1.02	1.29
2.0	1.38
3.0	1.70
4.0	1.72
4.25	1.08
4.47	1.17
5.0	0.55
6.0	0.39
8.03	0.22

END

DATA F60_1b (T, CTCOH)

0.58	0.32
1.02	0.49
2.0	0.85
3.0	0.97
4.0	1.20
4.25	1.14
4.47	1.18
5.0	1.13
9.98	0.70
12.0	0.60
14.02	0.52
16.0	0.55
18.03	0.54
20.0	0.45
22.0	0.35

END

DATA F60_1c (T, CBldTCA)

0.58	0.16
1.02	0.46
2.0	1.15
3.0	1.53
4.0	1.90
4.25	2.10
4.47	2.18
5.0	2.13
6.0	2.56
8.03	3.32
9.98	2.83
12.0	2.98
14.02	3.42
16.0	3.44
18.03	3.31
20.0	4.15
22.0	4.07
44.33	3.70
68.32	3.31
93.38	1.02

END

DATA F60_1d (T, AUrnTCA)

4.58	0.64
5.26	0.76
6.12	0.85
8.12	1.83

10.18	2.57
12.18	3.36
14.32	3.94
16.18	5.12
18.16	6.03
20.25	6.67
22.53	7.30
23.25	7.60
25.25	7.96
27.58	8.60
29.5	8.89
30.92	9.21
32.92	9.86
35.0	9.66
39.83	11.19
42.0	11.85
43.08	12.35
44.72	12.73
46.5	13.49
49.83	14.31
52.00	15.73
53.59	16.12
54.53	16.34
56.83	16.93
58.5	17.24
59.25	17.85
63.83	18.13
68.28	18.53
70.67	19.18
72.78	19.42
74.75	20.00
76.92	20.58
80.33	20.79
81.50	20.93
82.42	21.82
83.5	21.37
90.25	21.56
91.42	21.69
92.33	21.87

END

DATA F60_1e (T, AUrnTCOGTCOH)

4.58	20.08
5.26	22.91
6.12	24.87
8.12	28.94
10.18	36.46
12.18	39.14
14.32	42.64
16.18	45.16
18.16	53.64
20.25	56.34
22.53	57.08
23.25	57.64
25.25	58.45
27.58	60.33
29.5	61.44

30.92	62.83
32.92	67.36
35.0	68.30
39.83	69.92
42.0	70.88
43.08	71.09
44.72	71.59
46.5	71.99
49.83	72.60
52.00	73.60
53.59	73.93
54.53	74.27
56.83	74.26
58.5	74.56
59.25	74.71
63.83	74.77
68.28	75.16
70.67	75.34
72.78	75.52
74.75	75.75
76.92	75.81
80.33	76.05
81.50	76.06
82.42	76.12
83.5	76.15
90.25	76.30
91.42	76.34
92.33	76.39

END

PROCED M100_1

! Data from Fisher et al. (1998)

! Data from procedure M100_1 (in Bld_M and Urine_M) in HumanB.cmd

! Male 100 ppm exposure

Human

ResetDoses

SET BW=71.4, VFatC=0.17

SET Conc=105.5, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=100.0

START /NC

PLOT /DATA=m100_1a CVen

PLOT /DATA=m100_1b CTCOH

PLOT /DATA=m100_1c CBldTCA

PLOT /DATA=m100_1d AUrnTCA

PLOT /DATA=m100_1e AUrnTCOGTCOH

END

DATA M100_1a (T, CVen)

0.52	1.98
1.0	2.69
2.0	3.38
3.0	3.76
4.0	3.95
4.25	3.26
4.5	2.54
5.0	1.12
6.0	0.72

8.0	0.52
10.0	0.31
12.0	0.28
14.0	0.23
16.0	0.17
18.0	0.15

END

DATA M100_1b (T, CTCOH)

1.0	0.39
2.0	1.30
3.0	2.18
4.0	2.83
4.25	2.94
4.5	3.21
5.0	2.78
6.0	2.84
8.0	2.52
10.0	2.03
12.0	1.56
14.0	1.56
16.0	1.31
18.0	1.21
20.03	1.15

END

DATA M100_1c (T, CBldTCA)

0.52	0.15
1.0	0.50
2.0	1.07
3.0	2.11
4.0	3.12
4.25	2.87
4.5	3.39
5.0	4.00
6.0	4.09
8.0	4.76
10.0	5.52
12.0	6.16
14.0	6.48
16.0	8.12
18.0	7.18
20.03	8.56
22.02	8.14
45.83	9.30
69.74	7.37
93.75	6.97

END

DATA M100_1d (T, AUrnTCA)

4.5	1.47
6.1	2.82
8.0	5.02
10.1	7.10
11.4	8.87
12.1	10.22
14.1	12.67

16.0	15.33
18.0	16.85
20.23	22.83
21.97	25.23
26.0	30.03
31.5	33.10
34.25	39.59
35.5	42.21
36.75	48.47
44.75	52.39
52.0	55.28
54.5	58.64
56.5	59.80
59.5	62.40
60.5	65.00
68.5	79.17
70.25	83.51
73.00	88.15
79.5	99.19
81.5	100.11
84.67	100.62

END

DATA M100_1e (T, AUrnTCOGTCOH)

4.5	13.94
6.1	23.22
8.0	30.95
10.1	37.58
11.4	43.49
12.1	46.17
14.1	50.32
16.0	56.69
18.0	61.37
20.23	65.35
21.97	68.94
26.0	74.63
31.5	79.76
34.25	82.89
35.5	84.29
36.75	86.91
44.75	90.23
52.0	91.80
54.5	93.75
56.5	94.88
59.5	96.10
60.5	96.99
68.5	99.59
70.25	100.64
73.00	102.16
79.5	104.07
81.5	104.74
84.67	104.94

END

PROCED M100_2
! Data from Fisher et al. (1998)

```

! Data from procedure M100_2 (in Bld_M and Urine_M) in HumanB.cmd
! Male 100 ppm exposure
Human
ResetDoses
SET BW=82.3, VFatC=0.14
SET Conc=105.5, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=100.0
START /NC
PLOT /DATA=m100_2a CVen
PLOT /DATA=m100_2b CTCOH
PLOT /DATA=m100_2c CBldTCA
PLOT /DATA=m100_2d CDCA
PLOT /DATA=m100_2e AUrnTCA
PLOT /DATA=m100_2f AUrnTCOGTCOH
END

```

DATA M100_2a (T, CVen)

0.52	1.69
1.0	2.50
2.02	3.50
3.02	4.24
4.02	4.75
4.27	3.76
4.52	2.20
5.02	0.96
6.42	0.53
8.0	0.26
10.0	0.17
12.0	0.17

END

DATA M100_2b (T, CTCOH)

1.0	0.37
2.02	1.41
3.02	2.40
4.02	3.59
4.27	4.16
4.52	3.73
5.02	3.65
6.42	3.63
8.0	2.60
10.0	2.82
12.0	1.84
14.0	1.55
16.0	1.59
18.0	1.06
20.0	1.23
22.03	0.75

