```
# USEPA TCE MODEL VERSION 1.2.3.3
# Include non-detects for DCVG in blood
# Error variances at study level
# Priors for most uniformly distributed parameters
#       based on combined mouse and rat posteriors
# Removed unused individual-level parameters to increase
# computational speed as follows:
#       FISHER -- removed DCVC parameters
#       PAYCOK -- kept only physiological and TCA parameter
#       KIMMERLE, MONSTER, CHIU -- removed DCVG and DCVC parameters
#       MULLER -- kept only physiological, TCA, TCOH, and TCOG parameters
# Muller -- both studies use same parameters (grouped data anyway)

Integrate(Lsodes, 0.3e-5, 0.3e-5, 1);
MCMC ("TCE.1.2.3.3.Human.pop.example.out", "" , "", 250 , 0 , 5 , 250 , 1.23456);

Level { #Population level

# Population means
Distrib(        M_lnQCC TruncNormal     0.0     0.2     -0.8    0.8     );

Distrib(        M_lnVPRC        TruncNormal     0.0     0.2     -0.8    0.8     );

Distrib(        M_QFatC TruncNormal     1.0     0.46    0.08    1.92    );
Distrib(        M_QGutC TruncNormal     1.0     0.18    0.64    1.36    );
Distrib(        M_QLivC TruncNormal     1.0     0.45    0.1     1.9     );
Distrib(        M_QSlwC TruncNormal     1.0     0.32    0.36    1.64    );
Distrib(        M_lnDRespC      TruncNormal     0.61    1.43    -11.513 2.303   );
Distrib(        M_QKidC TruncNormal     1.0     0.12    0.76    1.24    );
Distrib(        M_FracPlasC     TruncNormal     1.0     0.05    0.85    1.15    );


Distrib(        M_VFatC TruncNormal     1.0     0.45    0.1     1.9     );
Distrib(        M_VGutC TruncNormal     1.0     0.08    0.84    1.16    );
Distrib(        M_VLivC TruncNormal     1.0     0.23    0.54    1.46    );
Distrib(        M_VRapC TruncNormal     1.0     0.08    0.84    1.16    );
Distrib(        M_VRespLumC     TruncNormal     1.0     0.2     0.6     1.4     );
Distrib(        M_VRespEffC     TruncNormal     1.0     0.2     0.6     1.4     );
Distrib(        M_VKidC TruncNormal     1.0     0.17    0.66    1.34    );
Distrib(        M_VBldC TruncNormal     1.0     0.12    0.76    1.24    );





Distrib(        M_lnPBC TruncNormal     0.0     0.2     -0.6    0.6     );
Distrib(        M_lnPFatC       TruncNormal     0.0     0.2     -0.6    0.6     );
Distrib(        M_lnPGutC       TruncNormal     0.0     0.4     -1.2    1.2     );
Distrib(        M_lnPLivC       TruncNormal     0.0     0.4     -1.2    1.2     );
Distrib(        M_lnPRapC       TruncNormal     0.0     0.4     -1.2    1.2     );
Distrib(        M_lnPRespC      TruncNormal     0.0     0.4     -1.2    1.2     );
Distrib(        M_lnPKidC       TruncNormal     0.0     0.2     -0.6    0.6     );
Distrib(        M_lnPSlwC       TruncNormal     0.0     0.3     -0.9    0.9     );


Distrib(        M_lnPRBCPlasTCAC        Uniform                 -4.605  4.605   );
Distrib(        M_lnPBodTCAC    TruncNormal     0.0     0.336   -1.008  1.008   );
Distrib(        M_lnPLivTCAC    TruncNormal     0.0     0.336   -1.008  1.008   );


Distrib(        M_lnkDissocC    TruncNormal     0.0     0.06    -0.18   0.18    );
Distrib(        M_lnBMaxkDC     TruncNormal     0.0     0.182   -0.546  0.546   );


Distrib(        M_lnPBodTCOHC   TruncNormal     0.0     0.336   -1.008  1.008   );
Distrib(        M_lnPLivTCOHC   TruncNormal     0.0     0.336   -1.008  1.008   );
Distrib(        M_lnPBodTCOGC   TruncNormal     -0.21   1.63    -4.605  4.605   );
Distrib(        M_lnPLivTCOGC   TruncNormal     1.07    1.46    -4.605  4.605   );
Distrib(        M_lnPeffDCVG    Uniform                 -6.908  6.908   );


####Distrib(    M_lnkTSD        Uniform                 -4.269  4.942   );
####Distrib(    M_lnkAS Uniform                 -6.571  7.244   );
####Distrib(    M_lnkTD Uniform                 -4.605  0       );
####Distrib(    M_lnkAD Uniform                 -7.195  6.62    );
Distrib(        M_lnkASTCA      Uniform                 -7.195  6.62    );
Distrib(        M_lnkASTCOH     Uniform                 -7.195  6.62    );


Distrib(        M_lnVMaxC       TruncNormal     0.0     0.693   -2.079  2.079   );
#Distrib(       M_lnKMC Normal                  0       1       );
Distrib(        M_lnClC TruncNormal     0.0     1.386   -4.158  4.158   );
Distrib(        M_lnFracOtherC  TruncNormal     -1.98   1.56    -6.908  6.908   );
Distrib(        M_lnFracTCAC    TruncNormal     0.0     1.163   -3.489  3.489   );
#Distrib(       M_lnVMaxDCVGC   Normal                  0       1       );
Distrib(        M_lnClDCVGC     TruncNormal     0.0     4.605   -13.815 13.815  );
Distrib(        M_lnKMDCVGC     TruncNormal     0.0     1.386   -4.158  4.158   );
#Distrib(       M_lnVMaxKidDCVGC        Normal                  0       1       );
Distrib(        M_lnClKidDCVGC  TruncNormal     0.0     4.605   -13.815 13.815  );
```

```
Distrib(        M_lnKMKidDCVGC  TruncNormal     0.0     1.386   -4.158  4.158   );
Distrib(        M_lnVMaxLungLivC        TruncNormal     1.03    1.55    -3.297  3.297   );
Distrib(        M_lnKMClara     TruncNormal     -3.93   1.58    -6.908  6.908   );
Distrib(        M_lnFracLungSysC        TruncNormal     1.13    2.09    -6.908  6.908   );


#Distrib(       M_lnVMaxTCOHC   Normal                  0       1       );
Distrib(        M_lnClTCOHC     TruncNormal     -1      1.49    -11.513 6.908   );
Distrib(        M_lnKMTCOH      TruncNormal     1.57    1.51    -9.21   9.21    );
#Distrib(       M_lnVMaxGlucC   Normal                  0       1       );
Distrib(        M_lnClGlucC     TruncNormal     1.22    1.47    -9.21   4.605   );
Distrib(        M_lnKMGluc      TruncNormal     2.41    1.52    -6.908  6.908   );
Distrib(        M_lnkMetTCOHC   TruncNormal     0.87    1.53    -11.513 6.908   );


Distrib(        M_lnkUrnTCAC    TruncNormal     -2.42   1.44    -4.605  4.605   );
Distrib(        M_lnkMetTCAC    TruncNormal     -0.8    1.45    -9.21   4.605   );


Distrib(        M_lnkBileC      TruncNormal     1.22    1.49    -9.21   4.605   );
Distrib(        M_lnkEHRC       TruncNormal     -1.51   1.55    -9.21   4.605   );
Distrib(        M_lnkUrnTCOGC   TruncNormal     2.78    1.57    -6.908  6.908   );


##Distrib(      M_lnFracKidDCVCC        Uniform                 -6.908  6.908   );
Distrib(        M_lnkDCVGC      Uniform                 -9.21   4.605   );


Distrib(        M_lnkNATC       TruncNormal     -6.12   1.81    -9.21   4.605   );
Distrib(        M_lnkKidBioactC TruncNormal     -5.12   1.87    -9.21   4.605   );


#### Population variance parameters

Distrib(        V_lnQCC InvGamma        2.25    0.05    );

Distrib(        V_lnVPRC        InvGamma        2.25    0.05    );

Distrib(        V_QFatC InvGamma        6       1.058   );
Distrib(        V_QGutC InvGamma        6       0.162   );
Distrib(        V_QLivC InvGamma        6       1.0125  );
Distrib(        V_QSlwC InvGamma        6       0.512   );
Distrib(        V_lnDRespC      InvGamma        6       0.2     );
Distrib(        V_QKidC InvGamma        6       0.072   );
Distrib(        V_FracPlasC     InvGamma        6       0.0125  );


Distrib(        V_VFatC InvGamma        6       1.0125  );
Distrib(        V_VGutC InvGamma        6       0.032   );
Distrib(        V_VLivC InvGamma        6       0.2645  );
Distrib(        V_VRapC InvGamma        6       0.032   );
Distrib(        V_VRespLumC     InvGamma        6       0.2     );
Distrib(        V_VRespEffC     InvGamma        6       0.2     );
Distrib(        V_VKidC InvGamma        6       0.1445  );
Distrib(        V_VBldC InvGamma        6       0.072   );





Distrib(        V_lnPBC InvGamma        11.00018        0.342256161     );
Distrib(        V_lnPFatC       InvGamma        3       0.08    );
Distrib(        V_lnPGutC       InvGamma        2.25    0.2     );
Distrib(        V_lnPLivC       InvGamma        2.5     0.24    );
Distrib(        V_lnPRapC       InvGamma        2.25    0.2     );
Distrib(        V_lnPRespC      InvGamma        2.25    0.2     );
Distrib(        V_lnPKidC       InvGamma        2.5     0.06    );
Distrib(        V_lnPSlwC       InvGamma        2.5     0.135   );


Distrib(        V_lnPRBCPlasTCAC        InvGamma        2.25    0.14112 );
Distrib(        V_lnPBodTCAC    InvGamma        2.25    0.14112 );
Distrib(        V_lnPLivTCAC    InvGamma        2.25    0.14112 );


Distrib(        V_lnkDissocC    InvGamma        2.25    0.0045  );
Distrib(        V_lnBMaxkDC     InvGamma        2.25    0.041405        );


Distrib(        V_lnPBodTCOHC   InvGamma        2.25    0.14112 );
Distrib(        V_lnPLivTCOHC   InvGamma        2.25    0.14112 );
Distrib(        V_lnPBodTCOGC   InvGamma        2.25    0.2     );
Distrib(        V_lnPLivTCOGC   InvGamma        2.25    0.2     );
Distrib(        V_lnPeffDCVG    InvGamma        2.25    0.2     );


####Distrib(    V_lnkTSD        InvGamma        2.25    5       );
####Distrib(    V_lnkAS InvGamma        2.25    5       );
####Distrib(    V_lnkTD InvGamma        2.25    5       );
```

```
####Distrib(    V_lnkAD InvGamma        2.25    5       );
Distrib(        V_lnkASTCA      InvGamma        2.25    5       );
Distrib(        V_lnkASTCOH     InvGamma        2.25    5       );


Distrib(        V_lnVMaxC       InvGamma        16.79289941     7.91721238      );
#Distrib(       V_lnKMC InvGamma        #DIV/0! #DIV/0! );
Distrib(        V_lnClC InvGamma        2.502992807     1.339103986     );
Distrib(        V_lnFracOtherC  InvGamma        2.25    0.3125  );
Distrib(        V_lnFracTCAC    InvGamma        2.25    4.05    );
#Distrib(       V_lnVMaxDCVGC   InvGamma        #DIV/0! #DIV/0! );
Distrib(        V_lnClDCVGC     InvGamma        2.25    0.3125  );
Distrib(        V_lnKMDCVGC     InvGamma        2.25    0.3125  );
#Distrib(       V_lnVMaxKidDCVGC        InvGamma        #DIV/0! #DIV/0! );
Distrib(        V_lnClKidDCVGC  InvGamma        2.25    0.3125  );
Distrib(        V_lnKMKidDCVGC  InvGamma        2.25    0.3125  );
Distrib(        V_lnVMaxLungLivC        InvGamma        2.25    0.3125  );
Distrib(        V_lnKMClara     InvGamma        2.25    0.3125  );
Distrib(        V_lnFracLungSysC        InvGamma        2.25    0.3125  );


#Distrib(       V_lnVMaxTCOHC   InvGamma        #DIV/0! #DIV/0! );
Distrib(        V_lnClTCOHC     InvGamma        2.25    0.3125  );
Distrib(        V_lnKMTCOH      InvGamma        2.25    0.3125  );
#Distrib(       V_lnVMaxGlucC   InvGamma        #DIV/0! #DIV/0! );
Distrib(        V_lnClGlucC     InvGamma        2.25    0.3125  );
Distrib(        V_lnKMGluc      InvGamma        2.25    0.3125  );
Distrib(        V_lnkMetTCOHC   InvGamma        2.25    0.3125  );


Distrib(        V_lnkUrnTCAC    InvGamma        2.25    0.3125  );
Distrib(        V_lnkMetTCAC    InvGamma        2.25    0.3125  );


Distrib(        V_lnkBileC      InvGamma        2.25    0.3125  );
Distrib(        V_lnkEHRC       InvGamma        2.25    0.3125  );
Distrib(        V_lnkUrnTCOGC   InvGamma        2.25    0.3125  );


##Distrib(      V_lnFracKidDCVCC        InvGamma        2.25    0.3125  );
Distrib(        V_lnkDCVGC      InvGamma        2.25    0.3125  );


Distrib(        V_lnkNATC       InvGamma        2.25    0.3125  );
Distrib(        V_lnkKidBioactC InvGamma        2.25    0.3125  );

Level { # Study Level

#Error distributions

        Distrib( Ve_RetDose , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CAlv , LogUniform , 0.01 , 3.3 );
        Distrib( Ve_CAlvPPM , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CInhPPM , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CInh , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CMixExh , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CArt , LogUniform , 0.01 , 3.3 );
        Distrib( Ve_CVen , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CBldMix , LogUniform , 0.01 , 3.3 );
#
#       Distrib( Ve_CFat , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CGut , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CRap , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CSlw , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CHrt , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CKid , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CLiv , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CLung , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CMus , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CSpl , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CBrn , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_zAExh , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_zAExhpost , LogUniform , 0.01 , 3.3 );
#
#
        Distrib( Ve_CTCOH , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CKidTCOH , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CLivTCOH , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CLungTCOH , LogUniform , 0.01 , 3.3 );
#
#
        Distrib( Ve_CPlasTCA , LogUniform , 0.01 , 3.3 );
        Distrib( Ve_CBldTCA , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CBodTCA , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CKidTCA , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CLivTCA , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CLungTCA , LogUniform , 0.01 , 3.3 );
        Distrib( Ve_zAUrnTCA , LogUniform , 0.01 , 3.3 );
        Distrib( Ve_zAUrnTCA_collect , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_zAUrnTCA_sat , LogUniform , 0.01 , 3.3 );
```

```
#
#
#       Distrib( Ve_zABileTCOG , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CTCOG , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CTCOGTCOH , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CKidTCOGTCOH , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CLivTCOGTCOH , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CLungTCOGTCOH , LogUniform , 0.01 , 3.3 );
        Distrib( Ve_AUrnTCOGTCOH , LogUniform , 0.01 , 3.3 );
        Distrib( Ve_AUrnTCOGTCOH_collect , LogUniform , 0.01 , 3.3 );
#
#       Distrib( Ve_AUrnTCOGTCOH_sat , LogUniform , 0.01 , 3.3 );
#
#
        Distrib( Ve_CDCVGmol , LogUniform , 0.01 , 3.3 );
        Distrib( Ve_zAUrnNDCVC , LogUniform , 0.01 , 3.3 );
        Distrib( Ve_AUrnTCTotMole , LogUniform , 0.01 , 3.3 );
        Distrib( Ve_TotCTCOH , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_QPsamp , LogUniform , 0.01 , 3.3 );

#Likelihoods

        Likelihood( RetDose , LogNormal_v , Prediction( RetDose ) , Ve_RetDose );
#       Likelihood( CAlv , LogNormal_v , Prediction( CAlv ) , Ve_CAlv );
        Likelihood( CAlvPPM , LogNormal_v , Prediction( CAlvPPM ) , Ve_CAlvPPM );
#       Likelihood( CInhPPM , LogNormal_v , Prediction( CInhPPM ) , Ve_CInhPPM );
#       Likelihood( CInh , LogNormal_v , Prediction( CInh ) , Ve_CInh );
#       Likelihood( CMixExh , LogNormal_v , Prediction( CMixExh ) , Ve_CMixExh );
#       Likelihood( CArt , LogNormal_v , Prediction( CArt ) , Ve_CArt );
        Likelihood( CVen , LogNormal_v , Prediction( CVen ) , Ve_CVen );
#       Likelihood( CBldMix , LogNormal_v , Prediction( CBldMix ) , Ve_CBldMix );
#
#       Likelihood( CFat , LogNormal_v , Prediction( CFat ) , Ve_CFat );
#       Likelihood( CGut , LogNormal_v , Prediction( CGut ) , Ve_CGut );
#       Likelihood( CRap , LogNormal_v , Prediction( CRap ) , Ve_CRap );
#       Likelihood( CSlw , LogNormal_v , Prediction( CSlw ) , Ve_CSlw );
#       Likelihood( CHrt , LogNormal_v , Prediction( CHrt ) , Ve_CHrt );
#       Likelihood( CKid , LogNormal_v , Prediction( CKid ) , Ve_CKid );
#       Likelihood( CLiv , LogNormal_v , Prediction( CLiv ) , Ve_CLiv );
#       Likelihood( CLung , LogNormal_v , Prediction( CLung ) , Ve_CLung );
#       Likelihood( CMus , LogNormal_v , Prediction( CMus ) , Ve_CMus );
#       Likelihood( CSpl , LogNormal_v , Prediction( CSpl ) , Ve_CSpl );
#       Likelihood( CBrn , LogNormal_v , Prediction( CBrn ) , Ve_CBrn );
#       Likelihood( zAExh , LogNormal_v , Prediction( zAExh ) , Ve_zAExh );
#       Likelihood( zAExhpost , LogNormal_v , Prediction( zAExhpost ) , Ve_zAExhpost );
#
#
        Likelihood( CTCOH , LogNormal_v , Prediction( CTCOH ) , Ve_CTCOH );
#       Likelihood( CKidTCOH , LogNormal_v , Prediction( CKidTCOH ) , Ve_CKidTCOH );
#       Likelihood( CLivTCOH , LogNormal_v , Prediction( CLivTCOH ) , Ve_CLivTCOH );
#       Likelihood( CLungTCOH , LogNormal_v , Prediction( CLungTCOH ) , Ve_CLungTCOH );
#
#
        Likelihood( CPlasTCA , LogNormal_v , Prediction( CPlasTCA ) , Ve_CPlasTCA );
        Likelihood( CBldTCA , LogNormal_v , Prediction( CBldTCA ) , Ve_CBldTCA );
#       Likelihood( CBodTCA , LogNormal_v , Prediction( CBodTCA ) , Ve_CBodTCA );
#       Likelihood( CKidTCA , LogNormal_v , Prediction( CKidTCA ) , Ve_CKidTCA );
#       Likelihood( CLivTCA , LogNormal_v , Prediction( CLivTCA ) , Ve_CLivTCA );
#       Likelihood( CLungTCA , LogNormal_v , Prediction( CLungTCA ) , Ve_CLungTCA );
        Likelihood( zAUrnTCA , LogNormal_v , Prediction( zAUrnTCA ) , Ve_zAUrnTCA );
        Likelihood( zAUrnTCA_collect , LogNormal_v , Prediction( zAUrnTCA_collect ) , Ve_zAUrnTCA_collect );
#       Likelihood( zAUrnTCA_sat , LogNormal_v , Prediction( zAUrnTCA_sat ) , Ve_zAUrnTCA_sat );
#
#
#       Likelihood( zABileTCOG , LogNormal_v , Prediction( zABileTCOG ) , Ve_zABileTCOG );
#       Likelihood( CTCOG , LogNormal_v , Prediction( CTCOG ) , Ve_CTCOG );
#       Likelihood( CTCOGTCOH , LogNormal_v , Prediction( CTCOGTCOH ) , Ve_CTCOGTCOH );
#       Likelihood( CKidTCOGTCOH , LogNormal_v , Prediction( CKidTCOGTCOH ) , Ve_CKidTCOGTCOH );
#       Likelihood( CLivTCOGTCOH , LogNormal_v , Prediction( CLivTCOGTCOH ) , Ve_CLivTCOGTCOH );
#       Likelihood( CLungTCOGTCOH , LogNormal_v , Prediction( CLungTCOGTCOH ) , Ve_CLungTCOGTCOH );
        Likelihood( AUrnTCOGTCOH , LogNormal_v , Prediction( AUrnTCOGTCOH ) , Ve_AUrnTCOGTCOH );
        Likelihood( AUrnTCOGTCOH_collect , LogNormal_v , Prediction( AUrnTCOGTCOH_collect ) , Ve_AUrnTCOGTCOH_collect );
#
#       Likelihood( AUrnTCOGTCOH_sat , LogNormal_v , Prediction( AUrnTCOGTCOH_sat ) , Ve_AUrnTCOGTCOH_sat );
#
#
        Likelihood( CDCVGmol , LogNormal_v , Prediction( CDCVGmol ) , Ve_CDCVGmol );
        Likelihood( zAUrnNDCVC , LogNormal_v , Prediction( zAUrnNDCVC ) , Ve_zAUrnNDCVC );
        Likelihood( AUrnTCTotMole , LogNormal_v , Prediction( AUrnTCTotMole ) , Ve_AUrnTCTotMole );
        Likelihood( TotCTCOH , LogNormal_v , Prediction( TotCTCOH ) , Ve_TotCTCOH );
#       Likelihood( QPsamp , LogNormal_v , Prediction( QPsamp ) , Ve_QPsamp );
        Likelihood( CDCVG_ND , Poisson , Prediction( CDCVG_ND ) );