END

DATA M100_2c (T, CBldTCA)

0.52	0.24
1.0	0.60
2.02	1.24
3.02	2.71
4.27	4.23
4.52	3.86
5.02	3.92

6.42	4.54
8.0	5.71
10.0	6.21
14.0	7.96
16.0	9.08
18.0	8.30
20.0	8.43
22.03	8.95
69.72	5.51
93.61	3.55

END

DATA M100_2d (T, CDCA)

0.52	0.004
1.0	0.004
2.02	0.004
3.02	0.004
4.27	0.005
8.0	0.007

END

DATA M100_2e (T, AUrnTCA)

4.38	1.74
6.0	2.77
8.0	3.94
10.0	5.52
12.0	7.66
14.0	9.62
16.0	11.69
18.0	13.57
20.0	20.39
22.0	26.25
24.42	30.32
31.0	40.91
35.42	50.70
44.90	65.02
49.75	65.02
53.75	78.15
54.76	79.79
59.42	83.82
68.9	93.09
70.83	98.82
72.0	100.66
74.58	112.13
77.0	117.83
83.92	118.82
86.0	119.30
92.67	120.02

END

DATA M100_2f (T, AUrnTCOGTCOH)

6.0	8.69
8.0	18.39
10.0	27.48
12.0	37.49
14.0	44.58
16.0	51.78

18.0	56.11
20.0	60.47
22.0	64.77
24.42	66.98
31.0	75.49
35.42	79.43
44.90	82.13
49.75	85.29
53.75	88.15
54.76	88.66
59.42	89.44
68.9	90.60
70.83	91.71
72.0	91.84
74.58	92.37
77.0	93.07
83.92	93.79
86.0	94.17
92.67	94.55

END

PROCED M100_3

! Data from Fisher et al. (1998)

! Data from procedure M100_3 (in Bld_M and Urine_M) in HumanB.cmd

! Male 100 ppm exposure

Human

ResetDoses

SET BW=82.7, VFatC=0.14

SET Conc=102.6, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=100.0

START /NC

PLOT /DATA=m100_3a CVen

PLOT /DATA=m100_3b CTCOH

PLOT /DATA=m100_3c CBldTCA

PLOT /DATA=m100_3d AUrnTCA

PLOT /DATA=m100_3e AUrnTCOGTCOH

END

DATA M100_3a (T, CVen)

0.5	1.93
1.07	2.34
2.0	2.84
3.0	3.40
3.98	3.41
4.25	2.20
4.5	1.66
5.0	0.89
6.0	0.38

END

DATA M100_3b (T, CTCOH)

0.5	0.45
1.07	0.77
2.0	1.51
3.0	2.41
3.98	3.3
4.25	3.64

4.5	3.67
5.0	3.48
6.0	3.05
8.0	2.52
10.02	2.38
12.0	2.16
14.0	1.73
16.02	1.48
18.07	1.12
20.0	1.01
22.0	0.85

END

DATA M100_3c (T, CBldTCA)

0.5	0.23
1.07	0.49
2.0	1.07
3.0	1.89
3.98	2.87
4.25	3.69
4.5	3.87
5.0	3.59
6.0	4.18
8.0	4.71
10.02	5.46
12.0	5.67
14.0	5.97
16.02	6.05
18.07	6.22
20.0	7.54
22.0	7.26
46.85	8.43
71.47	3.86
95.50	3.55

END

DATA M100_3d (T, AUrnTCA)

3.03	0.488
4.75	0.961
6.7	2.09
8.25	2.96
10.17	5.56
12.08	7.17
14.19	8.37
15.58	9.09
17.6	9.70
18.23	10.13
19.58	10.99
20.05	11.24
21.33	11.88
22.17	12.36
23.2	13.03
35.42	14.18
40.67	16.14
46.67	18.07
47.17	19.06
52.33	20.35

55.25	23.68
68.17	24.71
69.75	27.02

END

DATA M100_3e (T, AUrnTCOGTCOH)

3.03	32.70
4.75	60.26
6.7	97.98
8.25	130.67
10.17	182.90
12.08	204.64
14.19	224.53
15.58	233.79
17.6	240.99
18.23	245.36
19.58	253.46
20.05	255.90
21.33	261.17
22.17	265.40
23.2	269.76
35.42	271.64
40.67	276.15
46.67	277.54
47.17	277.83
52.33	278.12
55.25	278.81
68.17	278.88
69.75	279.07

END

PROCED M100_4

! Data from Fisher et al. (1998)
! Data from procedure M100_4 (in Bld_M and Urine_M) in HumanB.cmd
! Male 100 ppm exposure
Human
ResetDoses
SET BW=71.1, VFatC=0.14
SET Conc=101.5, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=100.0
START /NC
PLOT /DATA=m100_4a CVen
PLOT /DATA=m100_4b CTCOH
PLOT /DATA=m100_4c CBldTCA
PLOT /DATA=m100_4d AUrnTCA
PLOT /DATA=m100_4e AUrnTCOGTCOH
END

DATA M100_4a (T, CVen)

0.5	3.10
1.0	3.76
2.0	3.46
3.0	3.83
4.02	3.78
4.25	2.90
4.5	2.11
5.0	1.09

END

DATA M100_4b (T, CTCOH)

0.5	0.56
1.0	1.12
2.0	1.75
3.0	2.55
4.02	3.48
4.25	3.73
4.5	3.52
5.0	3.78
6.0	3.79
8.0	3.30
10.0	2.96
12.05	2.71
14.0	2.38
16.0	2.04
18.0	1.89
20.0	1.57
22.05	1.40

END

DATA M100_4c (T, CBldTCA)

0.5	0.3
1.0	0.75
2.0	1.42
3.0	2.34
4.02	3.01
4.25	2.58
4.5	3.10
5.0	3.26
6.0	4.21
8.0	4.99
10.0	5.46
12.05	5.74
14.0	6.69
16.0	6.85
18.0	7.14
20.0	9.85
22.05	9.32
50.52	8.87
74.03	8.08
98.58	3.82

END

DATA M100_4d (T, AUrnTCA)

4.35	0.98
5.03	1.21
6.07	1.42
8.07	2.05
10.04	3.12
12.07	3.60
14.06	4.09
16.03	4.57
18.02	4.86
20.04	5.28
22.13	5.98

25.5	8.14
36.5	8.94
44.1	10.97
47.0	11.58
54.0	13.48
61.45	15.33
69.3	17.47
85.0	21.65
93.55	21.65

END

DATA M100_4e (T, AUrnTCOGTCOH)

4.35	28.92
5.03	31.85
6.07	40.01
8.07	56.31
10.04	68.48
12.07	78.80
14.06	89.82
16.03	98.66
18.02	105.25
20.04	112.29
22.13	122.73
25.5	141.62
36.5	150.29
44.1	162.32
47.0	165.74
54.0	173.84
61.45	178.30
69.3	182.24
85.0	185.01
93.55	186.89