#### For non-detects, LD = 5e-5 mM, where LD is the detection limit.
#### Code calculates -lnlikelihood, so poisson(0,lambda) gives
#### likelihood

Species = 1;
lnFracKidDCVCC = 10; # All kidney GSH conjugation is locally processed

################### BEGIN Individual Data ########################
```

```
############# BEGIN FISHER et al. 1998 individual data ######
Level { #Subject level
### FOR FISHER, NO DCVC

Distrib(        lnQCC   TruncNormal_v   M_lnQCC V_lnQCC -0.8    0.8     );

Distrib(        lnVPRC  TruncNormal_v   M_lnVPRC        V_lnVPRC        -0.8    0.8     );

Distrib(        QFatC   TruncNormal_v   M_QFatC V_QFatC 0.08    1.92    );
Distrib(        QGutC   TruncNormal_v   M_QGutC V_QGutC 0.64    1.36    );
Distrib(        QLivC   TruncNormal_v   M_QLivC V_QLivC 0.1     1.9     );
Distrib(        QSlwC   TruncNormal_v   M_QSlwC V_QSlwC 0.36    1.64    );
Distrib(        lnDRespC        TruncNormal_v   M_lnDRespC      V_lnDRespC      -11.513 2.303   );
Distrib(        QKidC   TruncNormal_v   M_QKidC V_QKidC 0.76    1.24    );
Distrib(        FracPlasC       TruncNormal_v   M_FracPlasC     V_FracPlasC     0.85    1.15    );


Distrib(        VFatC   TruncNormal_v   M_VFatC V_VFatC 0.1     1.9     );
Distrib(        VGutC   TruncNormal_v   M_VGutC V_VGutC 0.84    1.16    );
Distrib(        VLivC   TruncNormal_v   M_VLivC V_VLivC 0.54    1.46    );
Distrib(        VRapC   TruncNormal_v   M_VRapC V_VRapC 0.84    1.16    );
Distrib(        VRespLumC       TruncNormal_v   M_VRespLumC     V_VRespLumC     0.6     1.4     );
Distrib(        VRespEffC       TruncNormal_v   M_VRespEffC     V_VRespEffC     0.6     1.4     );
Distrib(        VKidC   TruncNormal_v   M_VKidC V_VKidC 0.66    1.34    );
Distrib(        VBldC   TruncNormal_v   M_VBldC V_VBldC 0.76    1.24    );





Distrib(        lnPBC   TruncNormal_v   M_lnPBC V_lnPBC -0.6    0.6     );
Distrib(        lnPFatC TruncNormal_v   M_lnPFatC       V_lnPFatC       -0.6    0.6     );
Distrib(        lnPGutC TruncNormal_v   M_lnPGutC       V_lnPGutC       -1.2    1.2     );
Distrib(        lnPLivC TruncNormal_v   M_lnPLivC       V_lnPLivC       -1.2    1.2     );
Distrib(        lnPRapC TruncNormal_v   M_lnPRapC       V_lnPRapC       -1.2    1.2     );
Distrib(        lnPRespC        TruncNormal_v   M_lnPRespC      V_lnPRespC      -1.2    1.2     );
Distrib(        lnPKidC TruncNormal_v   M_lnPKidC       V_lnPKidC       -0.6    0.6     );
Distrib(        lnPSlwC TruncNormal_v   M_lnPSlwC       V_lnPSlwC       -0.9    0.9     );


Distrib(        lnPRBCPlasTCAC  TruncNormal_v   M_lnPRBCPlasTCAC        V_lnPRBCPlasTCAC        -4.605  4.605   );
Distrib(        lnPBodTCAC      TruncNormal_v   M_lnPBodTCAC    V_lnPBodTCAC    -1.008  1.008   );
Distrib(        lnPLivTCAC      TruncNormal_v   M_lnPLivTCAC    V_lnPLivTCAC    -1.008  1.008   );


Distrib(        lnkDissocC      TruncNormal_v   M_lnkDissocC    V_lnkDissocC    -0.18   0.18    );
Distrib(        lnBMaxkDC       TruncNormal_v   M_lnBMaxkDC     V_lnBMaxkDC     -0.546  0.546   );


Distrib(        lnPBodTCOHC     TruncNormal_v   M_lnPBodTCOHC   V_lnPBodTCOHC   -1.008  1.008   );
Distrib(        lnPLivTCOHC     TruncNormal_v   M_lnPLivTCOHC   V_lnPLivTCOHC   -1.008  1.008   );
Distrib(        lnPBodTCOGC     TruncNormal_v   M_lnPBodTCOGC   V_lnPBodTCOGC   -4.605  4.605   );
Distrib(        lnPLivTCOGC     TruncNormal_v   M_lnPLivTCOGC   V_lnPLivTCOGC   -4.605  4.605   );
Distrib(        lnPeffDCVG      TruncNormal_v   M_lnPeffDCVG    V_lnPeffDCVG    -6.908  6.908   );


####Distrib(     lnkTSD  TruncNormal_v   M_lnkTSD        V_lnkTSD        -4.269  4.942   );
####Distrib(     lnkAS   TruncNormal_v   M_lnkAS V_lnkAS -6.571  7.244   );
####Distrib(     lnkTD   TruncNormal_v   M_lnkTD V_lnkTD -4.605  0       );
####Distrib(     lnkAD   TruncNormal_v   M_lnkAD V_lnkAD -7.195  6.62    );
####Distrib(     lnkASTCA        TruncNormal_v   M_lnkASTCA      V_lnkASTCA      -7.195  6.62    );
####Distrib(     lnkASTCOH       TruncNormal_v   M_lnkASTCOH     V_lnkASTCOH     -7.195  6.62    );


Distrib(        lnVMaxC TruncNormal_v   M_lnVMaxC       V_lnVMaxC       -2.079  2.079   );
#Distrib(       lnKMC   TruncNormal_v   M_lnKMC V_lnKMC 0       1       );
Distrib(        lnClC   TruncNormal_v   M_lnClC V_lnClC -4.158  4.158   );
Distrib(        lnFracOtherC    TruncNormal_v   M_lnFracOtherC  V_lnFracOtherC  -6.908  6.908   );
Distrib(        lnFracTCAC      TruncNormal_v   M_lnFracTCAC    V_lnFracTCAC    -3.489  3.489   );
#Distrib(       lnVMaxDCVGC     TruncNormal_v   M_lnVMaxDCVGC   V_lnVMaxDCVGC   0       1       );
Distrib(        lnClDCVGC       TruncNormal_v   M_lnClDCVGC     V_lnClDCVGC     -13.815 13.815  );
Distrib(        lnKMDCVGC       TruncNormal_v   M_lnKMDCVGC     V_lnKMDCVGC     -4.158  4.158   );
#Distrib(       lnVMaxKidDCVGC  TruncNormal_v   M_lnVMaxKidDCVGC        V_lnVMaxKidDCVGC        0       1       );
Distrib(        lnClKidDCVGC    TruncNormal_v   M_lnClKidDCVGC  V_lnClKidDCVGC  -13.815 13.815  );
Distrib(        lnKMKidDCVGC    TruncNormal_v   M_lnKMKidDCVGC  V_lnKMKidDCVGC  -4.158  4.158   );
Distrib(        lnVMaxLungLivC  TruncNormal_v   M_lnVMaxLungLivC        V_lnVMaxLungLivC        -3.297  3.297   );
Distrib(        lnKMClara       TruncNormal_v   M_lnKMClara     V_lnKMClara     -6.908  6.908   );
Distrib(        lnFracLungSysC  TruncNormal_v   M_lnFracLungSysC        V_lnFracLungSysC        -6.908  6.908   );


#Distrib(       lnVMaxTCOHC     TruncNormal_v   M_lnVMaxTCOHC   V_lnVMaxTCOHC   0       1       );
Distrib(        lnClTCOHC       TruncNormal_v   M_lnClTCOHC     V_lnClTCOHC     -11.513 6.908   );
Distrib(        lnKMTCOH        TruncNormal_v   M_lnKMTCOH      V_lnKMTCOH      -9.21   9.21    );
#Distrib(       lnVMaxGlucC     TruncNormal_v   M_lnVMaxGlucC   V_lnVMaxGlucC   0       1       );
Distrib(        lnClGlucC       TruncNormal_v   M_lnClGlucC     V_lnClGlucC     -9.21   4.605   );
Distrib(        lnKMGluc        TruncNormal_v   M_lnKMGluc      V_lnKMGluc      -6.908  6.908   );
Distrib(        lnkMetTCOHC     TruncNormal_v   M_lnkMetTCOHC   V_lnkMetTCOHC   -11.513 6.908   );
```

```
Distrib(        lnkUrnTCAC      TruncNormal_v   M_lnkUrnTCAC    V_lnkUrnTCAC    -4.605  4.605   );
Distrib(        lnkMetTCAC      TruncNormal_v   M_lnkMetTCAC    V_lnkMetTCAC    -9.21   4.605   );


Distrib(        lnkBileC        TruncNormal_v   M_lnkBileC      V_lnkBileC      -9.21   4.605   );
Distrib(        lnkEHRC TruncNormal_v   M_lnkEHRC       V_lnkEHRC       -9.21   4.605   );
Distrib(        lnkUrnTCOGC     TruncNormal_v   M_lnkUrnTCOGC   V_lnkUrnTCOGC   -6.908  6.908   );


##Distrib(      lnFracKidDCVCC  TruncNormal_v   M_lnFracKidDCVCC        V_lnFracKidDCVCC        -6.908  6.908   );
Distrib(        lnkDCVGC        TruncNormal_v   M_lnkDCVGC      V_lnkDCVGC      -9.21   4.605   );


####Distrib(    lnkNATC TruncNormal_v   M_lnkNATC       V_lnkNATC       -9.21   4.605   );
####Distrib(    lnkKidBioactC   TruncNormal_v   M_lnkKidBioactC V_lnkKidBioactC -9.21   4.605   );

Level { # Fisher et al. 1998 Male subject 1

 Experiment { # 1
         #Subject=13;
 # 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
 # Male vol 1
# lnBW=4.27; VFatC=0.79; lnPB=2.44;
 BWmeas = 71.4;
 VFatCmeas = 0.17;
 PBmeas = 11.49;

# CC= 0;
 Conc=NDoses(2, 105.5 0, 0.0 4.0);

 # M100_1a (T, CVen)
 Print (CVen, 0.52, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16, 18);
 Data (CVen, 1.98, 2.69, 3.38, 3.76, 3.95, 3.26, 2.54, 1.12, 0.72, 0.52, 0.31, 0.28, 0.23, 0.17, 0.15);
 # M100_1b (T, CTCOH)
 Print (CTCOH, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16, 18, 20.03);
 Data (CTCOH, 0.39, 1.3, 2.18, 2.83, 2.94, 3.21, 2.78, 2.84, 2.52, 2.03, 1.56, 1.56, 1.31, 1.21, 1.15);
 # M100_1c (T, CBldTCA)
 Print (CBldTCA, 0.52, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16, 18, 20.03, 22.02, 45.83, 69.74, 93.75);
 Data (CBldTCA, 0.15, 0.5, 1.07, 2.11, 3.12, 2.87, 3.39, 4, 4.09, 4.76, 5.52, 6.16, 6.48, 8.12, 7.18, 8.56, 8.14, 9.3, 7.37,
 # M100_1d (T, AUrnTCA),
 Print (zAUrnTCA, 4.5, 6.1, 8, 10.1, 11.4, 12.1, 14.1, 16, 18, 20.23, 21.97, 26, 31.5, 34.25, 35.5, 36.75, 44.75, 52, 54.5,
 Data (zAUrnTCA, 1.47, 2.82, 5.02, 7.1, 8.87, 10.22, 12.67, 15.33, 16.85, 22.83, 25.23, 30.03, 33.1, 39.59, 42.21, 48.47, 52
 # M100_1e (T, AUrnTCOGTCOH),
 Print (AUrnTCOGTCOH, 4.5, 6.1, 8, 10.1, 11.4, 12.1, 14.1, 16, 18, 20.23, 21.97, 26, 31.5, 34.25, 35.5, 36.75, 44.75, 52, 54
 Data (AUrnTCOGTCOH, 13.94, 23.22, 30.95, 37.58, 43.49, 46.17, 50.32, 56.69, 61.37, 65.35, 68.94, 74.63, 79.76, 82.89, 84.29
# Total = Free in Fisher data
 Print (TotCTCOH, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16, 18, 20.03);
 Data (TotCTCOH, 0.39, 1.3, 2.18, 2.83, 2.94, 3.21, 2.78, 2.84, 2.52, 2.03, 1.56, 1.56, 1.31, 1.21, 1.15);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
#
Print(CDCVGmol, 0.579   1.01    2       3       4.02    4.24    4.5     5.01    6.02    8.01);
Data(CDCVGmol, 0.00886  0.0349  0.0461  0.0337  0.0313  0.0241  0.0132  0.00552 0.00417 0.000671);
Print(CDCVGmol0, 12);      # No detect at 12 hr in males
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 12);      # No detect at 12 hr in males
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };
```

```
}

Level { # Fisher et al. 1998 Male subject 2

 Experiment { # 2
         #Subject=14;
 # 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
 # Male vol #2
# lnBW=4.24; VFatC=1.3; lnPB=2.31;
# CC= 0;
 BWmeas = 69.3;
 VFatCmeas = 0.27;
 PBmeas = 10.1;

 Conc=NDoses(2, 49.3 0, 0.0 4.0);
 # M50_2a (T, CVen),
 Print (CVen, 0.5, 1, 2, 3, 4, 4.25, 4.5);
 Data (CVen, 0.61, 0.74, 1.11, 1.01, 1.05, 0.81, 0.46);
 # M50_2b (T, CTCOH),
 Print (CTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 14, 16, 18, 20);
 Data (CTCOH, 0.44, 0.55, 0.83, 1.08, 1.35, 1.26, 1.34, 1.11, 1.01, 0.9, 0.76, 0.66, 0.63, 0.56, 0.51);
 # M50_2c (T, CBldTCA),
 Print (CBldTCA, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16, 18, 20, 22, 49.08, 71.72, 97.47);
 Data (CBldTCA, 0.29, 0.65, 1.47, 2.27, 2.91, 2.99, 3.12, 3.49, 3.66, 4.29, 4.69, 5.11, 5.17, 5.26, 5.66, 5.18, 5.69, 6.67,
 # M50_2d (T, AUrnTCA),
 Print (zAUrnTCA, 4.55, 5.08, 6.06, 8.08, 10.06, 12.08, 14.08, 16.08, 18.08, 20.08, 22.17, 31.33, 49, 64.33, 77, 86.25);
 Data (zAUrnTCA, 0.041, 0.062, 0.15, 0.26, 0.41, 0.53, 0.65, 0.8, 0.92, 1.05, 1.18, 1.46, 2.2, 3.61, 4.36, 5.03);
 # M50_2e (T, AUrnTCOGTCOH),
 Print (AUrnTCOGTCOH, 4.55, 5.08, 6.06, 8.08, 10.06, 12.08, 14.08, 16.08, 18.08, 20.08, 22.17, 31.33, 49, 64.33, 77, 86.25);
 Data (AUrnTCOGTCOH, 8.45, 15.2, 21.6, 28.09, 35.67, 39.98, 43.78, 47.68, 50.54, 53.03, 55.3, 60.62, 69.8, 73.15, 74.82, 76.
# Total = Free in Fisher data
 Print (TotCTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 14, 16, 18, 20);
 Data (TotCTCOH, 0.44, 0.55, 0.83, 1.08, 1.35, 1.26, 1.34, 1.11, 1.01, 0.9, 0.76, 0.66, 0.63, 0.56, 0.51);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

Print(CDCVGmol, 0);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 0);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}

Level { # Fisher et al. 1998 Male subject 3

 Experiment { # 3 ## Low exposure
         #Subject=15;
 # 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
 # Male vol 3
# lnBW=4.26; VFatC=0.654; lnPB=2.41;
# CC= 0;
 BWmeas = 71.1;
 VFatCmeas = 0.14;
 PBmeas = 11.1;

 Conc=NDoses(2, 55.2 0, 0.0 4.0);
```

```
 # M60a (T, CVen),
 Print (CVen, 0.58, 0.98, 2.02, 3.02, 4.02, 4.25, 4.44, 5.02, 5.83, 8);
 Data (CVen, 1.89, 1.36, 2.68, 2.67, 2.79, 2.42, 1.52, 0.82, 0.37, 0.29);
 # M60b (T, CTCOH),
 Print (CTCOH, 0.58, 0.98, 2.02, 3.02, 4.02, 4.25, 4.44, 5.02, 5.83, 8, 10, 12, 14.17, 16.02, 18.02, 20);
 Data (CTCOH, 0.63, 1.07, 1.57, 1.9, 1.94, 2.02, 2.26, 1.02, 0.96, 1.65, 1.38, 1.26, 1.13, 1.03, 1.05, 0.9);
 # M60c (T, CBldTCA),
 Print (CBldTCA, 0.58, 0.98, 2.02, 3.02, 4.02, 4.25, 4.44, 5.02, 5.83, 8, 10, 12, 14.17, 16.02, 18.02, 20, 22, 44.83, 68.72,
 Data (CBldTCA, 0.43, 0.55, 1.07, 1.57, 1.96, 2.01, 2.19, 2.28, 2.52, 2.92, 3.2, 3.56, 4.19, 3.9, 4.95, 5.04, 5.08, 5.51, 9.