END

PROCED M100_5

! Data from Fisher et al. (1998)

! Data from procedure M100_5 (in Bld_M, Exh_M and Urine_M) in HumanB.cmd

! Male 100 ppm exposure

Human

ResetDoses

SET BW=73.2, VFatC=0.18

SET Conc=102.0, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=110.0

START /NC

PLOT /DATA=m100_5a CVen

PLOT /DATA=m100_5b CTCOH

PLOT /DATA=m100_5c CBldTCA

PLOT /DATA=m100_5d CALvPPM

PLOT /DATA=m100_5e AUrnTCA

PLOT /DATA=m100_5f AUrnTCOGTCOH

END

DATA M100_5a (T, CVen)

0.5	0.76
1.0	0.86
2.0	1.15
3.0	1.15

4.0	1.23
4.25	0.77
4.53	0.46
5.0	0.34
6.0	0.21
8.0	0.15

END

DATA M100_5b (T, CTCOH)

1.0	0.52
2.0	1.35
3.0	1.87
4.0	2.50
4.25	2.59
4.53	2.58
5.0	2.25
6.0	2.15
8.0	1.98
10.0	1.56
12.0	1.02
14.0	1.26
16.03	0.89
18.0	0.79
20.0	0.73
22.0	0.70

END

DATA M100_5c (T, CBldTCA)

0.5	0.11
1.0	0.36
2.0	1.07
3.0	1.55
4.0	2.31
4.25	2.03
4.53	2.16
5.0	2.35
6.0	2.53
8.0	3.61
10.0	3.93
12.0	4.57
14.0	4.50
16.03	5.02
18.0	5.10
20.0	5.07
22.0	5.91
51.0	6.38
78.08	5.33
100.83	4.01

END

DATA M100_5d (T, CALvPPM)

4.0	12.386
4.25	3.305
4.53	2.478
5.0	1.567
6.0	0.577
8.0	0.317

10.0 0.286
END

DATA M100_5e (T, AUrnTCA)

4.67	1.36
5.05	1.66
6.3	2.70
8.05	4.22
10.07	6.04
12.07	8.04
14.07	10.37
16.15	13.33
18.08	16.55
20.05	20.04
22.15	23.89
25.33	30.02
31.92	35.07
35.33	38.42
43.58	43.06
51.08	46.65
53.25	48.88
56.92	54.83
58.33	57.31
59.67	59.49
63.75	62.36
67.42	66.44
73.08	70.15
78.0	73.57
80.58	75.42
82.75	77.73
84.25	78.87
84.92	80.37
87.58	83.60
91.83	86.81

END

DATA M100_5f (T, AUrnTCOGTCOH)

4.67	16.05
5.05	18.22
6.3	25.28
8.05	34.46
10.07	43.49
12.07	49.91
14.07	55.78
16.15	59.33
18.08	65.07
20.05	68.36
22.15	71.48
25.33	76.10
31.92	81.25
35.33	83.82
43.58	86.11
51.08	87.66
53.25	88.38
56.92	89.39
58.33	89.71
59.67	89.92

63.75	89.92
67.42	90.38
73.08	91.07
78.0	91.55
80.58	91.79
82.75	91.94
84.25	92.03
84.92	92.22
87.58	92.37
91.83	92.55

END

PROCED M100_6

! Data from Fisher et al. (1998)

! Data from procedure M100_6 (in Bld_M, Exh_M and Urine_M) in HumanB.cmd

! Male 100 ppm exposure

Human

ResetDoses

SET BW=52.3, VFatC=0.06

SET Conc=97.8, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=110.0

START /NC

PLOT /DATA=m100_6a CVen

PLOT /DATA=m100_6b CTCOH

PLOT /DATA=m100_6c CBldTCA

PLOT /DATA=m100_6d CALvPPM

PLOT /DATA=m100_6e AUrnTCA

PLOT /DATA=m100_6f AUrnTCOGTCOH

END

DATA M100_6a (T, CVen)

0.5	0.64
1.0	0.94
2.02	1.35
3.0	1.62
4.02	1.56
4.25	1.16
4.5	0.77
5.0	0.37
6.0	0.23
8.0	0.19
10.03	0.17

END

DATA M100_6b (T, CTCOH)

1.0	0.47
2.02	1.10
3.0	1.58
4.02	2.10
4.25	2.21
4.5	2.20
5.0	2.15
6.0	1.94
8.0	1.88
10.03	1.61
12.02	1.39
14.03	1.26

16.0	1.06
18.0	0.95
19.97	0.88
22.07	0.77

END

DATA M100_6c (T, CBldTCA)

0.5	0.21
1.0	0.49
2.02	1.10
3.0	1.67
4.02	2.52
4.25	2.44
4.5	2.71
5.0	3.18
6.0	3.46
8.0	4.26
10.03	4.93
12.02	5.43
14.03	5.85
16.0	6.02
18.0	6.18
19.97	6.35
22.07	6.52
48.0	12.88
71.83	6.25
101.08	5.07

END

DATA M100_6d (T, CALvPPM)

4.02	24.679
4.25	6.422
4.5	4.394
5.0	2.691
6.0	1.388
8.0	1.198
10.03	0.592
12.02	0.470
14.03	0.369
16.0	0.351

END

DATA M100_6e (T, AUrnTCA)

4.55	0.32
5.12	0.41
6.08	1.04
8.13	1.32
10.13	2.51
12.1	4.77
14.1	7.29
16.1	10.23
18.12	11.50
20.08	13.03
22.3	14.26
30.42	17.65
35.67	18.58
51.83	18.58

56.67	18.58
61.5	18.95
70.17	20.95
72.67	22.77
76.92	25.76
82.67	30.01
85.75	30.70
93.67	34.88

END

DATA M100_6f (T, AUrnTCOGTCOH)

4.55	11.60
5.12	13.64
6.08	18.54
8.13	25.00
10.13	33.99
12.1	42.10
14.1	50.19
16.1	60.58
18.12	64.73
20.08	70.85
22.3	77.69
30.42	79.75
35.67	80.14
51.83	80.23
56.67	80.32
61.5	80.66
70.17	81.44
72.67	82.38
76.92	82.74
82.67	83.28
85.75	83.35
93.67	83.79

END

PROCED M100_7Param

SET VMaxC=3.0

END

PROCED M100_7

! Data from Fisher et al. (1998)

! Data from procedure M100_7 (in Bld_M, Exh_M and Urine_M) in HumanB.cmd

! Male 100 ppm exposure

Human

ResetDoses

M100_7Param

SET BW=60.9, VFatC=0.10

SET Conc=101.1, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=300.0

START /NC

PLOT /DATA=m100_7a CVen

PLOT /DATA=m100_7b CTCOH

PLOT /DATA=m100_7c CBldTCA

PLOT /DATA=m100_7d CALvPPM

PLOT /DATA=m100_7e CDCA

PLOT /DATA=m100_7f AUrnTCA

PLOT /DATA=m100_7g AUrnTCOGTCOH

END

DATA M100_7a (T, CVen)

0.5	0.59
1.0	0.85
2.0	1.1
3.0	1.04
4.0	1.18
4.3	0.64
4.5	0.42
5.0	0.19

END

DATA M100_7b (T, CTCOH)

0.5	0.28
1.0	0.76
2.0	1.92
3.0	1.69
4.0	2.34
4.3	2.34
4.5	2.16
5.0	2.13
6.0	1.95
8.0	1.61
10.0	1.33
12.0	1.58
14.0	0.84
16.0	0.77
18.0	0.57
20.03	0.76

END

DATA M100_7c (T, CBldTCA)

0.5	0.36
1.0	0.84
2.0	1.73
3.0	2.60
4.0	3.42
4.3	3.90
4.5	3.67
5.0	4.47
6.0	5.00
8.0	5.95
10.0	6.74
12.0	7.12
14.0	7.75
16.0	8.22
18.0	8.17
20.03	9.01
49.75	10.66
73.8	8.6
95.24	7.46
264.0	3.13

END

DATA M100_7d (T, CALvPPM)

4.0	21.575
-----	--------

4.03	14.272
4.05	10.770
4.08	7.056
4.167	5.876
4.3	5.773
4.5	5.010
5.0	2.498
6.0	1.713
8.0	1.263
10.0	1.029
12.0	0.936
14.0	0.809
16.0	0.738
18.0	0.683

END

DATA M100_7e (T, CDCA)

1.0	0.006
2.0	0.008
4.0	0.012

END

DATA M100_7f (T, AUrnTCA)

4.75	0.93
7.95	3.02
14.08	5.95
16.08	7.07
18.1	8.28
20.25	9.63
24.67	13.46
29.17	15.73
32.67	20.11
35.33	22.71
38.83	24.07
44.25	25.60
49.67	27.51
55.92	29.60
58.75	33.36
68.25	39.61
73.83	43.70
75.92	45.78
77.92	48.52
81.17	51.21
82.58	53.54
92.17	60.72

END

DATA M100_7g (T, AUrnTCOGTCOH)

4.75	40.71
7.95	69.81
14.08	89.76
16.08	96.80
18.1	102.69
20.25	107.93
24.67	121.30
29.17	128.51
32.67	135.51

35.33	138.05
38.83	140.20
44.25	142.48
49.67	144.47
55.92	144.96
58.75	145.55
68.25	146.67
73.83	147.09
75.92	147.25
77.92	147.38
81.17	147.50
82.58	147.62
92.17	147.98

END

PROCED M100_8

! Data from Fisher et al. (1998)

! Data from procedure M100_8 (in Bld_M and Urine_M) in HumanB.cmd

! Male 100 ppm exposure

Human

ResetDoses

SET BW=70.9, VFatC=0.18

SET Conc=103.4, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=300.0

START /NC

PLOT /DATA=m100_8a CVen

PLOT /DATA=m100_8b CTCOH

PLOT /DATA=m100_8c CBldTCA

PLOT /DATA=m100_8d CDCA

PLOT /DATA=m100_8e AUrnTCA

PLOT /DATA=m100_8f AUrnTCOGTCOH

END

DATA M100_8a (T, CVen)

0.5	2.69
1.0	2.98
2.0	3.51
3.0	3.58
4.0	2.88
4.25	1.96
4.5	1.53
5.75	0.81
6.0	0.52
8.0	0.32
10.0	0.27
12.0	0.24
14.0	0.22
16.0	0.22
18.0	0.20
20.0	0.16
22.0	0.16

END

DATA M100_8b (T, CTCOH)

0.5	0.47
1.0	0.68
2.0	1.51

3.0	3.58
4.0	2.72
4.25	2.87
4.5	2.77
5.75	2.63
6.0	2.30
8.0	1.90
10.0	1.59
12.0	1.28
14.0	1.23
16.0	1.06
18.0	0.98
20.0	0.72
22.0	0.71

END

DATA M100_8c (T, CBldTCA)

0.5	0.43
1.0	1.00
2.0	2.15
3.0	3.40
4.0	4.94
4.25	5.42
4.5	5.67
5.75	5.83
6.0	5.99
8.0	7.23
10.0	7.96
12.0	8.14
14.0	8.39
16.0	8.36
18.0	8.83
20.0	8.96
22.0	9.51
44.98	10.75
68.9	9.21
93.08	7.94
264.0	1.94

END

DATA M100_8d (T, CDCA)

2.0	0.004
3.0	0.010
4.0	0.008
4.25	0.005
4.5	0.005
5.75	0.004
8.0	0.005
16.0	0.005

END

DATA M100_8e (T, AUrnTCA)

4.58	40.02
5.03	40.67
6.03	57.48
8.05	76.60
10.03	99.19

12.03	115.98
14.07	126.00
16.05	136.55
18.03	143.51
20.02	150.54
22.08	163.57
45.42	196.37
47.42	197.62
48.92	198.48
50.42	199.33
53.92	201.12
57.33	201.12
59.17	201.73
60.92	202.15
63.92	202.88
67.92	203.60
74.58	204.11
80.25	204.47
82.42	204.92
84.33	205.07
85.58	205.15
86.92	205.30

END

DATA M100_8f (T, AUrnTCOGTCOH)

4.58	0.935
5.03	1.34
6.03	4.10
8.05	6.10
10.03	9.74
12.03	13.29
14.07	16.29
16.05	20.29
18.03	22.87
20.02	24.83
22.08	29.98
45.42	56.81
47.42	61.82
48.92	64.84
50.42	67.02
53.92	74.27
57.33	76.87
59.17	78.68
60.92	61.05
63.92	88.53
67.92	90.31
74.58	92.43
80.25	95.17
82.42	97.12
84.33	100.02
85.58	100.76
86.92	103.23

END

PROCED F100_1

! Data from Fisher et al. (1998)

```

! Data from procedure F100_1 (in Bld_F and Urine_F) in HumanB.cmd
! Female 100 ppm exposure
Human
ResetDoses
SET BW=57.5, VFatC=0.21
SET Conc=102.5, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=100.0
START /NC
PLOT /DATA=f100_1a CVen
PLOT /DATA=f100_1b CTCOH
PLOT /DATA=f100_1c CBldTCA
PLOT /DATA=f100_1d AUrnTCA
PLOT /DATA=f100_1e AUrnTCOGTCOH
END

```

DATA F100_1a (T, CVen)

0.5	1.11
1.0	1.36
2.0	2.11
3.0	1.92
4.0	2.30
4.25	1.56
4.50	1.26
5.0	0.73
6.0	0.42

END

DATA F100_1b (T, CTCOH)

0.5	0.22
1.0	0.46
2.0	1.18
3.0	2.18
4.0	3.03
4.25	3.29
4.50	3.67
5.0	3.13
6.0	2.57
8.0	2.46
10.0	1.93
12.0	1.57
14.0	1.30
16.05	1.08
18.0	0.89
20.02	0.56
22.02	0.65
46.17	0.3

END

DATA F100_1c (T, CBldTCA)