 # M60d (T, AUrnTCA),
 Print (zAUrnTCA, 0.5, 3.12, 4.63, 5.45, 6.45, 8.13, 10.17, 12.15, 14.27, 16.13, 18.15, 20.2, 22.22, 24.22, 32.85, 34.22, 39
 Data (zAUrnTCA, 0.002, 0.082, 0.184, 0.249, 0.307, 0.539, 0.852, 1.35, 1.78, 2.12, 2.48, 2.89, 3.48, 4.28, 5.35, 5.66, 6.72
 # M60e (T, AUrnTCOGTCOH),
 Print (AUrnTCOGTCOH, 3.12, 4.63, 5.45, 6.45, 8.13, 10.17, 12.15, 14.27, 16.13, 18.15, 20.2, 22.22, 24.22, 32.85, 34.22, 39.
 Data (AUrnTCOGTCOH, 8.24, 11.6, 13.64, 15.64, 19.73, 23.26, 28.95, 28.95, 29.79, 32.07, 34.21, 38.49, 43.06, 47.48, 48.6, 5
# Total = Free in Fisher data
 Print (TotCTCOH, 0.58, 0.98, 2.02, 3.02, 4.02, 4.25, 4.44, 5.02, 5.83, 8, 10, 12, 14.17, 16.02, 18.02, 20);
 Data (TotCTCOH, 0.63, 1.07, 1.57, 1.9, 1.94, 2.02, 2.26, 1.02, 0.96, 1.65, 1.38, 1.26, 1.13, 1.03, 1.05, 0.9);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

Print(CDCVGmol, 0);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 0);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };


 Experiment { # 4 ## High exposure
         #Subject=15; # 16
 # 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
 # Male vol 3
# lnBW=4.26; VFatC=0.654; lnPB=2.41;
# CC= 0;
 BWmeas = 71.1;
 VFatCmeas = 0.14;
 PBmeas = 11.1;

 Conc=NDoses(2, 101.5 0, 0.0 4.0);

 # M100_4a (T, CVen)
 Print (CVen, 0.5, 1, 2, 3, 4.02, 4.25, 4.5, 5);
 Data (CVen, 3.1, 3.76, 3.46, 3.83, 3.78, 2.9, 2.11, 1.09);
 # M100_4b (T, CTCOH)
 Print (CTCOH, 0.5, 1, 2, 3, 4.02, 4.25, 4.5, 5, 6, 8, 10, 12.05, 14, 16, 18, 20, 22.05);
 Data (CTCOH, 0.56, 1.12, 1.75, 2.55, 3.48, 3.73, 3.52, 3.78, 3.79, 3.3, 2.96, 2.71, 2.38, 2.04, 1.89, 1.57, 1.4);
 # M100_4c (T, CBldTCA)
 Print (CBldTCA, 0.5, 1, 2, 3, 4.02, 4.25, 4.5, 5, 6, 8, 10, 12.05, 14, 16, 18, 20, 22.05, 50.52, 74.03, 98.58);
 Data (CBldTCA, 0.3, 0.75, 1.42, 2.34, 3.01, 2.58, 3.1, 3.26, 4.21, 4.99, 5.46, 5.74, 6.69, 6.85, 7.14, 9.85, 9.32, 8.87, 8.
 # M100_4d (T, zAUrnTCA),
 Print (zAUrnTCA, 4.35, 5.03, 6.07, 8.07, 10.04, 12.07, 14.06, 16.03, 18.02, 20.04, 22.13, 25.5, 36.5, 44.1, 47, 54, 61.45,
 Data (zAUrnTCA, 0.98, 1.21, 1.42, 2.05, 3.12, 3.6, 4.09, 4.57, 4.86, 5.28, 5.98, 8.14, 8.94, 10.97, 11.58, 13.48, 15.33, 17
 # M100_4e (T, AUrnTCOGTCOH),
 Print (AUrnTCOGTCOH, 4.35, 5.03, 6.07, 8.07, 10.04, 12.07, 14.06, 16.03, 18.02, 20.04, 22.13, 25.5, 36.5, 44.1, 47, 54, 61.
 Data (AUrnTCOGTCOH, 28.92, 31.85, 40.01, 56.31, 68.48, 78.8, 89.82, 98.66, 105.25, 112.29, 122.73, 141.62, 150.29, 162.32,
# Total = Free in Fisher data
 Print (TotCTCOH, 0.5, 1, 2, 3, 4.02, 4.25, 4.5, 5, 6, 8, 10, 12.05, 14, 16, 18, 20, 22.05);
 Data (TotCTCOH, 0.56, 1.12, 1.75, 2.55, 3.48, 3.73, 3.52, 3.78, 3.79, 3.3, 2.96, 2.71, 2.38, 2.04, 1.89, 1.57, 1.4);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
```

```
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
#
Print(CDCVGmol, 0.579   1.01    2       3       4.02    4.24    4.5     5.01    6.02    8.01);
Data(CDCVGmol, 0.00886  0.0349  0.0461  0.0337  0.0313  0.0241  0.0132  0.00552 0.00417 0.000671);
Print(CDCVGmol0, 12);      # No detect at 12 hr in males
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 12);      # No detect at 12 hr in males
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}


Level { # Fisher et al. 1998 Male subject 4

 Experiment { # 5 ## Low exposure
         #Subject=16; # 17
 # 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
 # Male vol 4
# lnBW=3.96; VFatC=0.467; lnPB=2.49;
# CC= 0;

 BWmeas = 52.3;
 VFatCmeas = 0.1;
 PBmeas = 12.1;

 Conc=NDoses(2, 53.1 0, 0.0 4.0);
 # M50_1a (T, CVen)
 Print (CVen, 0.5, 1, 2.03, 3, 4.02, 4.25, 4.5, 5.02, 6.02, 8.08, 10);
 Data (CVen, 0.67, 1.37, 1.96, 1.92, 2.08, 1.13, 0.76, 0.42, 0.3, 0.21, 0.15);
 # M50_1b (T, CTCOH)
 Print (CTCOH, 1, 2.03, 3, 4.02, 4.25, 4.5, 5.02, 6.02, 8.08, 10, 12, 14, 16, 18, 20, 22);
 Data (CTCOH, 0.43, 1.2, 1.26, 1.69, 1.66, 1.6, 1.58, 1.51, 1.44, 1.52, 1.14, 1.05, 1.04, 1.06, 0.45, 0.75);
 # M50_1c (T, CBldTCA)
 Print (CBldTCA, 1, 2.03, 3, 4.02, 4.25, 4.5, 5.02, 6.02, 8.08, 10, 12, 14, 16, 18, 20, 22, 44.78, 68.72, 100.4);
 Data (CBldTCA, 0.29, 0.77, 1.33, 1.84, 1.93, 2.07, 2.27, 2.94, 3.58, 3.72, 3.98, 4.4, 4.58, 4.86, 5.73, 4.22, 5, 4.72, 4.47
 # M50_1d (T, AUrnTCA)
 Print (zAUrnTCA, 5.25, 5.97, 8, 10.17, 12.17, 14.17, 16.17, 18.17, 20.17, 22.17, 25, 29.83, 37.83, 44.83, 45.67, 49.67, 53.
 Data (zAUrnTCA, 1, 1.53, 3.34, 6.01, 7.6, 13.02, 14.83, 16.67, 18.69, 21.3, 21.95, 26.24, 31.79, 40.44, 40.86, 42.64, 42.94
 # M50_1e (T, AUrnTCOGTCOH),
 Print (AUrnTCOGTCOH, 5.25, 5.97, 8, 10.17, 12.17, 14.17, 16.17, 18.17, 20.17, 22.17, 25, 29.83, 37.83, 44.83, 45.67, 49.67,
 Data (AUrnTCOGTCOH, 5.26, 8.23, 13.05, 16.3, 19.05, 24.62, 26.97, 29.06, 30.62, 32.53, 33.35, 35.43, 37.99, 38.21, 39.06, 3
# Total = Free in Fisher data
 Print (TotCTCOH, 1, 2.03, 3, 4.02, 4.25, 4.5, 5.02, 6.02, 8.08, 10, 12, 14, 16, 18, 20, 22);
 Data (TotCTCOH, 0.43, 1.2, 1.26, 1.69, 1.66, 1.6, 1.58, 1.51, 1.44, 1.52, 1.14, 1.05, 1.04, 1.06, 0.45, 0.75);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

Print(CDCVGmol, 0);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 0);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
```

```
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };



 Experiment { # 6 ## High exposure
         #Subject=16; # 18
 # 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
 # Male vol 4
# lnBW=3.96; VFatC=0.467; lnPB=2.49;
# CC= 0;

 BWmeas = 52.3;
 VFatCmeas = 0.1;
 PBmeas = 12.1;

 Conc=NDoses(2, 97.8 0, 0.0 4.0);

 # M100_6a (T, CVen),
 Print (CVen, 0.5, 1, 2.02, 3, 4.02, 4.25, 4.5, 5, 6, 8, 10.03);
 Data (CVen, 0.64, 0.94, 1.35, 1.62, 1.56, 1.16, 0.77, 0.37, 0.23, 0.19, 0.17);
 # M100_6b (T, CTCOH),
 Print (CTCOH, 1, 2.02, 3, 4.02, 4.25, 4.5, 5, 6, 8, 10.03, 12.02, 14.03, 16, 18, 19.97, 22.07);
 Data (CTCOH, 0.47, 1.1, 1.58, 2.1, 2.21, 2.2, 2.15, 1.94, 1.88, 1.61, 1.39, 1.26, 1.06, 0.95, 0.88, 0.77);
 # M100_6c (T, CBldTCA),
 Print (CBldTCA, 0.5, 1, 2.02, 3, 4.02, 4.25, 4.5, 5, 6, 8, 10.03, 12.02, 14.03, 16, 18, 19.97, 22.07, 48, 71.83, 101.08);
 Data (CBldTCA, 0.21, 0.49, 1.1, 1.67, 2.52, 2.44, 2.71, 3.18, 3.46, 4.26, 4.93, 5.43, 5.85, 6.02, 6.18, 6.35, 6.52, 12.88,
 # M100_6d (T, CAlvPPM),
 Print (CAlvPPM, 4.02, 4.25, 4.5, 5, 6, 8, 10.03, 12.02, 14.03, 16);
 Data (CAlvPPM, 24.679, 6.422, 4.394, 2.691, 1.388, 1.198, 0.592, 0.47, 0.369, 0.351);
 # M100_6e (T, zAUrnTCA),
 Print (zAUrnTCA, 4.55, 5.12, 6.08, 8.13, 10.13, 12.1, 14.1, 16.1, 18.12, 20.08, 22.3, 30.42, 35.67, 51.83, 56.67, 61.5, 70.
 Data (zAUrnTCA, 0.32, 0.41, 1.04, 1.32, 2.51, 4.77, 7.29, 10.23, 11.5, 13.03, 14.26, 17.65, 18.58, 18.58, 18.58, 18.95, 20.
 # M100_6f (T, AUrnTCOGTCOH),
 Print (AUrnTCOGTCOH, 4.55, 5.12, 6.08, 8.13, 10.13, 12.1, 14.1, 16.1, 18.12, 20.08, 22.3, 30.42, 35.67, 51.83, 56.67, 61.5,
 Data (AUrnTCOGTCOH, 11.6, 13.64, 18.54, 25, 33.99, 42.1, 50.19, 60.58, 64.73, 70.85, 77.69, 79.75, 80.14, 80.23, 80.32, 80.
# Total = Free in Fisher data
 Print (TotCTCOH, 1, 2.02, 3, 4.02, 4.25, 4.5, 5, 6, 8, 10.03, 12.02, 14.03, 16, 18, 19.97, 22.07);
 Data (TotCTCOH, 0.47, 1.1, 1.58, 2.1, 2.21, 2.2, 2.15, 1.94, 1.88, 1.61, 1.39, 1.26, 1.06, 0.95, 0.88, 0.77);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
#
Print(CDCVGmol, 0.579   1.01    2       3       4.02    4.24    4.5     5.01    6.02    8.01);
Data(CDCVGmol, 0.00886  0.0349  0.0461  0.0337  0.0313  0.0241  0.0132  0.00552 0.00417 0.000671);
Print(CDCVGmol0, 12);      # No detect at 12 hr in males
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 12);      # No detect at 12 hr in males
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
```

```
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}


Level { # Fisher et al. 1998 Male subject 5

 Experiment { # 7
         #Subject=17; # 19
 # 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
 # Male vol 5
# lnBW=4.41; VFatC=0.65; lnPB=2.48;
# CC= 0;
 BWmeas = 82.3;
 VFatCmeas = 0.14;
 PBmeas = 11.91;

 Conc=NDoses(2, 105.5 0, 0.0 4.0);

 # M100_2a (T, CVen),
 Print (CVen, 0.52, 1, 2.02, 3.02, 4.02, 4.27, 4.52, 5.02, 6.42, 8, 10, 12);
 Data (CVen, 1.69, 2.5, 3.5, 4.24, 4.75, 3.76, 2.2, 0.96, 0.53, 0.26, 0.17, 0.17);
 # M100_2b (T, CTCOH)
 Print (CTCOH, 1, 2.02, 3.02, 4.02, 4.27, 4.52, 5.02, 6.42, 8, 10, 12, 14, 16, 18, 20, 22.03);
 Data (CTCOH, 0.37, 1.41, 2.4, 3.59, 4.16, 3.73, 3.65, 3.63, 2.6, 2.82, 1.84, 1.55, 1.59, 1.06, 1.23, 0.75);
 # M100_2c (T, CBldTCA)
 Print (CBldTCA, 0.52, 1, 2.02, 3.02, 4.27, 4.52, 5.02, 6.42, 8, 10, 14, 16, 18, 20, 22.03, 69.72, 93.61);
 Data (CBldTCA, 0.24, 0.6, 1.24, 2.71, 4.23, 3.86, 3.92, 4.54, 5.71, 6.21, 7.96, 9.08, 8.3, 8.43, 8.95, 5.51, 3.55);
 # M100_2d (T, CDCA)
 #Print (CDCA, 0.52, 1, 2.02, 3.02, 4.27, 8);
 #Data (CDCA, 0.004, 0.004, 0.004, 0.004, 0.005, 0.007);
 # M100_2e (T, AUrnTCA),
 Print (zAUrnTCA, 4.38, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24.42, 31, 35.42, 44.9, 49.75, 53.75, 54.76, 59.42, 68.9, 70.83, 7
 Data (zAUrnTCA, 1.74, 2.77, 3.94, 5.52, 7.66, 9.62, 11.69, 13.57, 20.39, 26.25, 30.32, 40.91, 50.7, 65.02, 65.02, 78.15, 79
 # M100_2f (T, AUrnTCOGTCOH),
 Print (AUrnTCOGTCOH, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24.42, 31, 35.42, 44.9, 49.75, 53.75, 54.76, 59.42, 68.9, 70.83, 72,
 Data (AUrnTCOGTCOH, 8.69, 18.39, 27.48, 37.49, 44.58, 51.78, 56.11, 60.47, 64.77, 66.98, 75.49, 79.43, 82.13, 85.29, 88.15,
# Total = Free
 Print (TotCTCOH, 1, 2.02, 3.02, 4.02, 4.27, 4.52, 5.02, 6.42, 8, 10, 12, 14, 16, 18, 20, 22.03);
 Data (TotCTCOH, 0.37, 1.41, 2.4, 3.59, 4.16, 3.73, 3.65, 3.63, 2.6, 2.82, 1.84, 1.55, 1.59, 1.06, 1.23, 0.75);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
#
Print(CDCVGmol, 0.579   1.01    2       3       4.02    4.24    4.5     5.01    6.02    8.01);
Data(CDCVGmol, 0.00886  0.0349  0.0461  0.0337  0.0313  0.0241  0.0132  0.00552 0.00417 0.000671);
Print(CDCVGmol0, 12);      # No detect at 12 hr in males
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 12);      # No detect at 12 hr in males
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}


Level { # Fisher et al. 1998 Male subject 6
```

```
 Experiment { # 8
         #Subject=18;# 20
 # 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
 # Male vol 6
# lnBW=4.42; VFatC=0.65; lnPB=2.39;
# CC= 0;
 BWmeas = 82.7;
 VFatCmeas = 0.14;
 PBmeas = 10.85;

 Conc=NDoses(2, 102.6 0, 0.0 4.0);

 # M100_3a (T, CVen),
 Print (CVen, 0.5, 1.07, 2, 3, 3.98, 4.25, 4.5, 5, 6);
 Data (CVen, 1.93, 2.34, 2.84, 3.4, 3.41, 2.2, 1.66, 0.89, 0.38);
 # M100_3b (T, CTCOH)
 Print (CTCOH, 0.5, 1.07, 2, 3, 3.98, 4.25, 4.5, 5, 6, 8, 10.02, 12, 14, 16.02, 18.07, 20, 22);
 Data (CTCOH, 0.45, 0.77, 1.51, 2.41, 3.3, 3.64, 3.67, 3.48, 3.05, 2.52, 2.38, 2.16, 1.73, 1.48, 1.12, 1.01, 0.85);
 # M100_3c (T, CBldTCA)
 Print (CBldTCA, 0.5, 1.07, 2, 3, 3.98, 4.25, 4.5, 5, 6, 8, 10.02, 12, 14, 16.02, 18.07, 20, 22, 46.85, 71.47, 95.5);
 Data (CBldTCA, 0.23, 0.49, 1.07, 1.89, 2.87, 3.69, 3.87, 3.59, 4.18, 4.71, 5.46, 5.67, 5.97, 6.05, 6.22, 7.54, 7.26, 8.43,
 # M100_3d (T, zAUrnTCA)
 Print (zAUrnTCA, 3.03, 4.75, 6.7, 8.25, 10.17, 12.08, 14.19, 15.58, 17.6, 18.23, 19.58, 20.05, 21.33, 22.17, 23.2, 35.42, 4
 Data (zAUrnTCA, 0.488, 0.961, 2.09, 2.96, 5.56, 7.17, 8.37, 9.09, 9.7, 10.13, 10.99, 11.24, 11.88, 12.36, 13.03, 14.18, 16.
 # M100_3e (T, AUrnTCOGTCOH)
 Print (AUrnTCOGTCOH, 3.03, 4.75, 6.7, 8.25, 10.17, 12.08, 14.19, 15.58, 17.6, 18.23, 19.58, 20.05, 21.33, 22.17, 23.2, 35.4
 Data (AUrnTCOGTCOH, 32.7, 60.26, 97.98, 130.67, 182.9, 204.64, 224.53, 233.79, 240.99, 245.36, 253.46, 255.9, 261.17, 265.4
# Total = Free in Fisher data
 Print (TotCTCOH, 0.5, 1.07, 2, 3, 3.98, 4.25, 4.5, 5, 6, 8, 10.02, 12, 14, 16.02, 18.07, 20, 22);
 Data (TotCTCOH, 0.45, 0.77, 1.51, 2.41, 3.3, 3.64, 3.67, 3.48, 3.05, 2.52, 2.38, 2.16, 1.73, 1.48, 1.12, 1.01, 0.85);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
#
Print(CDCVGmol, 0.579   1.01    2       3       4.02    4.24    4.5     5.01    6.02    8.01);
Data(CDCVGmol, 0.00886  0.0349  0.0461  0.0337  0.0313  0.0241  0.0132  0.00552 0.00417 0.000671);
Print(CDCVGmol0, 12);      # No detect at 12 hr in males
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 12);      # No detect at 12 hr in males
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}

Level { # Fisher et al. 1998 Male subject 7

 Experiment { # 9
         #Subject=19;# 21
 # 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
 # Male vol 7
# lnBW=4.29; VFatC=0.84; lnPB=2.35;
# CC= 0;

 BWmeas = 73.2;
 VFatCmeas = 0.18;
 PBmeas = 10.47;
```

```
 Conc=NDoses(2, 102.0 0, 0.0 4.0);

 # M100_5a (T, CVen),
 Print (CVen, 0.5, 1, 2, 3, 4, 4.25, 4.53, 5, 6, 8);
 Data (CVen, 0.76, 0.86, 1.15, 1.15, 1.23, 0.77, 0.46, 0.34, 0.21, 0.15);
 # M100_5b (T, CTCOH),
 Print (CTCOH, 1, 2, 3, 4, 4.25, 4.53, 5, 6, 8, 10, 12, 14, 16.03, 18, 20, 22);
 Data (CTCOH, 0.52, 1.35, 1.87, 2.5, 2.59, 2.58, 2.25, 2.15, 1.98, 1.56, 1.02, 1.26, 0.89, 0.79, 0.73, 0.7);
 # M100_5c (T, CBldTCA),
 Print (CBldTCA, 0.5, 1, 2, 3, 4, 4.25, 4.53, 5, 6, 8, 10, 12, 14, 16.03, 18, 20, 22, 51, 78.08, 100.83);
 Data (CBldTCA, 0.11, 0.36, 1.07, 1.55, 2.31, 2.03, 2.16, 2.35, 2.53, 3.61, 3.93, 4.57, 4.5, 5.02, 5.1, 5.07, 5.91, 6.38, 5.
 # M100_5d (T, CAlvPPM),
 Print (CAlvPPM, 4, 4.25, 4.53, 5, 6, 8, 10);
 Data (CAlvPPM, 12.386, 3.305, 2.478, 1.567, 0.577, 0.317, 0.286);
 # M100_5e (T, zAUrnTCA),
 Print (zAUrnTCA, 4.67, 5.05, 6.3, 8.05, 10.07, 12.07, 14.07, 16.15, 18.08, 20.05, 22.15, 25.33, 31.92, 35.33, 43.58, 51.08,
 Data (zAUrnTCA, 1.36, 1.66, 2.7, 4.22, 6.04, 8.04, 10.37, 13.33, 16.55, 20.04, 23.89, 30.02, 35.07, 38.42, 43.06, 46.65, 48
 # M100_5f (T, AUrnTCOGTCOH),
 Print (AUrnTCOGTCOH, 4.67, 5.05, 6.3, 8.05, 10.07, 12.07, 14.07, 16.15, 18.08, 20.05, 22.15, 25.33, 31.92, 35.33, 43.58, 51
 Data (AUrnTCOGTCOH, 16.05, 18.22, 25.28, 34.46, 43.49, 49.91, 55.78, 59.33, 65.07, 68.36, 71.48, 76.1, 81.25, 83.82, 86.11,
# Total = Free in Fisher data
 Print (TotCTCOH, 1, 2, 3, 4, 4.25, 4.53, 5, 6, 8, 10, 12, 14, 16.03, 18, 20, 22);
 Data (TotCTCOH, 0.52, 1.35, 1.87, 2.5, 2.59, 2.58, 2.25, 2.15, 1.98, 1.56, 1.02, 1.26, 0.89, 0.79, 0.73, 0.7);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
#
Print(CDCVGmol, 0.579   1.01    2       3       4.02    4.24    4.5     5.01    6.02    8.01);
Data(CDCVGmol, 0.00886  0.0349  0.0461  0.0337  0.0313  0.0241  0.0132  0.00552 0.00417 0.000671);
Print(CDCVGmol0, 12);      # No detect at 12 hr in males
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 12);      # No detect at 12 hr in males
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}


Level { # Fisher et al. 1998 Male subject 8

 Experiment { # 10
         #Subject=20;#22
 # 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
 # Male vol 8
# lnBW=4.11; VFatC=0.47;
# CC= 0;
 BWmeas = 60.9;
 VFatCmeas = 0.1;

 Conc=NDoses(2, 101.1 0, 0.0 4.0);

 # M100_7a (T, CVen),
 Print (CVen, 0.5, 1, 2, 3, 4, 4.3, 4.5, 5);
 Data (CVen, 0.59, 0.85, 1.1, 1.04, 1.18, 0.64, 0.42, 0.19);
 # M100_7b (T, CTCOH),
 Print (CTCOH, 0.5, 1, 2, 3, 4, 4.3, 4.5, 5, 6, 8, 10, 12, 14, 16, 18, 20.03);
 Data (CTCOH, 0.28, 0.76, 1.92, 1.69, 2.34, 2.34, 2.16, 2.13, 1.95, 1.61, 1.33, 1.58, 0.84, 0.77, 0.57, 0.76);
 # M100_7c (T, CBldTCA),
 Print (CBldTCA, 0.5, 1, 2, 3, 4, 4.3, 4.5, 5, 6, 8, 10, 12, 14, 16, 18, 20.03, 49.75, 73.8, 95.24, 264);
 Data (CBldTCA, 0.36, 0.84, 1.73, 2.6, 3.42, 3.9, 3.67, 4.47, 5, 5.95, 6.74, 7.12, 7.75, 8.22, 8.17, 9.01, 10.66, 8.6, 7.46,
 # M100_7d (T, CAlvPPM),
```

```
 Print (CAlvPPM, 4, 4.03, 4.05, 4.08, 4.167, 4.3, 4.5, 5, 6, 8, 10, 12, 14, 16, 18);
 Data (CAlvPPM, 21.575, 14.272, 10.77, 7.056, 5.876, 5.773, 5.01, 2.498, 1.713, 1.263, 1.029, 0.936, 0.809, 0.738, 0.683);
 # M100_7e (T, CDCA),
 #Print (CDCA, 1, 2, 4);
 #Data (CDCA, 0.006, 0.008, 0.012);
 # M100_7f (T, zAUrnTCA),
 Print (zAUrnTCA, 4.75, 7.95, 14.08, 16.08, 18.1, 20.25, 24.67, 29.17, 32.67, 35.33, 38.83, 44.25, 49.67, 55.92, 58.75, 68.2
 Data (zAUrnTCA, 0.93, 3.02, 5.95, 7.07, 8.28, 9.63, 13.46, 15.73, 20.11, 22.71, 24.07, 25.6, 27.51, 29.6, 33.36, 39.61, 43.
 # M100_7g (T, AUrnTCOGTCOH),
 Print (AUrnTCOGTCOH, 4.75, 7.95, 14.08, 16.08, 18.1, 20.25, 24.67, 29.17, 32.67, 35.33, 38.83, 44.25, 49.67, 55.92, 58.75,
 Data (AUrnTCOGTCOH, 40.71, 69.81, 89.76, 96.8, 102.69, 107.93, 121.3, 128.51, 135.51, 138.05, 140.2, 142.48, 144.47, 144.96
# Total = Free in Fisher data
 Print (TotCTCOH, 0.5, 1, 2, 3, 4, 4.3, 4.5, 5, 6, 8, 10, 12, 14, 16, 18, 20.03);
 Data (TotCTCOH, 0.28, 0.76, 1.92, 1.69, 2.34, 2.34, 2.16, 2.13, 1.95, 1.61, 1.33, 1.58, 0.84, 0.77, 0.57, 0.76);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
#
Print(CDCVGmol, 0.579   1.01    2       3       4.02    4.24    4.5     5.01    6.02    8.01);
Data(CDCVGmol, 0.00886  0.0349  0.0461  0.0337  0.0313  0.0241  0.0132  0.00552 0.00417 0.000671);
Print(CDCVGmol0, 12);      # No detect at 12 hr in males
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 12);      # No detect at 12 hr in males
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}


Level { # Fisher et al. 1998 Male subject 9

 Experiment { # 11
         #Subject=21;#23
 # 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
 # Male vol 9
# lnBW=4.26; VFatC=0.84;
# CC= 0;
 BWmeas = 70.9;
 VFatCmeas = 0.18;

 Conc=NDoses(2, 103.4 0, 0.0 4.0);

 # M100_8a (T, CVen),
 Print (CVen, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5.75, 6, 8, 10, 12, 14, 16, 18, 20, 22);
 Data (CVen, 2.69, 2.98, 3.51, 3.58, 2.88, 1.96, 1.53, 0.81, 0.52, 0.32, 0.27, 0.24, 0.22, 0.22, 0.2, 0.16, 0.16);
 # M100_8b (T, CTCOH)
 Print (CTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5.75, 6, 8, 10, 12, 14, 16, 18, 20, 22);
 Data (CTCOH, 0.47, 0.68, 1.51, 3.58, 2.72, 2.87, 2.77, 2.63, 2.3, 1.9, 1.59, 1.28, 1.23, 1.06, 0.98, 0.72, 0.71);
 # M100_8c (T, CBldTCA)
 Print (CBldTCA, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5.75, 6, 8, 10, 12, 14, 16, 18, 20, 22, 44.98, 68.9, 93.08, 264);
 Data (CBldTCA, 0.43, 1, 2.15, 3.4, 4.94, 5.42, 5.67, 5.83, 5.99, 7.23, 7.96, 8.14, 8.39, 8.36, 8.83, 8.96, 9.51, 10.75, 9.2
 # M100_8d (T, CDCA)
 #Print (CDCA, 2, 3, 4, 4.25, 4.5, 5.75, 8, 16);
 #Data (CDCA, 0.004, 0.01, 0.008, 0.005, 0.005, 0.004, 0.005, 0.005);
 # M100_8e (T, zAUrnTCA)
 Print (zAUrnTCA, 4.58, 5.03, 6.03, 8.05, 10.03, 12.03, 14.07, 16.05, 18.03, 20.02, 22.08, 45.42, 47.42, 48.92, 50.42, 53.92
 Data (zAUrnTCA, 40.02, 40.67, 57.48, 76.6, 99.19, 115.98, 126, 136.55, 143.51, 150.54, 163.57, 196.37, 197.62, 198.48, 199.
 # M100_8f (T, AUrnTCOGTCOH)
 Print (AUrnTCOGTCOH, 4.58, 5.03, 6.03, 8.05, 10.03, 12.03, 14.07, 16.05, 18.03, 20.02, 22.08, 45.42, 47.42, 48.92, 50.42, 5
 Data (AUrnTCOGTCOH, 0.935, 1.34, 4.1, 6.1, 9.74, 13.29, 16.29, 20.29, 22.87, 24.83, 29.98, 56.81, 61.82, 64.84, 67.02, 74.2
# Total = Free in Fisher data
 Print (TotCTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5.75, 6, 8, 10, 12, 14, 16, 18, 20, 22);
```

```
 Data (TotCTCOH, 0.47, 0.68, 1.51, 3.58, 2.72, 2.87, 2.77, 2.63, 2.3, 1.9, 1.59, 1.28, 1.23, 1.06, 0.98, 0.72, 0.71);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
#
Print(CDCVGmol, 0.579   1.01    2       3       4.02    4.24    4.5     5.01    6.02    8.01);
Data(CDCVGmol, 0.00886  0.0349  0.0461  0.0337  0.0313  0.0241  0.0132  0.00552 0.00417 0.000671);
Print(CDCVGmol0, 12);      # No detect at 12 hr in males
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 12);      # No detect at 12 hr in males
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}


Level { # Fisher et al. 1998 Female subject 1

 Experiment { # 12 ## Low exposure
         #Subject=22;#24
 # 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
 # Female vol 1
# lnBW=4.20; VFatC=1.50; lnPB=2.29;
# CC= 0;

 BWmeas = 66.5;
 VFatCmeas = 0.32;
 PBmeas = 9.88;
 Male = 0.0;

 Conc=NDoses(2, 55.1 0, 0.0 4.0);

 # F60_1a (T, CVen)
 Print (CVen, 0.58, 1.02, 2, 3, 4, 4.25, 4.47, 5, 6, 8.03);
 Data (CVen, 1, 1.29, 1.38, 1.7, 1.72, 1.08, 1.17, 0.55, 0.39, 0.22);
 # F60_1b (T, CTCOH)
 Print (CTCOH, 0.58, 1.02, 2, 3, 4, 4.25, 4.47, 5, 9.98, 12, 14.02, 16, 18.03, 20, 22);
 Data (CTCOH, 0.32, 0.49, 0.85, 0.97, 1.2, 1.14, 1.18, 1.13, 0.7, 0.6, 0.52, 0.55, 0.54, 0.45, 0.35);
 # F60_1c (T, CBldTCA)
 Print (CBldTCA, 0.58, 1.02, 2, 3, 4, 4.25, 4.47, 5, 6, 8.03, 9.98, 12, 14.02, 16, 18.03, 20, 22, 44.33, 68.32, 93.38);
 Data (CBldTCA, 0.16, 0.46, 1.15, 1.53, 1.9, 2.1, 2.18, 2.13, 2.56, 3.32, 2.83, 2.98, 3.42, 3.44, 3.31, 4.15, 4.07, 3.7, 3.3
 # F60_1d (T, AUrnTCA)
 Print (zAUrnTCA, 4.58, 5.26, 6.12, 8.12, 10.18, 12.18, 14.32, 16.18, 18.16, 20.25, 22.53, 23.25, 25.25, 27.58, 29.5, 30.92,
 Data (zAUrnTCA, 0.64, 0.76, 0.85, 1.83, 2.57, 3.36, 3.94, 5.12, 6.03, 6.67, 7.3, 7.6, 7.96, 8.6, 8.89, 9.21, 9.86, 9.66, 11
 # F60_1e (T, AUrnTCOGTCOH)
 Print (AUrnTCOGTCOH, 4.58, 5.26, 6.12, 8.12, 10.18, 12.18, 14.32, 16.18, 18.16, 20.25, 22.53, 23.25, 25.25, 27.58, 29.5, 30
 Data (AUrnTCOGTCOH, 20.08, 22.91, 24.87, 28.94, 36.46, 39.14, 42.64, 45.16, 53.64, 56.34, 57.08, 57.64, 58.45, 60.33, 61.44
# Total = Free in Fisher data
 Print (TotCTCOH, 0.58, 1.02, 2, 3, 4, 4.25, 4.47, 5, 9.98, 12, 14.02, 16, 18.03, 20, 22);
 Data (TotCTCOH, 0.32, 0.49, 0.85, 0.97, 1.2, 1.14, 1.18, 1.13, 0.7, 0.6, 0.52, 0.55, 0.54, 0.45, 0.35);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

Print(CDCVGmol, 0);
```

```
Data(CDCVGmol, -1);
Print(CDCVG_ND, 0);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };


 Experiment { # 13 ## high exposure
        #Subject=22;#25
 # 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
 # Female vol 1
# lnBW=4.20; VFatC=1.50; lnPB=2.29;
# CC= 0;

 BWmeas = 66.5;
 VFatCmeas = 0.32;
 PBmeas = 9.88;
 Male = 0.0;

 Conc=NDoses(2, 101.4 0, 0.0 4.0);

 #F100_2a (T, CVen),
 Print (CVen, 0.5, 1, 2, 3, 4, 4.23, 4.5, 5, 6);
 Data (CVen, 1.18, 2.17, 2.3, 2.41, 2.65, 1.84, 1.17, 0.62, 0.38);
 # F100_2b (T, CTCOH),
 Print (CTCOH, 1, 2, 3, 4, 4.23, 4.5, 5, 6, 8.05, 10, 12, 14.02, 16, 18, 20, 22.02);
 Data (CTCOH, 0.74, 1.38, 1.93, 2.41, 2.4, 2.33, 2.17, 1.94, 1.81, 1.38, 1.17, 1.25, 1.01, 0.88, 0.74, 0.7);
 # F100_2c (T, CBldTCA),
 Print (CBldTCA, 2, 3, 4, 4.23, 4.5, 5, 6, 8.05, 10, 12, 14.02, 16, 18, 20, 22.02, 46.7, 70.25, 93.72);
 Data (CBldTCA, 0.91, 1.75, 2.65, 2.54, 2.65, 2.73, 3.26, 3.58, 4.5, 4.02, 4.17, 4.45, 4.9, 5.26, 5.94, 6.68, 5.2, 3.6);
 # F100_2d (T, zAUrnTCA)
 Print (zAUrnTCA, 4.37, 5.03, 6.1, 8.1, 10.07, 12.03, 14.1, 16.05, 18.05, 20.06, 22.15, 24.32, 27.05, 28.3, 30.1, 32.45, 34.
 Data (zAUrnTCA, 0.31, 0.39, 0.64, 1.21, 1.66, 2.16, 2.96, 3.66, 4.37, 5.44, 6.66, 7.63, 8.16, 8.71, 10.3, 10.92, 11.77, 12.