0.5	0.21
1.0	0.39
2.0	1.05
3.0	1.86
4.0	3.46
4.25	3.78
4.50	3.91
5.0	4.22
6.0	4.67

8.0	5.71
10.0	6.29
12.0	7.76
14.0	7.78
16.05	8.11
18.0	8.79
20.02	9.05
22.02	9.34
46.17	9.58
69.83	7.93
94.67	6.69

END

DATA F100_1d (T, AUrnTCA)

4.62	0.51
5.08	0.65
6.86	1.26
8.33	1.85
10.25	2.92
12.13	3.91
14.08	4.92
16.15	5.91
18.0	5.91
20.05	7.12
22.17	9.55
30.67	15.22
33.67	17.85
35.42	19.66
40.67	24.08
46.67	26.68
47.17	27.91
52.33	30.49
55.25	35.74
68.17	35.75
69.75	36.78
73.92	37.71
76.0	41.25
78.17	45.21
80.33	46.43
81.5	47.22
82.25	47.91
92.58	49.66
93.67	50.98
94.17	51.67

END

DATA F100_1e (T, AUrnTCOGTCOH)

4.62	44.83
5.08	52.08
6.86	77.84
8.33	89.76
10.25	108.58
12.13	122.65
14.08	133.38
16.15	140.85
18.0	147.19
20.05	151.76

22.17	155.86
30.67	169.38
33.67	174.67
35.42	175.78
40.67	179.31
46.67	179.77
47.17	179.97
52.33	180.44
55.25	181.52
68.17	184.09
69.75	184.16
73.92	184.26
76.0	184.70
78.17	185.20
80.33	185.35
81.5	185.42
82.25	185.51
92.58	185.81
93.67	185.91
94.17	185.95

END

PROCED F100_2

! Data from Fisher et al. (1998)

! Data from procedure F100_2 (in Bld_F and Urine_F) in HumanB.cmd

! Female 100 ppm exposure

Human

ResetDoses

SET BW=66.6, VFatC=0.32

SET Conc=101.4, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=100.0

START /NC

PLOT /DATA=f100_2a CVen

PLOT /DATA=f100_2b CTCOH

PLOT /DATA=f100_2c CBldTCA

PLOT /DATA=f100_2d AUrnTCA

PLOT /DATA=f100_2e AUrnTCOGTCOH

END

DATA F100_2a (T, CVen)

0.5	1.18
1.0	2.17
2.0	2.30
3.0	2.41
4.0	2.65
4.23	1.84
4.5	1.17
5.0	0.62
6.0	0.38

END

DATA F100_2b (T, CTCOH)

1.0	0.74
2.0	1.38
3.0	1.93
4.0	2.41
4.23	2.40

4.5	2.33
5.0	2.17
6.0	1.94
8.05	1.81
10.0	1.38
12.0	1.17
14.02	1.25
16.0	1.01
18.0	0.88
20.0	0.74
22.02	0.70

END

DATA F100_2c (T, CBldTCA)

2.0	0.91
3.0	1.75
4.0	2.65
4.23	2.54
4.5	2.65
5.0	2.73
6.0	3.26
8.05	3.58
10.0	4.50
12.0	4.02
14.02	4.17
16.0	4.45
18.0	4.90
20.0	5.26
22.02	5.94
46.70	6.68
70.25	5.20
93.72	3.60

END

DATA F100_2d (T, AUrnTCA)

4.37	0.31
5.03	0.39
6.1	0.64
8.1	1.21
10.07	1.66
12.03	2.16
14.1	2.96
16.05	3.66
18.05	4.37
20.06	5.44
22.15	6.66
24.32	7.63
27.05	8.16
28.3	8.71
30.1	10.30
32.45	10.92
34.2	11.77
36.1	12.45
43.2	13.71
45.4	14.04
48.0	15.07
51.4	15.98

54.05	16.51
56.4	17.0
58.2	17.60
59.55	19.57
67.55	19.76
70.20	20.25
72.20	21.31
75.0	22.08
77.55	22.65
81.55	24.79
84.1	30.86
89.1	31.05
91.35	31.06

END

DATA F100_2e (T, AUrnTCOGTCOH)

4.37	35.78
5.03	44.40
6.1	54.40
8.1	72.58
10.07	90.61
12.03	104.44
14.1	116.90
16.05	127.49
18.05	127.49
20.06	136.49
22.15	144.45
24.32	147.89
27.05	150.61
28.3	154.52
30.1	157.72
32.45	160.74
34.2	163.47
36.1	165.86
43.2	167.54
45.4	168.21
48.0	169.24
51.4	170.26
54.05	171.66
56.4	172.85
58.2	173.70
59.55	175.02
67.55	175.31
70.20	175.67
72.20	176.21
75.0	176.60
77.55	177.07
81.55	178.04
84.1	178.43
89.1	178.65
91.35	178.94

END

PROCED F100_3

! Data from Fisher et al. (1998)

! Data from procedure F100_3 (in Bld_F and Urine_F) in HumanB.cmd

```

! Female 100 ppm exposure
Human
ResetDoses
SET BW=55.5, VFatC=0.23
SET Conc=102.0, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=100.0
START /NC
PLOT /DATA=f100_3a CVen
PLOT /DATA=f100_3b CTCOH
PLOT /DATA=f100_3c CBldTCA
PLOT /DATA=f100_3d AUrnTCA
PLOT /DATA=f100_3e AUrnTCOGTCOH
END

```

DATA F100_3a (T, CVen)

0.58	0.81
1.0	0.88
2.0	1.09
3.0	1.03
4.0	1.13
4.17	0.59
4.5	0.47
5.0	0.30
6.0	0.18
8.02	0.15

END

DATA F100_3b (T, CTCOH)

0.58	0.33
1.0	0.57
2.0	1.01
3.0	1.25
4.0	1.79
4.17	1.64
4.5	1.54
5.0	1.43
6.0	1.27
8.02	0.95
10.02	1.01
12.02	0.90
14.03	0.88
16.0	0.74
18.0	0.69
20.0	0.63
22.0	0.61

END

DATA F100_3c (T, CBldTCA)

0.58	0.40
1.0	0.97
2.0	1.72
3.0	2.64
4.0	3.41
4.17	3.62
4.5	3.86
5.0	4.39
6.0	4.80
8.02	5.73

10.02	6.79
12.02	7.55
14.03	7.68
16.0	7.98
18.0	9.27
20.0	8.91
22.0	9.12
46.08	11.31
75.67	10.49
94.25	8.47

END

DATA F100_3d (T, AUrnTCA)

4.58	0.44
6.03	0.71
8.12	1.31
10.08	2.28
12.1	3.48
14.1	4.64
16.05	5.64
18.1	6.76
20.05	7.66
21.92	8.89
26.17	10.64
33.25	13.81
37.92	14.11
44.92	15.44
49.0	16.00
54.92	23.2
58.42	22.4
61.42	24.1
66.42	29.1
70.67	32.6
74.75	36.2
80.42	36.8
82.42	37.5
84.92	37.79
93.42	45.72

END

DATA F100_3e (T, AUrnTCOGTCOH)

4.58	12.63
6.03	17.83
8.12	26.05
10.08	30.40
12.1	36.72
14.1	41.26
16.05	44.27
18.1	47.94
20.05	50.31
21.92	53.17
26.17	57.90
33.25	65.27
37.92	65.80
44.92	69.74
49.0	69.74
54.92	72.07

58.42	73.58
61.42	75.39
66.42	76.98
70.67	79.89
74.75	80.98
80.42	82.20
82.42	82.57
84.92	82.74
93.42	83.41

END

PROCED F100_4

! Data from Fisher et al. (1998)

! Data from procedure F100_4 (in Bld_F and Urine_F) in HumanB.cmd

! Female 100 ppm exposure

Human

ResetDoses

SET BW=61.8, VFatC=0.33

SET Conc=102.0, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=100.0

START /NC

PLOT /DATA=f100_4a CVen

PLOT /DATA=f100_4b CTCOH

PLOT /DATA=f100_4c CBldTCA

PLOT /DATA=f100_4d AUrnTCA

PLOT /DATA=f100_4e AUrnTCOGTCOH

END

DATA F100_4a (T, CVen)

0.55	0.55
1.0	0.81
2.12	1.30
3.05	1.37
4.0	1.43
4.25	0.81
4.50	0.54
5.0	0.35
6.0	0.18

END

DATA F100_4b (T, CTCOH)

1.0	0.39
2.12	1.2
3.05	1.59
4.0	1.93
4.25	1.97
4.50	1.75
5.0	1.63
6.0	1.32
8.05	1.10
10.08	0.91
14.03	0.83
18.02	0.69
22.02	0.54

END

DATA F100_4c (T, CBldTCA)

0.55	0.47
1.0	1.05
2.12	2.73
3.05	3.85
4.0	4.82
4.25	5.02
4.50	5.29
5.0	5.37
6.0	6.01
8.05	7.60
10.08	6.77
14.03	8.65
18.02	9.49
22.02	10.64
46.08	9.58
75.67	8.55
94.25	7.82

END

DATA F100_4d (T, AUrnTCA)

2.33	0.29
4.57	1.62
5.12	2.09
6.12	4.01
8.12	5.81
10.33	8.27
12.08	10.21
14.12	13.06
16.0	16.29
18.08	19.09
20.0	21.96
21.92	24.17
25.08	27.09
29.25	29.05
32.58	35.13
35.83	45.84
38.33	56.12
41.0	65.21
45.0	75.98
48.83	81.05
50.33	83.74
53.67	87.89
56.33	91.72
59.33	97.13
66.83	100.34
73.25	102.88
80.58	106.50
83.5	110.02
86.0	113.61
93.0	117.51

END

DATA F100_4e (T, AUrnTCOGTCOH)

2.33	4.52
4.57	8.37
5.12	12.49
6.12	19.46

8.12	29.26
10.33	35.93
12.08	40.21
14.12	44.90
16.0	48.15
18.08	51.04
20.0	55.72
21.92	58.76
25.08	60.75
29.25	62.24
32.58	72.07
35.83	76.15
38.33	79.24
41.0	81.48
45.0	83.84
48.83	86.37
50.33	87.44
53.67	88.84
56.33	90.90
59.33	92.91
66.83	94.07
73.25	94.96
80.58	96.17
83.5	96.82
86.0	97.41
93.0	98.54

END

```

PROCED F100_5
! Data from Fisher et al. (1998)
! Data from procedure F100_5 (in Bld_F, Exh_F and Urine_F) in HumanB.cmd
! Female 100 ppm exposure
Human
ResetDoses
SET BW=67.3, VFatC=0.35
SET Conc=102.0, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=100.0
START /NC
PLOT /DATA=f100_5a CVen
PLOT /DATA=f100_5b CTCOH
PLOT /DATA=f100_5c CBldTCA
PLOT /DATA=f100_5d CALvPPM
PLOT /DATA=f100_5e AUrnTCA
PLOT /DATA=f100_5f AUrnTCOGTCOH
END

```

```

DATA F100_5a (T, CVen)
0.5    0.74
1.0    1.0
2.0    1.27
3.0    1.45
4.0    1.19
4.25   0.81
4.55   0.66
5.0    0.46
6.02   0.25
8.02   0.19

```

END

DATA F100_5b (T, CTCOH)

1.0	0.41
2.0	0.78
3.0	1.04
4.0	1.18
4.25	1.17
4.55	1.18
5.0	1.18
8.02	0.84
10.0	0.72
12.0	0.82
14.0	0.56
18.02	0.49
20.0	0.41

END

DATA F100_5c (T, CBldTCA)

0.5	0.25
1.0	0.76
2.0	1.48
3.0	2.21
4.0	2.79
4.25	2.78
4.55	3.12
5.0	3.23
6.02	3.52
8.02	4.76
10.0	4.95
12.0	5.29
14.0	5.33
18.02	6.46
20.0	6.91
22.0	7.10
46.58	6.63
70.5	5.28

END

DATA F100_5d (T, CALvPPM)

4.25	4.243
4.55	2.798
5.0	1.849
6.02	1.467
8.02	0.681
10.0	0.452
12.0	0.409
14.0	0.356

END

DATA F100_5e (T, AUrnTCA)

4.67	0.69
5.0	0.80
6.3	1.64
8.08	3.16
10.08	4.95
12.07	7.19

14.08	9.89
16.12	13.14
18.11	17.46
20.1	21.67
22.12	26.40
22.67	29.05
26.5	35.18
29.67	41.73
34.17	49.36
35.67	50.76
40.67	56.47
43.67	60.68
47.17	69.00
49.67	73.32
53.42	76.81
56.17	79.16
58.0	81.70
59.67	83.84
60.17	84.56
61.67	86.11
67.67	91.59
72.67	95.63
76.67	100.35
82.67	110.14
84.17	111.45
85.67	112.62
91.67	115.92

END

DATA F100_5f (T, AUrnTCOGTCOH)

4.67	9.98
5.0	9.98
6.3	12.41
8.08	16.09
10.08	18.99
12.07	20.96
14.08	23.08
16.12	24.46
18.11	26.22
20.1	27.92
22.12	29.05
22.67	29.64
26.5	32.31
29.67	34.40
34.17	36.58
35.67	37.14
40.67	38.80
43.67	39.86
47.17	40.61
49.67	41.58
53.42	42.31
56.17	42.94
58.0	43.30
59.67	43.53
60.17	43.60
61.67	43.78
67.67	44.79

72.67	45.19
76.67	45.69
82.67	46.42
84.17	46.54
85.67	46.60
91.67	47.13

END

PROCED F100_6Param

SET VMaxC=3.0

END

PROCED F100_6

! Data from Fisher et al. (1998)