 # F100_2e (T, AUrnTCOGTCOH)
 Print (AUrnTCOGTCOH, 4.37, 5.03, 6.1, 8.1, 10.07, 12.03, 14.1, 16.05, 18.05, 20.06, 22.15, 24.32, 27.05, 28.3, 30.1, 32.45,
 Data (AUrnTCOGTCOH, 35.78, 44.4, 54.4, 72.58, 90.61, 104.44, 116.9, 127.49, 127.49, 136.49, 144.45, 147.89, 150.61, 154.52,
# Total = Free in Fisher data
 Print (TotCTCOH, 1, 2, 3, 4, 4.23, 4.5, 5, 6, 8.05, 10, 12, 14.02, 16, 18, 20, 22.02);
 Data (TotCTCOH, 0.74, 1.38, 1.93, 2.41, 2.4, 2.33, 2.17, 1.94, 1.81, 1.38, 1.17, 1.25, 1.01, 0.88, 0.74, 0.7);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
#
Print(CDCVGmol, 0.51    0.985   1.99    2.96    4.02    4.23    4.52    5.01    6.03    );
Data(CDCVGmol, 0.0032   0.00868 0.0106  0.0127  0.0133  0.0087  0.00508 0.00229 0.00074 );
Print(CDCVGmol0, 10);      # No detect at 10 hr in females
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 10);      # No detect at 10 hr in females
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
```

```
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}


Level { # Fisher et al. 1998 Female subject 2

 Experiment { # 14 ## Low exposure
         #Subject=23;#26
 # 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
 # Female vol 2
# lnBW=4.13; VFatC=1.12; lnPB=2.25;
# CC= 0;

 BWmeas = 62.3;
 VFatCmeas = 0.24;
 PBmeas = 9.45;
 Male = 0.0;

 Conc=NDoses(2, 53.0 0, 0.0 4.0);

 # F50_1a (T, CVen)
 Print (CVen, 0.5, 1, 2, 3, 4, 4.27, 4.55, 5.1, 6);
 Data (CVen, 0.93, 1.33, 1.65, 1.85, 1.45, 0.94, 0.63, 0.32, 0.18);
 # F50_1b (T, CTCOH)
 Print (CTCOH, 1, 2, 3, 4, 4.27, 4.55, 5.1, 6, 8, 10, 12, 14, 16.05, 18, 22);
 Data (CTCOH, 0.33, 0.63, 0.79, 0.98, 0.83, 0.83, 0.9, 0.89, 0.76, 0.66, 0.67, 0.54, 0.48, 0.47, 0.35);
 # F50_1c (T, CBldTCA)
 Print (CBldTCA, 1, 2, 3, 4, 4.27, 4.55, 5.1, 6, 8, 10, 12, 14, 16.05, 18, 20.02, 22, 44.92, 68.86, 100.44);
 Data (CBldTCA, 0.38, 1.23, 1.96, 2.8, 2.81, 3.23, 3.34, 3.72, 4.88, 4.93, 5.28, 5.18, 5.37, 6.03, 4.87, 6.66, 6.66, 5.27, 2
 # F50_1d (T, AUrnTCA)
 Print (zAUrnTCA, 5.25, 5.97, 8, 10.17, 12.17, 14.17, 16.17, 18.17, 20.17, 22.17, 25, 29.83, 37.83, 44.83, 49.67, 53.33, 61.
 Data (zAUrnTCA, 1.35, 4.49, 7.17, 9.38, 10.36, 11.91, 13.46, 14.7, 15.64, 16.49, 22.11, 23.27, 26.03, 27.35, 33.94, 35.83,
 # F50_1e (T, AUrnTCOGTCOH)
 Print (AUrnTCOGTCOH, 5.25, 5.97, 8, 10.17, 12.17, 14.17, 16.17, 18.17, 20.17, 22.17, 25, 29.83, 37.83, 44.83, 49.67, 53.33,
 Data (AUrnTCOGTCOH, 4.42, 6.71, 12, 15.4, 16.73, 20.35, 23.49, 25.44, 25.44, 26.96, 30.55, 32.71, 34.38, 34.88, 37.25, 38.5
# Total = Free in Fisher data
 Print (TotCTCOH, 1, 2, 3, 4, 4.27, 4.55, 5.1, 6, 8, 10, 12, 14, 16.05, 18, 22);
 Data (TotCTCOH, 0.33, 0.63, 0.79, 0.98, 0.83, 0.83, 0.9, 0.89, 0.76, 0.66, 0.67, 0.54, 0.48, 0.47, 0.35);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

Print(CDCVGmol, 0);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 0);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };


 Experiment { # 15 ## High exposure
         #Subject=23;#27
 # 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
 # Female vol 2
# lnBW=4.13; VFatC=1.12; lnPB=2.25;
# CC= 0;

 BWmeas = 62.3;
 VFatCmeas = 0.24;
 PBmeas = 9.45;
 Male = 0.0;

 Conc=NDoses(2, 97.7 0, 0.0 4.0);

 # F100_6a (T, CVen)
 Print (CVen, 0.5, 1, 2.03, 3, 4.03, 4.25, 4.5, 5, 6, 8, 10);
 Data (CVen, 0.83, 0.99, 1.2, 1.59, 2.03, 1.33, 0.87, 0.42, 0.21, 0.22, 0.15);
 # F100_6b (T, CTCOH),
 Print (CTCOH, 2.03, 3, 4.03, 4.25, 4.5, 5, 6, 8, 10, 12, 14.03, 16.03, 18.07, 20);
 Data (CTCOH, 0.53, 0.83, 1.27, 0.92, 0.85, 1.17, 1.03, 0.86, 0.8, 0.71, 0.62, 0.55, 0.48, 0.41);
 # F100_6c (T, CBldTCA),
 Print (CBldTCA, 0.5, 1, 2.03, 3, 4.03, 4.25, 4.5, 5, 6, 8, 10, 12, 14.03, 16.03, 18.07, 20, 22, 47.95, 71.98, 101.22);
 Data (CBldTCA, 0.44, 0.97, 2.16, 3.79, 5.12, 5.35, 5.6, 5.88, 6.55, 7.3, 7.66, 8.61, 8.73, 9.65, 8.29, 8.6, 10.2, 6.15, 7.1
 # F100_6d (T, CAlvPPM),
 Print (CAlvPPM, 4.03, 4.25, 4.5, 5, 6, 8, 10, 12, 14.03);
 Data (CAlvPPM, 22.398, 7.317, 5.917, 2.903, 1.382, 0.982, 0.691, 0.524, 0.428);
 # F100_6e (T, CDCA),
 #Print (CDCA, 1, 2.03, 3);
 #Data (CDCA, 0.005, 0.014, 0.005);
 # F100_6f (T, zAUrnTCA),
 Print (zAUrnTCA, 4.55, 5.12, 6.08, 8.19, 10.19, 12.17, 14.33, 16.23, 18.19, 20.13, 22.38, 31.92, 34.25, 36.92, 48.67, 55.83
 Data (zAUrnTCA, 0.3, 0.56, 1.75, 1.97, 3.75, 6.58, 6.81, 8.64, 10.3, 12.13, 13.64, 15.77, 18.03, 18.16, 22.69, 28.52, 30.85
 # F100_6g (T, AUrnTCOGTCOH),
 Print (AUrnTCOGTCOH, 4.55, 5.12, 6.08, 8.19, 10.19, 12.17, 14.33, 16.23, 18.19, 20.13, 22.38, 31.92, 34.25, 36.92, 48.67, 5
 Data (AUrnTCOGTCOH, 11.67, 14.56, 20.78, 25.55, 34.83, 45.33, 45.98, 54.21, 60.91, 68.01, 73.35, 75.14, 79.52, 79.97, 85.95
# Total = Free in Fisher data
 Print (TotCTCOH, 2.03, 3, 4.03, 4.25, 4.5, 5, 6, 8, 10, 12, 14.03, 16.03, 18.07, 20);
 Data (TotCTCOH, 0.53, 0.83, 1.27, 0.92, 0.85, 1.17, 1.03, 0.86, 0.8, 0.71, 0.62, 0.55, 0.48, 0.41);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
#
Print(CDCVGmol, 0.51    0.985   1.99    2.96    4.02    4.23    4.52    5.01    6.03    );
Data(CDCVGmol, 0.0032   0.00868 0.0106  0.0127  0.0133  0.0087  0.00508 0.00229 0.00074 );
Print(CDCVGmol0, 10);      # No detect at 10 hr in females
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 10);      # No detect at 10 hr in females
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}

Level { # Fisher et al. 1998 Female subject 3

 Experiment { # 16
         #Subject=24;#28
 # 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
 # Female vol 3
# lnBW=4.05; VFatC=0.98; lnPB=1.87;
# CC= 0;
 BWmeas = 57.5;
 VFatCmeas = 0.21;
 PBmeas = 6.47;
```

```
 Male = 0.0;

 Conc=NDoses(2, 102.5 0, 0.0 4.0);

 # F100_1a (T, CVen)
 Print (CVen, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6);
 Data (CVen, 1.11, 1.36, 2.11, 1.92, 2.3, 1.56, 1.26, 0.73, 0.42);
 # F100_1b (T, CTCOH)
 Print (CTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16.05, 18, 20.02, 22.02, 46.17);
 Data (CTCOH, 0.22, 0.46, 1.18, 2.18, 3.03, 3.29, 3.67, 3.13, 2.57, 2.46, 1.93, 1.57, 1.3, 1.08, 0.89, 0.56, 0.65, 0.3);
 # F100_1c (T, CBldTCA),
 Print (CBldTCA, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16.05, 18, 20.02, 22.02, 46.17, 69.83, 94.67);
 Data (CBldTCA, 0.21, 0.39, 1.05, 1.86, 3.46, 3.78, 3.91, 4.22, 4.67, 5.71, 6.29, 7.76, 7.78, 8.11, 8.79, 9.05, 9.34, 9.58,
 # F100_1d (T, zAUrnTCA),
 Print (zAUrnTCA, 4.62, 5.08, 6.86, 8.33, 10.25, 12.13, 14.08, 16.15, 18, 20.05, 22.17, 30.67, 33.67, 35.42, 40.67, 46.67, 4
 Data (zAUrnTCA, 0.51, 0.65, 1.26, 1.85, 2.92, 3.91, 4.92, 5.91, 5.91, 7.12, 9.55, 15.22, 17.85, 19.66, 24.08, 26.68, 27.91,
 # F100_1e (T, AUrnTCOGTCOH),
 Print (AUrnTCOGTCOH, 4.62, 5.08, 6.86, 8.33, 10.25, 12.13, 14.08, 16.15, 18, 20.05, 22.17, 30.67, 33.67, 35.42, 40.67, 46.6
 Data (AUrnTCOGTCOH, 44.83, 52.08, 77.84, 89.76, 108.58, 122.65, 133.38, 140.85, 147.19, 151.76, 155.86, 169.38, 174.67, 175
# Total = Free in Fisher data
 Print (TotCTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16.05, 18, 20.02, 22.02, 46.17);
 Data (TotCTCOH, 0.22, 0.46, 1.18, 2.18, 3.03, 3.29, 3.67, 3.13, 2.57, 2.46, 1.93, 1.57, 1.3, 1.08, 0.89, 0.56, 0.65, 0.3);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
#
Print(CDCVGmol, 0.51    0.985   1.99    2.96    4.02    4.23    4.52    5.01    6.03    );
Data(CDCVGmol, 0.0032   0.00868 0.0106  0.0127  0.0133  0.0087  0.00508 0.00229 0.00074 );
Print(CDCVGmol0, 10);      # No detect at 10 hr in females
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 10);      # No detect at 10 hr in females
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}


Level { # Fisher et al. 1998 Female subject 4

 Experiment { # 17
         #Subject=25;#29
 # 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
 # Female vol 4
# lnBW=4.02; VFatC=1.07; lnPB=2.03;
# CC= 0;

 BWmeas = 55.5;
 VFatCmeas = 0.23;
 PBmeas = 7.63;
 Male = 0.0;

 Conc=NDoses(2, 102.0 0, 0.0 4.0);

 # F100_3a (T, CVen)
 Print (CVen, 0.58, 1, 2, 3, 4, 4.17, 4.5, 5, 6, 8.02);
 Data (CVen, 0.81, 0.88, 1.09, 1.03, 1.13, 0.59, 0.47, 0.3, 0.18, 0.15);
 # F100_3b (T, CTCOH)
 Print (CTCOH, 0.58, 1, 2, 3, 4, 4.17, 4.5, 5, 6, 8.02, 10.02, 12.02, 14.03, 16, 18, 20, 22);
 Data (CTCOH, 0.33, 0.57, 1.01, 1.25, 1.79, 1.64, 1.54, 1.43, 1.27, 0.95, 1.01, 0.9, 0.88, 0.74, 0.69, 0.63, 0.61);
 # F100_3c (T, CBldTCA)
```

```
 Print (CBldTCA, 0.58, 1, 2, 3, 4, 4.17, 4.5, 5, 6, 8.02, 10.02, 12.02, 14.03, 16, 18, 20, 22, 46.08, 75.67, 94.25);
 Data (CBldTCA, 0.4, 0.97, 1.72, 2.64, 3.41, 3.62, 3.86, 4.39, 4.8, 5.73, 6.79, 7.55, 7.68, 7.98, 9.27, 8.91, 9.12, 11.31, 1
 # F100_3d (T, zAUrnTCA)
 Print (zAUrnTCA, 4.58, 6.03, 8.12, 10.08, 12.1, 14.1, 16.05, 18.1, 20.05, 21.92, 26.17, 33.25, 37.92, 44.92, 49, 54.92, 58.
 Data (zAUrnTCA, 0.44, 0.71, 1.31, 2.28, 3.48, 4.64, 5.64, 6.76, 7.66, 8.89, 10.64, 13.81, 14.11, 15.44, 16, 23.2, 22.4, 24.
 # F100_3e (T, AUrnTCOGTCOH)
 Print (AUrnTCOGTCOH, 4.58, 6.03, 8.12, 10.08, 12.1, 14.1, 16.05, 18.1, 20.05, 21.92, 26.17, 33.25, 37.92, 44.92, 49, 54.92,
 Data (AUrnTCOGTCOH, 12.63, 17.83, 26.05, 30.4, 36.72, 41.26, 44.27, 47.94, 50.31, 53.17, 57.9, 65.27, 65.8, 69.74, 69.74, 7
# Total = Free in Fisher data
 Print (TotCTCOH, 0.58, 1, 2, 3, 4, 4.17, 4.5, 5, 6, 8.02, 10.02, 12.02, 14.03, 16, 18, 20, 22);
 Data (TotCTCOH, 0.33, 0.57, 1.01, 1.25, 1.79, 1.64, 1.54, 1.43, 1.27, 0.95, 1.01, 0.9, 0.88, 0.74, 0.69, 0.63, 0.61);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
#
Print(CDCVGmol, 0.51    0.985   1.99    2.96    4.02    4.23    4.52    5.01    6.03    );
Data(CDCVGmol, 0.0032   0.00868 0.0106  0.0127  0.0133  0.0087  0.00508 0.00229 0.00074 );
Print(CDCVGmol0, 10);      # No detect at 10 hr in females
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 10);      # No detect at 10 hr in females
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}


Level { # Fisher et al. 1998 Female subject 5

 Experiment { # 18
         #Subject=26;#30
 # 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
 # Female vol 5
# lnBW=4.21; VFatC=1.64; lnPB=2.40;
# CC= 0;

 BWmeas = 67.3;
 VFatCmeas = 0.35;
 PBmeas = 11.0;
 Male = 0.0;

 Conc=NDoses(2, 102.0 0, 0.0 4.0);

 # F100_5a (T, CVen),
 Print (CVen, 0.5, 1, 2, 3, 4, 4.25, 4.55, 5, 6.02, 8.02);
 Data (CVen, 0.74, 1, 1.27, 1.45, 1.19, 0.81, 0.66, 0.46, 0.25, 0.19);
 # F100_5b (T, CTCOH),
 Print (CTCOH, 1, 2, 3, 4, 4.25, 4.55, 5, 8.02, 10, 12, 14, 18.02, 20);
 Data (CTCOH, 0.41, 0.78, 1.04, 1.18, 1.17, 1.18, 1.18, 0.84, 0.72, 0.82, 0.56, 0.49, 0.41);
 # F100_5c (T, CBldTCA),
 Print (CBldTCA, 0.5, 1, 2, 3, 4, 4.25, 4.55, 5, 6.02, 8.02, 10, 12, 14, 18.02, 20, 22, 46.58, 70.5);
 Data (CBldTCA, 0.25, 0.76, 1.48, 2.21, 2.79, 2.78, 3.12, 3.23, 3.52, 4.76, 4.95, 5.29, 5.33, 6.46, 6.91, 7.1, 6.63, 5.28);
 # F100_5d (T, CAlvPPM),
 Print (CAlvPPM, 4.25, 4.55, 5, 6.02, 8.02, 10, 12, 14);
 Data (CAlvPPM, 4.243, 2.798, 1.849, 1.467, 0.681, 0.452, 0.409, 0.356);
 # F100_5e (T, zAUrnTCA)
 Print (zAUrnTCA, 4.67, 5, 6.3, 8.08, 10.08, 12.07, 14.08, 16.12, 18.11, 20.1, 22.12, 22.67, 26.5, 29.67, 34.17, 35.67, 40.6
 Data (zAUrnTCA, 0.69, 0.8, 1.64, 3.16, 4.95, 7.19, 9.89, 13.14, 17.46, 21.67, 26.4, 29.05, 35.18, 41.73, 49.36, 50.76, 56.4
 # F100_5f (T, AUrnTCOGTCOH)
 Print (AUrnTCOGTCOH, 4.67, 5, 6.3, 8.08, 10.08, 12.07, 14.08, 16.12, 18.11, 20.1, 22.12, 22.67, 26.5, 29.67, 34.17, 35.67,
```

```
 Data (AUrnTCOGTCOH, 9.98, 9.98, 12.41, 16.09, 18.99, 20.96, 23.08, 24.46, 26.22, 27.92, 29.05, 29.64, 32.31, 34.4, 36.58, 3
# Total = Free in Fisher data
 Print (TotCTCOH, 1, 2, 3, 4, 4.25, 4.55, 5, 8.02, 10, 12, 14, 18.02, 20);
 Data (TotCTCOH, 0.41, 0.78, 1.04, 1.18, 1.17, 1.18, 1.18, 0.84, 0.72, 0.82, 0.56, 0.49, 0.41);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
# This is average female data points -- high CV (~0.5, based on peaks)
#
Print(CDCVGmol, 0.51    0.985   1.99    2.96    4.02    4.23    4.52    5.01    6.03    );
Data(CDCVGmol, 0.0032   0.00868 0.0106  0.0127  0.0133  0.0087  0.00508 0.00229 0.00074 );
Print(CDCVGmol0, 10);      # No detect at 10 hr in females
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 10);      # No detect at 10 hr in females
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}

Level { # Fisher et al. 1998 Female subject 6

 Experiment { # 19
         #Subject=27;#31
 # 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
 # Female vol 6
# lnBW=4.15; VFatC=1.21;
# CC= 0;

 BWmeas = 63.2;
 VFatCmeas = 0.26;
 Male = 0.0;

 Conc=NDoses(2, 101.0 0, 0.0 4.0);

 # F100_7a (T, CVen),
 Print (CVen, 0.52, 1, 2, 3, 4, 4.28, 4.5, 5);
 Data (CVen, 0.53, 1, 0.97, 1.31, 1.48, 0.84, 0.58, 0.39);
 # F100_7b (T, CTCOH)
 Print (CTCOH, 0.52, 1, 2, 3, 4, 4.28, 4.5, 5, 6.05, 8, 10, 12);
 Data (CTCOH, 0.35, 0.58, 0.86, 1.6, 2.03, 2.04, 1.93, 1.95, 1.79, 1.29, 1.14, 1.03);
 # F100_7c (T, CBldTCA)
 Print (CBldTCA, 0.52, 1, 2, 3, 4, 4.28, 4.5, 5, 6.05, 8, 10, 12, 46.75, 73.97, 95.42);
 Data (CBldTCA, 0.39, 1.08, 1.9, 3.83, 4.48, 4.65, 4.8, 4.73, 6.02, 6.02, 7.12, 7.13, 9.1, 6.92, 6.14);
 # F100_7d (T, zAUrnTCA)
 Print (zAUrnTCA, 4.67, 5.17, 6.25, 8.08, 10.13, 12.08, 14.12, 16.02, 18.02, 20.17, 25.27, 25.75, 30, 34.5, 37.92, 45.08, 49
 Data (zAUrnTCA, 2.51, 3.07, 6.21, 9.97, 13.01, 16.35, 20.65, 23.23, 26.31, 26.31, 34.28, 34.84, 42.19, 51.62, 61.19, 75.52,
 # F100_7e (T, AUrnTCOGTCOH)
 Print (AUrnTCOGTCOH, 4.67, 5.17, 6.25, 8.08, 10.13, 12.08, 14.12, 16.02, 18.02, 20.17, 25.27, 25.75, 30, 34.5, 37.92, 45.08
 Data (AUrnTCOGTCOH, 37.76, 42.18, 48.68, 60.91, 72.32, 81.05, 86.76, 94.78, 100.92, 105.91, 115.12, 116.22, 125.29, 131.36,
# Total = Free in Fisher data
 Print (TotCTCOH, 0.52, 1, 2, 3, 4, 4.28, 4.5, 5, 6.05, 8, 10, 12);
 Data (TotCTCOH, 0.35, 0.58, 0.86, 1.6, 2.03, 2.04, 1.93, 1.95, 1.79, 1.29, 1.14, 1.03);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
#
Print(CDCVGmol, 0.51    0.985   1.99    2.96    4.02    4.23    4.52    5.01    6.03    );
```

```
Data(CDCVGmol, 0.0032   0.00868 0.0106  0.0127  0.0133  0.0087  0.00508 0.00229 0.00074 );
Print(CDCVGmol0, 10);      # No detect at 10 hr in females
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 10);      # No detect at 10 hr in females
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}

Level { # Fisher et al. 1998 Female subject 7

 Experiment { # 20
         #Subject=28;#32
 # 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
 # Female vol 7
# lnBW=3.88; VFatC=1.07;
# CC= 0;

 BWmeas = 48.6;
 VFatCmeas = 0.23;
 Male = 0.0;

 Conc=NDoses(2, 103.3 0, 0.0 4.0);

 # F100_8a (T, CVen)
 Print (CVen, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8.05, 10.03);
 Data (CVen, 1.32, 1.68, 1.86, 2.37, 2.66, 2.1, 1.23, 0.83, 0.42, 0.33, 0.3);
 # F100_8b (T, CTCOH)
 Print (CTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8.05, 10.03, 12.05, 14.02, 16, 18, 20, 22);
 Data (CTCOH, 0.47, 0.68, 1.51, 2.15, 2.72, 2.87, 2.77, 2.63, 2.3, 1.9, 1.59, 1.28, 1.23, 1.1, 0.98, 0.72, 0.71);
 # F100_8c (T, CBldTCA)
 Print (CBldTCA, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8.05, 10.03, 12.05, 14.02, 16, 18, 20, 22, 45.03, 69.03, 93.13, 264);
 Data (CBldTCA, 0.27, 0.7, 1.48, 2.8, 3.92, 3.86, 3.98, 4.55, 4.8, 5.96, 6.09, 6.41, 7.01, 7.23, 7.57, 7.68, 8.46, 8.75, 7.7
 # F100_8d (T, CDCA)
 #Print (CDCA, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8.05, 12.05, 16, 18, 22, 45.03, 69.03);
 #Data (CDCA, 0.008, 0.008, 0.007, 0.007, 0.006, 0.009, 0.013, 0.012, 0.011, 0.005, 0.005, 0.004, 0.004, 0.005, 0.006, 0.004
 # F100_8e (T, zAUrnTCA)
 Print (zAUrnTCA, 4.58, 5.05, 6.05, 8.08, 10.07, 12.08, 14.31, 16.05, 18.05, 20.03, 22.08, 43.33, 45.58, 47.58, 49.17, 53.58
 Data (zAUrnTCA, 2.34, 2.92, 5.27, 8.33, 12.15, 17.02, 21.46, 26.02, 28.88, 32.6, 37.96, 80.45, 85.25, 87.93, 91.55, 99.63,
 # F100_8f (T, AUrnTCOGTCOH)
 Print (AUrnTCOGTCOH, 4.58, 5.05, 6.05, 8.08, 10.07, 12.08, 14.31, 16.05, 18.05, 20.03, 22.08, 43.33, 45.58, 47.58, 49.17, 5
 Data (AUrnTCOGTCOH, 15.54, 18.22, 24.58, 33.76, 41.25, 47.8, 54.36, 59.99, 63.23, 68.23, 73.9, 110.18, 112.61, 113.7, 115.1
# Total = Free in Fisher data
 Print (TotCTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8.05, 10.03, 12.05, 14.02, 16, 18, 20, 22);
 Data (TotCTCOH, 0.47, 0.68, 1.51, 2.15, 2.72, 2.87, 2.77, 2.63, 2.3, 1.9, 1.59, 1.28, 1.23, 1.1, 0.98, 0.72, 0.71);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
#
Print(CDCVGmol, 0.51    0.985   1.99    2.96    4.02    4.23    4.52    5.01    6.03    );
Data(CDCVGmol, 0.0032   0.00868 0.0106  0.0127  0.0133  0.0087  0.00508 0.00229 0.00074 );
Print(CDCVGmol0, 10);      # No detect at 10 hr in females
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 10);      # No detect at 10 hr in females
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
```

```
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}

Level { # Fisher et al. 1998 Female subject 8

 Experiment { # 21
         #Subject=29;#33
 # 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
 # Female vol 8
# lnBW=4.12; VFatC=1.54; lnPB=2.34;
# CC= 0;

 BWmeas = 61.8;
 VFatCmeas = 0.33;
 PBmeas = 10.37;
 Male = 0.0;

 Conc=NDoses(2, 102.0 0, 0.0 4.0);

 # F100_4a (T, CVen)
 Print (CVen, 0.55, 1, 2.12, 3.05, 4, 4.25, 4.5, 5, 6);
 Data (CVen, 0.55, 0.81, 1.3, 1.37, 1.43, 0.81, 0.54, 0.35, 0.18);
 # F100_4b (T, CTCOH)
 Print (CTCOH, 1, 2.12, 3.05, 4, 4.25, 4.5, 5, 6, 8.05, 10.08, 14.03, 18.02, 22.02);
 Data (CTCOH, 0.39, 1.2, 1.59, 1.93, 1.97, 1.75, 1.63, 1.32, 1.1, 0.91, 0.83, 0.69, 0.54);
 # F100_4c (T, CBldTCA)
 Print (CBldTCA, 0.55, 1, 2.12, 3.05, 4, 4.25, 4.5, 5, 6, 8.05, 10.08, 14.03, 18.02, 22.02, 46.08, 75.67, 94.25);
 Data (CBldTCA, 0.47, 1.05, 2.73, 3.85, 4.82, 5.02, 5.29, 5.37, 6.01, 7.6, 6.77, 8.65, 9.49, 10.64, 9.58, 8.55, 7.82);
 # F100_4d (T, zAUrnTCA),
 Print (zAUrnTCA, 2.33, 4.57, 5.12, 6.12, 8.12, 10.33, 12.08, 14.12, 16, 18.08, 20, 21.92, 25.08, 29.25, 32.58, 35.83, 38.33
 Data (zAUrnTCA, 0.29, 1.62, 2.09, 4.01, 5.81, 8.27, 10.21, 13.06, 16.29, 19.09, 21.96, 24.17, 27.09, 29.05, 35.13, 45.84, 5
 # F100_4e (T, AUrnTCOGTCOH),
 Print (AUrnTCOGTCOH, 2.33, 4.57, 5.12, 6.12, 8.12, 10.33, 12.08, 14.12, 16, 18.08, 20, 21.92, 25.08, 29.25, 32.58, 35.83, 3
 Data (AUrnTCOGTCOH, 4.52, 8.37, 12.49, 19.46, 29.26, 35.93, 40.21, 44.9, 48.15, 51.04, 55.72, 58.76, 60.75, 62.24, 72.07, 7
# Total = Free in Fisher data
 Print (TotCTCOH, 1, 2.12, 3.05, 4, 4.25, 4.5, 5, 6, 8.05, 10.08, 14.03, 18.02, 22.02);
 Data (TotCTCOH, 0.39, 1.2, 1.59, 1.93, 1.97, 1.75, 1.63, 1.32, 1.1, 0.91, 0.83, 0.69, 0.54);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Data (CAlvPPM, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);
 Print(CAlvPPM, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
#
Print(CDCVGmol, 0.51    0.985   1.99    2.96    4.02    4.23    4.52    5.01    6.03    );
Data(CDCVGmol, 0.0032   0.00868 0.0106  0.0127  0.0133  0.0087  0.00508 0.00229 0.00074 );
Print(CDCVGmol0, 10);      # No detect at 10 hr in females
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 10);      # No detect at 10 hr in females
Data(CDCVG_ND, 0);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
```

```
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

 };

}

}
############# END FISHER et al. 1998 individual data ######

############# BEGIN Paykoc and Powell 1945 individual data ########
Level { #Subject level
### FOR PAYKOC, ONLY PHYSIOLOGICAL AND TCA PARAMETERS

Distrib(        lnQCC   TruncNormal_v   M_lnQCC V_lnQCC -0.8    0.8     );

Distrib(        lnVPRC  TruncNormal_v   M_lnVPRC        V_lnVPRC        -0.8    0.8     );

Distrib(        QFatC   TruncNormal_v   M_QFatC V_QFatC 0.08    1.92    );
Distrib(        QGutC   TruncNormal_v   M_QGutC V_QGutC 0.64    1.36    );
Distrib(        QLivC   TruncNormal_v   M_QLivC V_QLivC 0.1     1.9     );
Distrib(        QSlwC   TruncNormal_v   M_QSlwC V_QSlwC 0.36    1.64    );
####Distrib(    lnDRespC        TruncNormal_v   M_lnDRespC      V_lnDRespC      -11.513 2.303   );
Distrib(        QKidC   TruncNormal_v   M_QKidC V_QKidC 0.76    1.24    );
Distrib(        FracPlasC       TruncNormal_v   M_FracPlasC     V_FracPlasC     0.85    1.15    );


Distrib(        VFatC   TruncNormal_v   M_VFatC V_VFatC 0.1     1.9     );
Distrib(        VGutC   TruncNormal_v   M_VGutC V_VGutC 0.84    1.16    );
Distrib(        VLivC   TruncNormal_v   M_VLivC V_VLivC 0.54    1.46    );
Distrib(        VRapC   TruncNormal_v   M_VRapC V_VRapC 0.84    1.16    );
Distrib(        VRespLumC       TruncNormal_v   M_VRespLumC     V_VRespLumC     0.6     1.4     );
Distrib(        VRespEffC       TruncNormal_v   M_VRespEffC     V_VRespEffC     0.6     1.4     );
Distrib(        VKidC   TruncNormal_v   M_VKidC V_VKidC 0.66    1.34    );
Distrib(        VBldC   TruncNormal_v   M_VBldC V_VBldC 0.76    1.24    );





####Distrib(    lnPBC   TruncNormal_v   M_lnPBC V_lnPBC -0.6    0.6     );
####Distrib(    lnPFatC TruncNormal_v   M_lnPFatC       V_lnPFatC       -0.6    0.6     );
####Distrib(    lnPGutC TruncNormal_v   M_lnPGutC       V_lnPGutC       -1.2    1.2     );
####Distrib(    lnPLivC TruncNormal_v   M_lnPLivC       V_lnPLivC       -1.2    1.2     );
####Distrib(    lnPRapC TruncNormal_v   M_lnPRapC       V_lnPRapC       -1.2    1.2     );
####Distrib(    lnPRespC        TruncNormal_v   M_lnPRespC      V_lnPRespC      -1.2    1.2     );
####Distrib(    lnPKidC TruncNormal_v   M_lnPKidC       V_lnPKidC       -0.6    0.6     );
####Distrib(    lnPSlwC TruncNormal_v   M_lnPSlwC       V_lnPSlwC       -0.9    0.9     );


Distrib(        lnPRBCPlasTCAC  TruncNormal_v   M_lnPRBCPlasTCAC        V_lnPRBCPlasTCAC        -4.605  4.605   );
Distrib(        lnPBodTCAC      TruncNormal_v   M_lnPBodTCAC    V_lnPBodTCAC    -1.008  1.008   );
Distrib(        lnPLivTCAC      TruncNormal_v   M_lnPLivTCAC    V_lnPLivTCAC    -1.008  1.008   );


Distrib(        lnkDissocC      TruncNormal_v   M_lnkDissocC    V_lnkDissocC    -0.18   0.18    );
Distrib(        lnBMaxkDC       TruncNormal_v   M_lnBMaxkDC     V_lnBMaxkDC     -0.546  0.546   );


####Distrib(    lnPBodTCOHC     TruncNormal_v   M_lnPBodTCOHC   V_lnPBodTCOHC   -1.008  1.008   );
####Distrib(    lnPLivTCOHC     TruncNormal_v   M_lnPLivTCOHC   V_lnPLivTCOHC   -1.008  1.008   );
####Distrib(    lnPBodTCOGC     TruncNormal_v   M_lnPBodTCOGC   V_lnPBodTCOGC   -4.605  4.605   );
####Distrib(    lnPLivTCOGC     TruncNormal_v   M_lnPLivTCOGC   V_lnPLivTCOGC   -4.605  4.605   );
####Distrib(    lnPeffDCVG      TruncNormal_v   M_lnPeffDCVG    V_lnPeffDCVG    -6.908  6.908   );


####Distrib(    lnkTSD  TruncNormal_v   M_lnkTSD         V_lnkTSD        -4.269  4.942   );
####Distrib(    lnkAS   TruncNormal_v   M_lnkAS V_lnkAS -6.571  7.244   );
####Distrib(    lnkTD   TruncNormal_v   M_lnkTD V_lnkTD -4.605  0       );
####Distrib(    lnkAD   TruncNormal_v   M_lnkAD V_lnkAD -7.195  6.62    );
####Distrib(    lnkASTCA        TruncNormal_v   M_lnkASTCA      V_lnkASTCA      -7.195  6.62    );
####Distrib(    lnkASTCOH       TruncNormal_v   M_lnkASTCOH     V_lnkASTCOH     -7.195  6.62    );


####Distrib(    lnVMaxC TruncNormal_v   M_lnVMaxC        V_lnVMaxC       -2.079  2.079   );
#####Distrib(   lnKMC   TruncNormal_v   M_lnKMC V_lnKMC 0       1       );
####Distrib(    lnClC   TruncNormal_v   M_lnClC V_lnClC -4.158  4.158   );
####Distrib(    lnFracOtherC    TruncNormal_v   M_lnFracOtherC  V_lnFracOtherC  -6.908  6.908   );
####Distrib(    lnFracTCAC      TruncNormal_v   M_lnFracTCAC    V_lnFracTCAC    -3.489  3.489   );
#####Distrib(   lnVMaxDCVGC     TruncNormal_v   M_lnVMaxDCVGC   V_lnVMaxDCVGC   0       1       );
####Distrib(    lnClDCVGC       TruncNormal_v   M_lnClDCVGC     V_lnClDCVGC     -13.815 13.815  );
####Distrib(    lnKMDCVGC       TruncNormal_v   M_lnKMDCVGC     V_lnKMDCVGC     -4.158  4.158   );
#####Distrib(   lnVMaxKidDCVGC  TruncNormal_v   M_lnVMaxKidDCVGC        V_lnVMaxKidDCVGC        0       1       );
####Distrib(    lnClKidDCVGC    TruncNormal_v   M_lnClKidDCVGC  V_lnClKidDCVGC  -13.815 13.815  );
####Distrib(    lnKMKidDCVGC    TruncNormal_v   M_lnKMKidDCVGC  V_lnKMKidDCVGC  -4.158  4.158   );
####Distrib(    lnVMaxLungLivC  TruncNormal_v   M_lnVMaxLungLivC        V_lnVMaxLungLivC        -3.297  3.297   );
####Distrib(    lnKMClara       TruncNormal_v   M_lnKMClara     V_lnKMClara     -6.908  6.908   );
####Distrib(    lnFracLungSysC  TruncNormal_v   M_lnFracLungSysC        V_lnFracLungSysC        -6.908  6.908   );
```

```
#####Distrib(   lnVMaxTCOHC     TruncNormal_v   M_lnVMaxTCOHC   V_lnVMaxTCOHC   0       1       );
####Distrib(    lnClTCOHC       TruncNormal_v   M_lnClTCOHC     V_lnClTCOHC     -11.513 6.908   );
####Distrib(    lnKMTCOH        TruncNormal_v   M_lnKMTCOH      V_lnKMTCOH      -9.21   9.21    );
#####Distrib(   lnVMaxGlucC     TruncNormal_v   M_lnVMaxGlucC   V_lnVMaxGlucC   0       1       );
####Distrib(    lnClGlucC       TruncNormal_v   M_lnClGlucC     V_lnClGlucC     -9.21   4.605   );
####Distrib(    lnKMGluc        TruncNormal_v   M_lnKMGluc      V_lnKMGluc      -6.908  6.908   );
####Distrib(    lnkMetTCOHC     TruncNormal_v   M_lnkMetTCOHC   V_lnkMetTCOHC   -11.513 6.908   );


Distrib(        lnkUrnTCAC      TruncNormal_v   M_lnkUrnTCAC    V_lnkUrnTCAC    -4.605  4.605   );
Distrib(        lnkMetTCAC      TruncNormal_v   M_lnkMetTCAC    V_lnkMetTCAC    -9.21   4.605   );


####Distrib(    lnkBileC        TruncNormal_v   M_lnkBileC      V_lnkBileC      -9.21   4.605   );
####Distrib(    lnkEHRC TruncNormal_v   M_lnkEHRC       V_lnkEHRC       -9.21   4.605   );
####Distrib(    lnkUrnTCOGC     TruncNormal_v   M_lnkUrnTCOGC   V_lnkUrnTCOGC   -6.908  6.908   );


####Distrib(    lnFracKidDCVCC  TruncNormal_v   M_lnFracKidDCVCC        V_lnFracKidDCVCC        -6.908  6.908   );
####Distrib(    lnkDCVGC        TruncNormal_v   M_lnkDCVGC      V_lnkDCVGC      -9.21   4.605   );


####Distrib(    lnkNATC TruncNormal_v   M_lnkNATC       V_lnkNATC       -9.21   4.605   );
####Distrib(    lnkKidBioactC   TruncNormal_v   M_lnkKidBioactC V_lnkKidBioactC -9.21   4.605   );


Experiment { # 22 ## Paykoc and Powell 1945


 #  #Subject 1, TCA iv, 1.7 g sodium TCA, 45.6 kg
 #  0.03728 g sodium TCA/kg = 37.2 mg NaTCA/kg = 32.9 mg TCA/kg
 # NaTCA MW = 185.4
 # TCA MW = 163.5
 # 1 mg NaTCA equiv to  0.8819 mg TCA

#  lnBW=3.82; ## ln(45.6)

 BWmeas = 45.6;
 Hematocritmeas = 0.39;

# CC= 0;
#Conc=  0;


TChng = 1; # 1 hr infusion
IVDoseTCA=NDoses(2, 32.9 0, 0 1); # Converted to dose-rate in model

 Print( CBldTCA, 10     34      58      82      106     130     154);
 Data(  CBldTCA, 80     57      44      35      28      24      21);
 Print(CPlasTCA, 10     34      58      82      106     130     154);
 Data (CPlasTCA, 140    100     77      61      50      42      37);

Print(  zAUrnTCA,       10      34      58      82      106     130     154     178     202 );
Data(   zAUrnTCA,        189    453     703     928     1075    1148    1224    1284    1332);

Print(  AUrnTCOGTCOH,   0 );
Data(   AUrnTCOGTCOH,   -1 );
Print(  CVen,   0);
Data(   CVen,   -1);
Print(  CTCOH,  0);
Data(   CTCOH,  -1);
 Print( CAlvPPM,        0);
 Data(  CAlvPPM,        -1);
 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 0);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
```

```
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};


Experiment { # 23 ## Paykoc and Powell 1945
 #  Subject 2, TCA iv, 2.9 g sodium TCA, 48.2 kg
 #  0.06016 g sodium TCA/kg = 60.16 mg NaTCA/kg = 53.06 mg TCA/kg
 # NaTCA MW = 185.4
 # TCA MW = 163.5
 # 1 mg NaTCA equiv to  0.8819 mg TCA

#  lnBW=3.875; ## ln(48.2)

 BWmeas = 48.2;
 Hematocritmeas = 0.40;

# CC= 0;
#Conc=  0;
TChng = 1; # 1 hr infusion
IVDoseTCA=NDoses(2, 53.06 0, 0 1); # Converted to dose-rate in model

 Print( CBldTCA, 34     58      82      106     130);
 Data(  CBldTCA, 102    78      62      48      40);
 Print(CPlasTCA, 34     58      82      106     130);
 Data (CPlasTCA, 179    136     108     84      70);

Print(  zAUrnTCA,       34      58      82      106     130     154     178     202);
Data(   zAUrnTCA,       900     1260    1500    1690    1816    1856    1878    1932);


Print(  AUrnTCOGTCOH,   0 );
Data(   AUrnTCOGTCOH,   -1 );
Print(  CVen,   0);
Data(   CVen,   -1);
Print(  CTCOH,  0);
Data(   CTCOH,  -1);
 Print( CAlvPPM,        0);
 Data(  CAlvPPM,        -1);
 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};


Experiment { # 24 ## Paykoc and Powell 1945
 #  Subject 3, TCA iv, 1.8 g sodium TCA, 64 kg
 #  0.028125 g sodium TCA/kg = 28.125 mg NaTCA/kg = 24.80 mg TCA/kg
 # NaTCA MW = 185.4
 # TCA MW = 163.5
 # 1 mg NaTCA equiv to  0.8819 mg TCA

# CC= 0;
#Conc=  0;


 BWmeas = 64;
 Hematocritmeas = 0.45;
```

```
TChng = 1; # 1 hr infusion
IVDoseTCA=NDoses(2, 24.8 0, 0 1); # Converted to dose-rate in model

 Print( CBldTCA, 34     58      82      106);
 Data(  CBldTCA, 65     50      44      32);
 Print(CPlasTCA, 34     58      82      106);
 Data (CPlasTCA, 119    95      83      61);

Print(  zAUrnTCA,       0);
Data(   zAUrnTCA,       -1);

Print(  AUrnTCOGTCOH,   0 );
Data(   AUrnTCOGTCOH,   -1 );
Print(  CVen,   0);
Data(   CVen,   -1);
Print(  CTCOH,  0);
Data(   CTCOH,  -1);
 Print( CAlvPPM,        0);
 Data(  CAlvPPM,        -1);
 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};

}
############# END Paykoc and Powell 1945 individual data ########

############# BEGIN Kimmerle et al. 1973 individual data #########