! Data from procedure F100_6 (in Bld_F, Exh_F and Urine_F) in HumanB.cmd

! Female 100 ppm exposure

Human

ResetDoses

F100_6Param

SET BW=62.3, VFatC=0.24

SET Conc=97.7, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=110.0

START /NC

PLOT /DATA=f100_6a CVen

PLOT /DATA=f100_6b CTCOH

PLOT /DATA=f100_6c CBldTCA

PLOT /DATA=f100_6d CALvPPM

PLOT /DATA=f100_6e CDCA

PLOT /DATA=f100_6f AUrnTCA

PLOT /DATA=f100_6g AUrnTCOGTCOH

END

DATA F100_6a (T, CVen)

0.5	0.83
1.0	0.99
2.03	1.20
3.0	1.59
4.03	2.03
4.25	1.33
4.5	0.87
5.0	0.42
6.0	0.21
8.0	0.22
10.0	0.15

END

DATA F100_6b (T, CTCOH)

2.03	0.53
3.0	0.83
4.03	1.27
4.25	0.92
4.5	0.85
5.0	1.17
6.0	1.03
8.0	0.86
10.0	0.80
12.0	0.71

14.03	0.62
16.03	0.55
18.07	0.48
20.0	0.41

END

DATA F100_6c (T, CBldTCA)

0.5	0.44
1.0	0.97
2.03	2.16
3.0	3.79
4.03	5.12
4.25	5.35
4.5	5.60
5.0	5.88
6.0	6.55
8.0	7.30
10.0	7.66
12.0	8.61
14.03	8.73
16.03	9.65
18.07	8.29
20.0	8.60
22.0	10.2
47.95	6.15
71.98	7.11
101.22	6.73

END

DATA F100_6d (T, CALvPPM)

4.03	22.398
4.25	7.317
4.5	5.917
5.0	2.903
6.0	1.382
8.0	0.982
10.0	0.691
12.0	0.524
14.03	0.428

END

DATA F100_6e (T, CDCA)

1.0	0.005
2.03	0.014
3.0	0.005

END

DATA F100_6f (T, AUrnTCA)

4.55	0.30
5.12	0.56
6.08	1.75
8.19	1.97
10.19	3.75
12.17	6.58
14.33	6.81
16.23	8.64
18.19	10.30

20.13	12.13
22.38	13.64
31.92	15.77
34.25	18.03
36.92	18.16
48.67	22.69
55.83	28.52
59.0	30.85
63.5	31.36
70.8	33.88
76.0	37.20
85.5	41.32
87.25	42.86
88.08	49.42
94.75	54.14

END

DATA F100_6g (T, AUrnTCOGTCOH)

4.55	11.67
5.12	14.56
6.08	20.78
8.19	25.55
10.19	34.83
12.17	45.33
14.33	45.98
16.23	54.21
18.19	60.91
20.13	68.01
22.38	73.35
31.92	75.14
34.25	79.52
36.92	79.97
48.67	85.95
55.83	90.84
59.0	91.82
63.5	92.13
70.8	92.13
76.0	95.09
85.5	96.05
87.25	96.34
88.08	96.45
94.75	97.45

END

PROCED F100_7

```
! Data from Fisher et al. (1998)
! Data from procedure F100_7 (in Bld_F and Urine_F) in HumanB.cmd
! Female 100 ppm exposure
Human
ResetDoses
SET BW=63.2, VFatC=0.26
SET Conc=101.0, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=100.0
START /NC
PLOT /DATA=f100_7a CVen
PLOT /DATA=f100_7b CTCOH
PLOT /DATA=f100_7c CBldTCA
```

```
PLOT /DATA=f100_7d AUrnTCA
PLOT /DATA=f100_7e AUrnTCOGTCOH
END
```

```
DATA F100_7a (T, CVen)
```

0.52	0.53
1.0	1.0
2.0	0.97
3.0	1.31
4.0	1.48
4.28	0.84
4.5	0.58
5.0	0.39

```
END
```

```
DATA F100_7b (T, CTCOH)
```

0.52	0.35
1.0	0.58
2.0	0.86
3.0	1.60
4.0	2.03
4.28	2.04
4.5	1.93
5.0	1.95
6.05	1.79
8.0	1.29
10.0	1.14
12.0	1.03

```
END
```

```
DATA F100_7c (T, CBldTCA)
```

0.52	0.39
1.0	1.08
2.0	1.90
3.0	3.83
4.0	4.48
4.28	4.65
4.5	4.80
5.0	4.73
6.05	6.02
8.0	6.02
10.0	7.12
12.0	7.13
46.75	9.10
73.97	6.92
95.42	6.14

```
END
```

```
DATA F100_7d (T, AUrnTCA)
```

4.67	2.51
5.17	3.07
6.25	6.21
8.08	9.97
10.13	13.01
12.08	16.35
14.12	20.65
16.02	23.23

18.02	26.31
20.17	26.31
25.27	34.28
25.75	34.84
30.0	42.19
34.5	51.62
37.92	61.19
45.08	75.52
49.33	81.43
56.92	92.21
60.42	104.12
68.33	116.32
72.58	121.17
80.5	131.94
84.33	134.71
86.17	136.09
93.5	142.30

END

DATA F100_7d (T, AUrnTCOGTCOH)

4.67	37.76
5.17	42.18
6.25	48.68
8.08	60.91
10.13	72.32
12.08	81.05
14.12	86.76
16.02	94.78
18.02	100.92
20.17	105.91
25.27	115.12
25.75	116.22
30.0	125.29
34.5	131.36
37.92	135.91
45.08	143.62
49.33	146.34
56.92	149.70
60.42	151.17
68.33	153.38
72.58	154.28
80.5	155.70
84.33	155.93
86.17	156.09
93.5	156.70

END

PROCED F100_8

! Data from Fisher et al. (1998)

! Data from procedure F100_8 (in Bld_F and Urine_F) in HumanB.cmd

! Female 100 ppm exposure

Human

ResetDoses

SET BW=48.6, VFatC=0.23

SET Conc=103.3, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=300.0

START /NC


```
PLOT /DATA=f100_8a CVen
PLOT /DATA=f100_8b CTCOH
PLOT /DATA=f100_8c CBldTCA
PLOT /DATA=f100_8d CDCA
PLOT /DATA=f100_8e AUrnTCA
PLOT /DATA=f100_8f AUrnTCOGTCOH
END
```

```
DATA F100_8a (T, CVen)
```

0.5	1.32
1.0	1.68
2.0	1.86
3.0	2.37
4.0	2.66
4.25	2.10
4.5	1.23
5.0	0.83
6.0	0.42
8.05	0.33
10.03	0.30

```
END
```

```
DATA F100_8b (T, CTCOH)
```

0.5	0.47
1.0	0.68
2.0	1.51
3.0	2.15
4.0	2.72
4.25	2.87
4.5	2.77
5.0	2.63
6.0	2.30
8.05	1.90
10.03	1.59
12.05	1.28
14.02	1.23
16.0	1.10
18.0	0.98
20.0	0.72
22.0	0.71

```
END
```

```
DATA F100_8c (T, CBldTCA)
```

0.5	0.27
1.0	0.70
2.0	1.48
3.0	2.80
4.0	3.92
4.25	3.86
4.5	3.98
5.0	4.55
6.0	4.80
8.05	5.96
10.03	6.09
12.05	6.41
14.02	7.01
16.0	7.23

18.0	7.57
20.0	7.68
22.0	8.46
45.03	8.75
69.03	7.73
93.13	5.72
264.0	0.53

END

DATA F100_8d (T, CDCA)

0.5	0.008
1.0	0.008
2.0	0.007
3.0	0.007
4.0	0.006
4.25	0.009
4.5	0.013
5.0	0.012
6.0	0.011
8.05	0.005
12.05	0.005
16.0	0.004
18.0	0.004
22.0	0.005
45.03	0.006
69.03	0.004

END

DATA F100_8e (T, AUrnTCA)

4.58	2.34
5.05	2.92
6.05	5.27
8.08	8.33
10.07	12.15
12.08	17.02
14.31	21.46
16.05	26.02
18.05	28.88
20.03	32.60
22.08	37.96
43.33	80.45
45.58	85.25
47.58	87.93
49.17	91.55
53.58	99.63
61.33	110.21
67.33	114.43
70.58	118.52
74.58	123.23
77.25	128.78
83.25	133.51
84.25	134.95
85.17	136.29
90.5	143.83

END

DATA F100_8f (T, AUrnTCOGTCOH)

4.58	15.54
5.05	18.22
6.05	24.58
8.08	33.76
10.07	41.25
12.08	47.80
14.31	54.36
16.05	59.99
18.05	63.23
20.03	68.23
22.08	73.90
43.33	110.18
45.58	112.61
47.58	113.70
49.17	115.14
53.58	118.20
61.33	122.07
67.33	124.30
70.58	125.29
74.58	126.29
77.25	127.48
83.25	128.07
84.25	128.31
85.17	128.49
90.5	129.56

END

PROCED MaleHiM

! Data from Fisher et al. (1998)

! M file created Tue 18 Nov 2003

! Malehi.m

! Last Modified: 22 Jan 2004

! Modified by: Deborah Keys

! 100ppm 4 hr inhalation blood: fish,mahle,abbas

! Male

Human

ResetDoses

SET BW=60.9, VFatC=0.10

SET Conc=101.1, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=300.0

START /NC

PLOT /DATA=male100_7a CTCOH

PLOT /DATA=male100_7b CBldTCA

PLOT /DATA=male100_7c AUrnTCA

PLOT /DATA=male100_7d AUrnTCOGTCOH

END

DATA Male100_7a (T, CTCOH)

0.5	0.28
1.0	0.76
2.0	1.92
3.0	1.69
4.0	2.34
4.3	2.34
4.5	2.16
5.0	2.13

6.0	1.95
8.0	1.61
10.0	1.33
12.0	1.58
14.0	0.84
16.0	0.77
18.0	0.57
20.03	0.76

END

DATA Male100_7b (T, CBldTCA)

0.5	0.36
1.0	0.84
2.0	1.73
3.0	2.6
4.0	3.42
4.3	3.9
4.5	3.67
5.0	4.47
6.0	5.0
8.0	5.95
10.0	6.74
12.0	7.12
14.0	7.75
16.0	8.22
18.0	8.17
20.03	9.01
49.75	10.66
73.8	8.6
95.24	7.46
264.0	3.13

END

DATA Male100_7c (T, AUrnTCA)

4.75	0.93
7.95	3.02
14.08	5.95
16.08	7.07
18.1	8.28
20.25	9.63
24.67	13.46
29.17	15.73
32.67	20.11
35.33	22.71
38.83	24.07
44.25	25.6
49.67	27.51
55.92	29.6
58.75	33.36
68.25	39.61
73.83	43.7
75.92	45.78
77.92	48.52
81.17	51.21
82.58	53.54
92.17	60.72

END

DATA Male100_7d (T, AUrnTCOGTCOH)

4.75	40.71
7.95	69.81
14.08	89.76
16.08	96.8
18.1	102.69
20.25	107.93
24.67	121.3
29.17	128.51
32.67	135.51
35.33	138.05
38.83	140.2
44.25	142.48
49.67	144.47
55.92	144.96
58.75	145.55
68.25	146.67
73.83	147.09
75.92	147.25
77.92	147.38
81.17	147.5
82.58	147.62
92.17	147.98

END

PROCED MaleLoM

! Data from Fisher et al. (1998)

! M file created Tue 18 Nov 2003

! Malelo.m

! Last Modified: 22 Jan 2004

! Modified by: Deborah Keys

! 100ppm 4 hr inhalation blood: fish,mahle,abbas

! Male

Human

ResetDoses

SET BW=82.7, VFatC=0.14

SET Conc=102.6, CC=.FALSE., TChng=4.0, Days=1.0, TMax=24.0, TStp=100.0

START /NC

PLOT /DATA=male100_3a CTCOH

PLOT /DATA=male100_3b CBldTCA

PLOT /DATA=male100_3c AUrnTCA

PLOT /DATA=male100_3d AUrnTCOGTCOH

END

DATA Male100_3a (T, CTCOH)

0.5	0.45
1.07	0.77
2.0	1.51
3.0	2.41
3.98	3.3
4.25	3.64
4.5	3.67
5.0	3.48
6.0	3.05

8.0	2.52
10.02	2.38
12.0	2.16
14.0	1.73
16.02	1.48
18.07	1.12
20.0	1.01
22.0	0.85

END

DATA Male100_3b (T, CBldTCA)

0.5	0.23
1.07	0.49
2.0	1.07
3.0	1.89
3.98	2.87
4.25	3.69
4.5	3.87
5.0	3.59
6.0	4.18
8.0	4.71
10.02	5.46
12.0	5.67
14.0	5.97
16.02	6.05
18.07	6.22
20.0	7.54
22.0	7.26
46.85	8.43
71.47	3.86
95.5	3.55

END

DATA Male100_3c (T, AUrnTCA)

3.03	0.488
4.75	0.961
6.7	2.09
8.25	2.96
10.17	5.56
12.08	7.17
14.19	8.37
15.58	9.09
17.6	9.7
18.23	10.13
19.58	10.99
20.05	11.24
21.33	11.88
22.17	12.36
23.2	13.03
35.42	14.18
40.67	16.14
46.67	18.07
47.17	19.06
52.33	20.35
55.25	23.68
68.17	24.71
69.75	27.02

END

DATA Male100_3d (T, AUrnTCOGTCOH)

3.03	32.7
4.75	60.26
6.7	97.98
8.25	130.67
10.17	182.9
12.08	204.64
14.19	224.53
15.58	233.79
17.6	240.99
18.23	245.36
19.58	253.46
20.05	255.9
21.33	261.17
22.17	265.4
23.2	269.76
35.42	271.64
40.67	276.15
46.67	277.54
47.17	277.83
52.33	278.12
55.25	278.81
68.17	278.88
69.75	279.07

END

SET CMD=5