Level { #Subject level
### FOR KIMMERLE, NO DCVG, DCVC PARAMETERS

Distrib(        lnQCC   TruncNormal_v   M_lnQCC V_lnQCC -0.8    0.8     );

Distrib(        lnVPRC  TruncNormal_v   M_lnVPRC        V_lnVPRC        -0.8    0.8     );

Distrib(        QFatC   TruncNormal_v   M_QFatC V_QFatC 0.08    1.92    );
Distrib(        QGutC   TruncNormal_v   M_QGutC V_QGutC 0.64    1.36    );
Distrib(        QLivC   TruncNormal_v   M_QLivC V_QLivC 0.1     1.9     );
Distrib(        QSlwC   TruncNormal_v   M_QSlwC V_QSlwC 0.36    1.64    );
Distrib(        lnDRespC        TruncNormal_v   M_lnDRespC      V_lnDRespC      -11.513 2.303   );
Distrib(        QKidC   TruncNormal_v   M_QKidC V_QKidC 0.76    1.24    );
Distrib(        FracPlasC       TruncNormal_v   M_FracPlasC     V_FracPlasC     0.85    1.15    );


Distrib(        VFatC   TruncNormal_v   M_VFatC V_VFatC 0.1     1.9     );
Distrib(        VGutC   TruncNormal_v   M_VGutC V_VGutC 0.84    1.16    );
Distrib(        VLivC   TruncNormal_v   M_VLivC V_VLivC 0.54    1.46    );
Distrib(        VRapC   TruncNormal_v   M_VRapC V_VRapC 0.84    1.16    );
Distrib(        VRespLumC       TruncNormal_v   M_VRespLumC     V_VRespLumC     0.6     1.4     );
Distrib(        VRespEffC       TruncNormal_v   M_VRespEffC     V_VRespEffC     0.6     1.4     );
Distrib(        VKidC   TruncNormal_v   M_VKidC V_VKidC 0.66    1.34    );
Distrib(        VBldC   TruncNormal_v   M_VBldC V_VBldC 0.76    1.24    );





Distrib(        lnPBC   TruncNormal_v   M_lnPBC V_lnPBC -0.6    0.6     );
Distrib(        lnPFatC TruncNormal_v   M_lnPFatC       V_lnPFatC       -0.6    0.6     );
Distrib(        lnPGutC TruncNormal_v   M_lnPGutC       V_lnPGutC       -1.2    1.2     );
Distrib(        lnPLivC TruncNormal_v   M_lnPLivC       V_lnPLivC       -1.2    1.2     );
```

```
Distrib(        lnPRapC TruncNormal_v   M_lnPRapC       V_lnPRapC       -1.2    1.2     );
Distrib(        lnPRespC        TruncNormal_v   M_lnPRespC      V_lnPRespC      -1.2    1.2     );
Distrib(        lnPKidC TruncNormal_v   M_lnPKidC       V_lnPKidC       -0.6    0.6     );
Distrib(        lnPSlwC TruncNormal_v   M_lnPSlwC       V_lnPSlwC       -0.9    0.9     );


Distrib(        lnPRBCPlasTCAC  TruncNormal_v   M_lnPRBCPlasTCAC       V_lnPRBCPlasTCAC        -4.605  4.605   );
Distrib(        lnPBodTCAC      TruncNormal_v   M_lnPBodTCAC    V_lnPBodTCAC    -1.008  1.008   );
Distrib(        lnPLivTCAC      TruncNormal_v   M_lnPLivTCAC    V_lnPLivTCAC    -1.008  1.008   );


Distrib(        lnkDissocC      TruncNormal_v   M_lnkDissocC    V_lnkDissocC    -0.18   0.18    );
Distrib(        lnBMaxkDC       TruncNormal_v   M_lnBMaxkDC     V_lnBMaxkDC     -0.546  0.546   );


Distrib(        lnPBodTCOHC     TruncNormal_v   M_lnPBodTCOHC   V_lnPBodTCOHC   -1.008  1.008   );
Distrib(        lnPLivTCOHC     TruncNormal_v   M_lnPLivTCOHC   V_lnPLivTCOHC   -1.008  1.008   );
Distrib(        lnPBodTCOGC     TruncNormal_v   M_lnPBodTCOGC   V_lnPBodTCOGC   -4.605  4.605   );
Distrib(        lnPLivTCOGC     TruncNormal_v   M_lnPLivTCOGC   V_lnPLivTCOGC   -4.605  4.605   );
####Distrib(    lnPeffDCVG      TruncNormal_v   M_lnPeffDCVG    V_lnPeffDCVG    -6.908  6.908   );


####Distrib(    lnkTSD  TruncNormal_v   M_lnkTSD        V_lnkTSD        -4.269  4.942   );
####Distrib(    lnkAS   TruncNormal_v   M_lnkAS V_lnkAS -6.571  7.244   );
####Distrib(    lnkTD   TruncNormal_v   M_lnkTD V_lnkTD -4.605  0       );
####Distrib(    lnkAD   TruncNormal_v   M_lnkAD V_lnkAD -7.195  6.62    );
####Distrib(    lnkASTCA        TruncNormal_v   M_lnkASTCA      V_lnkASTCA      -7.195  6.62    );
####Distrib(    lnkASTCOH       TruncNormal_v   M_lnkASTCOH     V_lnkASTCOH     -7.195  6.62    );


Distrib(        lnVMaxC TruncNormal_v   M_lnVMaxC       V_lnVMaxC       -2.079  2.079   );
#Distrib(       lnKMC   TruncNormal_v   M_lnKMC V_lnKMC 0       1       );
Distrib(        lnClC   TruncNormal_v   M_lnClC V_lnClC -4.158  4.158   );
Distrib(        lnFracOtherC    TruncNormal_v   M_lnFracOtherC  V_lnFracOtherC  -6.908  6.908   );
Distrib(        lnFracTCAC      TruncNormal_v   M_lnFracTCAC    V_lnFracTCAC    -3.489  3.489   );
#Distrib(       lnVMaxDCVGC     TruncNormal_v   M_lnVMaxDCVGC   V_lnVMaxDCVGC   0       1       );
Distrib(        lnClDCVGC       TruncNormal_v   M_lnClDCVGC     V_lnClDCVGC     -13.815 13.815  );
Distrib(        lnKMDCVGC       TruncNormal_v   M_lnKMDCVGC     V_lnKMDCVGC     -4.158  4.158   );
#Distrib(       lnVMaxKidDCVGC  TruncNormal_v   M_lnVMaxKidDCVGC        V_lnVMaxKidDCVGC        0       1       );
Distrib(        lnClKidDCVGC    TruncNormal_v   M_lnClKidDCVGC  V_lnClKidDCVGC  -13.815 13.815  );
Distrib(        lnKMKidDCVGC    TruncNormal_v   M_lnKMKidDCVGC  V_lnKMKidDCVGC  -4.158  4.158   );
Distrib(        lnVMaxLungLivC  TruncNormal_v   M_lnVMaxLungLivC        V_lnVMaxLungLivC        -3.297  3.297   );
Distrib(        lnKMClara       TruncNormal_v   M_lnKMClara     V_lnKMClara     -6.908  6.908   );
Distrib(        lnFracLungSysC  TruncNormal_v   M_lnFracLungSysC        V_lnFracLungSysC        -6.908  6.908   );


#Distrib(       lnVMaxTCOHC     TruncNormal_v   M_lnVMaxTCOHC   V_lnVMaxTCOHC   0       1       );
Distrib(        lnClTCOHC       TruncNormal_v   M_lnClTCOHC     V_lnClTCOHC     -11.513 6.908   );
Distrib(        lnKMTCOH        TruncNormal_v   M_lnKMTCOH      V_lnKMTCOH      -9.21   9.21    );
#Distrib(       lnVMaxGlucC     TruncNormal_v   M_lnVMaxGlucC   V_lnVMaxGlucC   0       1       );
Distrib(        lnClGlucC       TruncNormal_v   M_lnClGlucC     V_lnClGlucC     -9.21   4.605   );
Distrib(        lnKMGluc        TruncNormal_v   M_lnKMGluc      V_lnKMGluc      -6.908  6.908   );
Distrib(        lnkMetTCOHC     TruncNormal_v   M_lnkMetTCOHC   V_lnkMetTCOHC   -11.513 6.908   );


Distrib(        lnkUrnTCAC      TruncNormal_v   M_lnkUrnTCAC    V_lnkUrnTCAC    -4.605  4.605   );
Distrib(        lnkMetTCAC      TruncNormal_v   M_lnkMetTCAC    V_lnkMetTCAC    -9.21   4.605   );


Distrib(        lnkBileC        TruncNormal_v   M_lnkBileC      V_lnkBileC      -9.21   4.605   );
Distrib(        lnkEHRC TruncNormal_v   M_lnkEHRC       V_lnkEHRC       -9.21   4.605   );
Distrib(        lnkUrnTCOGC     TruncNormal_v   M_lnkUrnTCOGC   V_lnkUrnTCOGC   -6.908  6.908   );


####Distrib(    lnFracKidDCVCC  TruncNormal_v   M_lnFracKidDCVCC        V_lnFracKidDCVCC        -6.908  6.908   );
####Distrib(    lnkDCVGC        TruncNormal_v   M_lnkDCVGC      V_lnkDCVGC      -9.21   4.605   );


####Distrib(    lnkNATC TruncNormal_v   M_lnkNATC       V_lnkNATC       -9.21   4.605   );
####Distrib(    lnkKidBioactC   TruncNormal_v   M_lnkKidBioactC V_lnkKidBioactC -9.21   4.605   );


Experiment { # 33 ## Kimmerle & Eben 1973; Single exposure;
 #  Subject A - Female, 40 +/- 4 ppm
 #
# CC= 0;

Male = 0.0;

Conc=   NDoses(2,       40      0,      0       4       );

Print(  CAlvPPM,        0); ## only group mean available
Data(   CAlvPPM,        -1);

Print(  CVen,   4       5       6
);
Data(   CVen,   0.196   0.104   0.078
);
Print(  CTCOH,  4       5       6       7       8       24      48      72
); ## Assume is free -- need to check
```

```
Data(   CTCOH,  0.706   0.693   0.614   0.574   0.602   0.473   0.244   0.2
);
Print(  AUrnTCOGTCOH,   4       8       24      48      72      96      120
);
Data(   AUrnTCOGTCOH,   12.046  15.644  41.741  61.959  75.097  81.615  85.263
);
Print(  zAUrnTCA,       4       8       24      48      72      96      120
);
Data(   zAUrnTCA,       1.32    1.645   5.803   18.403  32.335  40.805  48.605
);

# Separate the 8th day collection
UrnMissing=     NDoses( 3,      1       0       1
                                0       168     192);
Print(  AUrnTCOGTCOH_collect,   192);
Data(   AUrnTCOGTCOH_collect,   1.297);
Print(  zAUrnTCA_collect,       192);
Data(   zAUrnTCA_collect,       2.322);

 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
 Print( CBldTCA, 0);
 Data(  CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
};

Experiment { # 34 ## Kimmerle & Eben 1973; Single exposure;
 #  Subject B - Female, 44 +/- 4 ppm
 #
# CC= 0;

Male = 0.0;

Conc=   NDoses(2,       44      0,      0       4       );

Print(  CAlvPPM,        0); ## only group mean available
Data(   CAlvPPM,        -1);

Print(  CVen,   4       5       6       7
);
Data(   CVen,   0.479   0.151   0.109   0.077
);
Print(  CTCOH,  4       5       6       7       8       24      32      48      72
); ## Assume is free -- need to check
Data(   CTCOH,  1.636   1.621   1.335   1.195   1.302   0.525   0.659   0.134   0.096
);
Print(  AUrnTCOGTCOH,   4       8       24      48      72      96
);
Data(   AUrnTCOGTCOH,   8.816   24.94   44.218  60.919  68.921  70.903
);
Print(  zAUrnTCA,       4       8       24      48      72      96
);
Data(   zAUrnTCA,       0.294   1.842   7.027   19.845  31.698  38.408
);

# Separate the 8th day collection
UrnMissing=     NDoses( 3,      1       0       1
                                0       168     192);
Print(  AUrnTCOGTCOH_collect,   192);
Data(   AUrnTCOGTCOH_collect,   0.239);
Print(  zAUrnTCA_collect,       192);
Data(   zAUrnTCA_collect,       3.682);

 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
```

```
 Print( CBldTCA, 0);
 Data(  CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);

};

Experiment { # 35 ## Kimmerle & Eben 1973; Single exposure;
 #  Subject C - Female, 44 +/- 4 ppm
 #
# CC= 0;

Male = 0.0;

Conc=   NDoses(2,       44      0,      0       4       );

Print(  CAlvPPM,        0); ## only group mean available
Data(   CAlvPPM,        -1);

Print(  CVen,   4       5       6       7
);
Data(   CVen,   0.277   0.216   0.113   0.077
);
Print(  CTCOH,  4       5       6       7       8       24      32      48      72
); ## Assume is free -- need to check
Data(   CTCOH,  1.776   1.712   1.465   1.32    1.545   0.521   0.543   0.108   0.05
);
Print(  AUrnTCOGTCOH,   4       8       24      48      72      96
);
Data(   AUrnTCOGTCOH,   23.797  28.703  58.809  85.586  93.276  95.967
);
Print(  zAUrnTCA,       4       8       24      48      72      96
);
Data(   zAUrnTCA,       0.467   1.333   14.093  30.235  42.643  51.288
);

# Separate the 8th day collection
UrnMissing=     NDoses( 3,      1       0       1
                                0       168     192);
Print(  AUrnTCOGTCOH_collect,   192);
Data(   AUrnTCOGTCOH_collect,   0.268);
Print(  zAUrnTCA_collect,       192);
Data(   zAUrnTCA_collect,       1.518);

 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
 Print( CBldTCA, 0);
 Data(  CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
```

```
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);

};

Experiment { # 36 ## Kimmerle & Eben 1973; Single exposure;
 #  Subject D - Female, 44 +/- 4 ppm
 #
# CC= 0;

Male = 0.0;

Conc=   NDoses(2,       44      0,      0       4       );

Print(  CAlvPPM,        0); ## only group mean available
Data(   CAlvPPM,        -1);

Print(  CVen,   4       5       6       7
);
Data(   CVen,   0.256   0.194   0.097   0.077
);
Print(  CTCOH,  4       5       6       7       8       24      32      48      72
); ## Assume is free -- need to check
Data(   CTCOH,  1.49    1.335   1.239   1.172   1.356   0.696   0.668   0.232   0.129
);
Print(  AUrnTCOGTCOH,   4       8       24      48      72      96
);
Data(   AUrnTCOGTCOH,   14.848  44.609  82.283  113.34  126.783 131.251
);
Print(  zAUrnTCA,       4       8       24      48      72      96
);
Data(   zAUrnTCA,       1.273   3.715   18.435  40.529  57.932  69.431
);

# Separate the 8th day collection
UrnMissing=     NDoses( 3,      1       0       1
                                0       168     192);
Print(  AUrnTCOGTCOH_collect,   192);
Data(   AUrnTCOGTCOH_collect,   -1);
Print(  zAUrnTCA_collect,       192);
Data(   zAUrnTCA_collect,       -1);

 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
 Print( CBldTCA, 0);
 Data(  CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);

};

Experiment { # 37 ## Kimmerle & Eben 1973; Single exposure;
 #  Subject E - Male, 40 +/- 4 ppm
 #
# CC= 0;

Conc=   NDoses(2,       40      0,      0       4       );

Print(  CAlvPPM,        0); ## only group mean available
Data(   CAlvPPM,        -1);
```

```
Print(  CVen,   4       5       6
);
Data(   CVen,   0.322   0.117   0.117
);
Print(  CTCOH,  4       5       6       7       8       24      48      72
); ## Assume is free -- need to check
Data(   CTCOH,  0.775   0.66    0.638   0.585   0.574   0.438   0.2     0.141
);
Print(  AUrnTCOGTCOH,   4       8       24      48      72      96      120
);
Data(   AUrnTCOGTCOH,   6.262   15.15   29.19   36.782  42.539  44.553  46.221
);
Print(  zAUrnTCA,       4       8       24      48      72      96      120
);
Data(   zAUrnTCA,       0.426   1.195   6.565   11.965  23.235  32.775  37.96
);

# Separate the 8th day collection
UrnMissing=     NDoses( 3,      1       0       1
                                0       168     192);
Print(  AUrnTCOGTCOH_collect,   192);
Data(   AUrnTCOGTCOH_collect,   1.126);
Print(  zAUrnTCA_collect,       192);
Data(   zAUrnTCA_collect,       1.280);

 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
 Print( CBldTCA, 0);
 Data(  CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);

};

Experiment { # 38 ## Kimmerle & Eben 1973; Single exposure;
 #  Subject F - Male, 40 +/- 4 ppm
 #
# CC= 0;

Conc=   NDoses(2,       40      0,      0       4       );

Print(  CAlvPPM,        0); ## only group mean available
Data(   CAlvPPM,        -1);

Print(  CVen,   4       5       6
);
Data(   CVen,   0.252   0.132   0.08
);
Print(  CTCOH,  4       5       6       7       8       24      48
); ## Assume is free -- need to check
Data(   CTCOH,  0.806   0.681   0.614   0.551   0.504   0.243   0.08
);
Print(  AUrnTCOGTCOH,   4       8       24      48      72      96      120
);
Data(   AUrnTCOGTCOH,   12.878  24.712  58.083  72.72   76.4    77.744  78.599
);
Print(  zAUrnTCA,       4       8       24      48      72      96      120
);
Data(   zAUrnTCA,       0.205   0.489   4.818   17.241  28.511  38.051  43.199
);

# Separate the 8th day collection
UrnMissing=     NDoses( 3,      1       0       1
                                0       168     192);
Print(  AUrnTCOGTCOH_collect,   192);
```

```
Data(   AUrnTCOGTCOH_collect,   0.297);
Print(  zAUrnTCA_collect,       192);
Data(   zAUrnTCA_collect,       2.695);

 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
 Print( CBldTCA, 0);
 Data(  CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);

};

Experiment { # 39 ## Kimmerle & Eben 1973; Single exposure;
 #  Subject G - Male, 40 +/- 4 ppm
 #
# CC= 0;

Conc=   NDoses(2,       40      0,      0       4       );

Print(  CAlvPPM,        0); ## only group mean available
Data(   CAlvPPM,        -1);

Print(  CVen,   4       5       6
);
Data(   CVen,   0.266   0.127   0.078
);
Print(  CTCOH,  4       5       6       7       8       24      48      72
); ## Assume is free -- need to check
Data(   CTCOH,  0.939   0.69    0.812   0.696   0.658   0.339   0.128   0.09
);
Print(  AUrnTCOGTCOH,   4       8       24      48      72      96      120
);
Data(   AUrnTCOGTCOH,   15.053  21.897  62.789  85.28   93.302  95.789  97.177
);
Print(  zAUrnTCA,       4       8       24      48      72      96      120
);
Data(   zAUrnTCA,       0.462   0.822   8.42    19.045  27.681  33.457  39.762
);

# Separate the 8th day collection
UrnMissing=     NDoses( 3,      1       0       1
                                0       168     192);
Print(  AUrnTCOGTCOH_collect,   192);
Data(   AUrnTCOGTCOH_collect,   0.324);
Print(  zAUrnTCA_collect,       192);
Data(   zAUrnTCA_collect,       3.610);

 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
 Print( CBldTCA, 0);
 Data(  CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
```

```
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);

};

Experiment { # 40 ## Kimmerle & Eben 1973; Single exposure;
 #  Subject H - Male, 44 +/- 4 ppm
 #
# CC= 0;

Conc=   NDoses(2,       44      0,      0       4       );

Print(  CAlvPPM,        0); ## only group mean available
Data(   CAlvPPM,        -1);

Print(  CVen,   4       5       6       7
);
Data(   CVen,   0.246   0.131   0.077   0.077
);
Print(  CTCOH,  4       5       6       7       8       24      32      48      72      96
); ## Assume is free -- need to check
Data(   CTCOH,  1.323   1.283   1.191   1.035   1.093   0.551   0.403   0.155   0.098   0.044
);
Print(  AUrnTCOGTCOH,   4       8       24      48      72      96
);
Data(   AUrnTCOGTCOH,   11.722  37.419  92.855  114.296 121.185 123.768
);
Print(  zAUrnTCA,       8       24      48      72      96
);
Data(   zAUrnTCA,       0.585   4.673   11.492  18.063  23.734
);

# Separate the 8th day collection
UrnMissing=     NDoses( 3,      1       0       1
                                0       168     192);
Print(  AUrnTCOGTCOH_collect,   192);
Data(   AUrnTCOGTCOH_collect,   0.234);
Print(  zAUrnTCA_collect,       192);
Data(   zAUrnTCA_collect,       2.108);

 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
 Print( CBldTCA, 0);
 Data(  CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);

};

Experiment { # 41 ## Kimmerle & Eben 1973; Repeated exposure;
 #  Subject J - 48 +/- 3 ppm, 4 hr/day for 5 days
 #  Not clear if M or F (3 males, 1 female in these experiments)
# CC= 0;

Conc=   NDoses(10,      48 0 48 0  48 0  48 0  48 0,
                        0  4 24 28 48 52 72 76 96 100);
```

```
Print(  CVen,   4       5       8                               28      33              52                      76
);
Data(   CVen,   0.42    0.13    0.085                           0.51    0.17            0.408                   0.51
);
Print(  CTCOH,  4       5       8       9       10      24      28      33      48      52      57      72      76      81
); ## Assume is free -- need to check
Data(   CTCOH,  2.047   1.672   1.596   1.406   1.26    1.174   2.002   1.801   0.917   2.38    1.72    0.946   2.58    2.06
);
Print(  AUrnTCOGTCOH,   24      48      72      96      120     144     168
);
Data(   AUrnTCOGTCOH,   46.14   121.6   175.55  238.17  358.26  378.55  396.33
);
Print(  zAUrnTCA,       24      48      72      96      120     144     168
);
Data(   zAUrnTCA,       4.175   19.16   46.72   72.82   124.285 153.321 168.271
);

# Separate the 11-12th day post-exposure collection
UrnMissing=     NDoses( 3,      1       0       1
                                0       384     408);
Print(  AUrnTCOGTCOH_collect,   408);
Data(   AUrnTCOGTCOH_collect,   0.20);
Print(  zAUrnTCA_collect,       408);
Data(   zAUrnTCA_collect,       1.365);

 Print( CAlvPPM,        0);
 Data(  CAlvPPM,        -1);
 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
 Print( CBldTCA, 0);
 Data(  CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);

};

Experiment { # 42 ## Kimmerle & Eben 1973; Repeated exposure;
 #  Subject K - 48 +/- 3 ppm, 4 hr/day for 5 days
 #  Not clear if M or F (3 males, 1 female in these experiments)
# CC= 0;

Conc=   NDoses(10,      48 0 48 0  48 0  48 0  48 0,
                        0  4 24 28 48 52 72 76 96 100);

Print(  CVen,   4       5       8                               28                      52                      76
);
Data(   CVen,   0.34    0.23    0.13                            0.34                    0.476                   0.272
);
Print(  CTCOH,  4       5       8       9       10      24      28      33      48      52      57      72      76      81
); ## Assume is free -- need to check
Data(   CTCOH,  1.958   1.596   1.368   1.204   1.152   1.036   1.82    1.674   0.812   2.01    1.87    0.591   2.322   1.90
);
Print(  AUrnTCOGTCOH,   24      48      72      96      120     144     168     192     216     240     264
);
Data(   AUrnTCOGTCOH,   88.46   214.54  335.72  453.37  557.89  600.5   638.16  643.27  647.1   649.13  650.17
);
Print(  zAUrnTCA,       24      48      72      96      120     144     168     192     216     240     264
);
Data(   zAUrnTCA,       6.613   25.399  75.391  139.375 229.037 271.661 304.179 328.651 346.571 360.221 371.781
);

# Separate the 11-12th day post-exposure collection
UrnMissing=     NDoses( 3,      1       0       1
                                0       384     408);
Print(  AUrnTCOGTCOH_collect,   408);
```

```
Data(   AUrnTCOGTCOH_collect,   0.08);
Print(  zAUrnTCA_collect,       408);
Data(   zAUrnTCA_collect,       2.1);

 Print( CAlvPPM,        0);
 Data(  CAlvPPM,        -1);
 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
 Print( CBldTCA, 0);
 Data(  CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);

};

Experiment { # 43 ## Kimmerle & Eben 1973; Repeated exposure;
 #  Subject L - 48 +/- 3 ppm, 4 hr/day for 5 days
 #  Not clear if M or F (3 males, 1 female in these experiments)
# CC= 0;

Conc=   NDoses(10,      48 0 48 0  48 0  48 0  48 0,
                        0  4 24 28 48 52 72 76 96 100);

Print(  CVen,   4       5       8                               28                      52                      76
);
Data(   CVen,   0.28    1.18    0.09                            0.34                    0.34                    0.34
);
Print(  CTCOH,  4       5       8       9       10      24      28      33      48      52      57      72      76      81
); ## Assume is free -- need to check
Data(   CTCOH,  1.275   1.014   0.9     0.803   0.72    0.567   1.44    1.85    0.55    2.09    1.4     0.676   1.565   1.24
);
Print(  AUrnTCOGTCOH,   24      48      72      96      120     144     168     192     216     240     264
);
Data(   AUrnTCOGTCOH,   63.33   149.89  234.33  320.33  409.94  434.46  440.59  444.02  446.58  447.9   448.61
);
Print(  zAUrnTCA,       24      48      72      96      120     144     168     192     216     240     264
);
Data(   zAUrnTCA,       5.341   17.631  49.311  110.463 187.167 234.983 283.309 319.077 337.788 356.118 372.468
);

# Separate the 11-12th day post-exposure collection
UrnMissing=     NDoses( 3,      1       0       1
                                0       384     408);
Print(  AUrnTCOGTCOH_collect,   408);
Data(   AUrnTCOGTCOH_collect,   0.07);
Print(  zAUrnTCA_collect,       408);
Data(   zAUrnTCA_collect,       2.184);

 Print( CAlvPPM,        0);
 Data(  CAlvPPM,        -1);
 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
 Print( CBldTCA, 0);
 Data(  CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);
```

```
 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);

};

Experiment { # 44 ## Kimmerle & Eben 1973; Repeated exposure;
 #  Subject M - 48 +/- 3 ppm, 4 hr/day for 5 days
 #  Not clear if M or F (3 males, 1 female in these experiments)
# CC= 0;

Conc=   NDoses(10,      48 0 48 0  48 0  48 0  48 0,
                        0  4 24 28 48 52 72 76 96 100);

Print(  CVen,   4       5       8                               28                      52
);
Data(   CVen,   0.17    0.17    0.09                            0.34                    0.272
);
Print(  CTCOH,  4       5       8       9       10      24      28      33      48      52      57      72      76      81
); ## Assume is free -- need to check
Data(   CTCOH,  2.849   2.394   2.28    2.052   1.976   1.296   2.912   2.429   0.825   2.53    2.26    0.473   2.322   2.41
);
Print(  AUrnTCOGTCOH,   24      48      72      96      120     144     168     192     216     240     264
);
Data(   AUrnTCOGTCOH,   116.1   246.68  363.79  458.92  556.48  597.53  638.45  641.52  642.45  642.84  642.97
);
Print(  zAUrnTCA,       24      48      72      96      120     144     168     192     216     240     264
);
Data(   zAUrnTCA,       2.928   12.19   29.482  48.094  111.934 169.81  186.895 206.764 218.839 230.578 239.119
);

# Separate the 11-12th day post-exposure collection
UrnMissing=     NDoses( 3,      1       0       1
                                0       384     408);
Print(  AUrnTCOGTCOH_collect,   408);
Data(   AUrnTCOGTCOH_collect,   -1);
Print(  zAUrnTCA_collect,       408);
Data(   zAUrnTCA_collect,       3.564);

 Print( CAlvPPM,        0);
 Data(  CAlvPPM,        -1);
 Print(TotCTCOH, 1);
 Data (TotCTCOH, -1);
 Print( CBldTCA, 0);
 Data(  CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);

};

}

############# END Kimmerle et al. 1973 individual data #########

############## BEGIN Monster et al. 1976 individual data ####
```

```
Level { #Subject level
### FOR MONSTER, NO DCVG OR DCVC PARAMETERS

Distrib(        lnQCC   TruncNormal_v   M_lnQCC V_lnQCC -0.8    0.8     );

Distrib(        lnVPRC  TruncNormal_v   M_lnVPRC        V_lnVPRC        -0.8    0.8     );

Distrib(        QFatC   TruncNormal_v   M_QFatC V_QFatC 0.08    1.92    );
Distrib(        QGutC   TruncNormal_v   M_QGutC V_QGutC 0.64    1.36    );
Distrib(        QLivC   TruncNormal_v   M_QLivC V_QLivC 0.1     1.9     );
Distrib(        QSlwC   TruncNormal_v   M_QSlwC V_QSlwC 0.36    1.64    );
Distrib(        lnDRespC        TruncNormal_v   M_lnDRespC      V_lnDRespC      -11.513 2.303   );
Distrib(        QKidC   TruncNormal_v   M_QKidC V_QKidC 0.76    1.24    );
Distrib(        FracPlasC       TruncNormal_v   M_FracPlasC     V_FracPlasC     0.85    1.15    );


Distrib(        VFatC   TruncNormal_v   M_VFatC V_VFatC 0.1     1.9     );
Distrib(        VGutC   TruncNormal_v   M_VGutC V_VGutC 0.84    1.16    );
Distrib(        VLivC   TruncNormal_v   M_VLivC V_VLivC 0.54    1.46    );
Distrib(        VRapC   TruncNormal_v   M_VRapC V_VRapC 0.84    1.16    );
Distrib(        VRespLumC       TruncNormal_v   M_VRespLumC     V_VRespLumC     0.6     1.4     );
Distrib(        VRespEffC       TruncNormal_v   M_VRespEffC     V_VRespEffC     0.6     1.4     );
Distrib(        VKidC   TruncNormal_v   M_VKidC V_VKidC 0.66    1.34    );
Distrib(        VBldC   TruncNormal_v   M_VBldC V_VBldC 0.76    1.24    );





Distrib(        lnPBC   TruncNormal_v   M_lnPBC V_lnPBC -0.6    0.6     );
Distrib(        lnPFatC TruncNormal_v   M_lnPFatC       V_lnPFatC       -0.6    0.6     );
Distrib(        lnPGutC TruncNormal_v   M_lnPGutC       V_lnPGutC       -1.2    1.2     );
Distrib(        lnPLivC TruncNormal_v   M_lnPLivC       V_lnPLivC       -1.2    1.2     );
Distrib(        lnPRapC TruncNormal_v   M_lnPRapC       V_lnPRapC       -1.2    1.2     );
Distrib(        lnPRespC        TruncNormal_v   M_lnPRespC      V_lnPRespC      -1.2    1.2     );
Distrib(        lnPKidC TruncNormal_v   M_lnPKidC       V_lnPKidC       -0.6    0.6     );
Distrib(        lnPSlwC TruncNormal_v   M_lnPSlwC       V_lnPSlwC       -0.9    0.9     );


Distrib(        lnPRBCPlasTCAC  TruncNormal_v   M_lnPRBCPlasTCAC        V_lnPRBCPlasTCAC        -4.605  4.605   );
Distrib(        lnPBodTCAC      TruncNormal_v   M_lnPBodTCAC    V_lnPBodTCAC    -1.008  1.008   );
Distrib(        lnPLivTCAC      TruncNormal_v   M_lnPLivTCAC    V_lnPLivTCAC    -1.008  1.008   );


Distrib(        lnkDissocC      TruncNormal_v   M_lnkDissocC    V_lnkDissocC    -0.18   0.18    );
Distrib(        lnBMaxkDC       TruncNormal_v   M_lnBMaxkDC     V_lnBMaxkDC     -0.546  0.546   );


Distrib(        lnPBodTCOHC     TruncNormal_v   M_lnPBodTCOHC   V_lnPBodTCOHC   -1.008  1.008   );
Distrib(        lnPLivTCOHC     TruncNormal_v   M_lnPLivTCOHC   V_lnPLivTCOHC   -1.008  1.008   );
Distrib(        lnPBodTCOGC     TruncNormal_v   M_lnPBodTCOGC   V_lnPBodTCOGC   -4.605  4.605   );
Distrib(        lnPLivTCOGC     TruncNormal_v   M_lnPLivTCOGC   V_lnPLivTCOGC   -4.605  4.605   );
####Distrib(    lnPeffDCVG      TruncNormal_v   M_lnPeffDCVG    V_lnPeffDCVG    -6.908  6.908   );


####Distrib(    lnkTSD  TruncNormal_v   M_lnkTSD        V_lnkTSD        -4.269  4.942   );
####Distrib(    lnkAS   TruncNormal_v   M_lnkAS V_lnkAS -6.571  7.244   );
####Distrib(    lnkTD   TruncNormal_v   M_lnkTD V_lnkTD -4.605  0       );
####Distrib(    lnkAD   TruncNormal_v   M_lnkAD V_lnkAD -7.195  6.62    );
####Distrib(    lnkASTCA        TruncNormal_v   M_lnkASTCA      V_lnkASTCA      -7.195  6.62    );
####Distrib(    lnkASTCOH       TruncNormal_v   M_lnkASTCOH     V_lnkASTCOH     -7.195  6.62    );


Distrib(        lnVMaxC TruncNormal_v   M_lnVMaxC        V_lnVMaxC       -2.079  2.079   );
#Distrib(       lnKMC   TruncNormal_v   M_lnKMC V_lnKMC 0       1       );
Distrib(        lnClC   TruncNormal_v   M_lnClC V_lnClC -4.158  4.158   );
Distrib(        lnFracOtherC    TruncNormal_v   M_lnFracOtherC  V_lnFracOtherC  -6.908  6.908   );
Distrib(        lnFracTCAC      TruncNormal_v   M_lnFracTCAC    V_lnFracTCAC    -3.489  3.489   );
#Distrib(       lnVMaxDCVGC     TruncNormal_v   M_lnVMaxDCVGC   V_lnVMaxDCVGC   0       1       );
Distrib(        lnClDCVGC       TruncNormal_v   M_lnClDCVGC     V_lnClDCVGC     -13.815 13.815  );
Distrib(        lnKMDCVGC       TruncNormal_v   M_lnKMDCVGC     V_lnKMDCVGC     -4.158  4.158   );
#Distrib(       lnVMaxKidDCVGC  TruncNormal_v   M_lnVMaxKidDCVGC        V_lnVMaxKidDCVGC        0       1       );
Distrib(        lnClKidDCVGC    TruncNormal_v   M_lnClKidDCVGC  V_lnClKidDCVGC  -13.815 13.815  );
Distrib(        lnKMKidDCVGC    TruncNormal_v   M_lnKMKidDCVGC  V_lnKMKidDCVGC  -4.158  4.158   );
Distrib(        lnVMaxLungLivC  TruncNormal_v   M_lnVMaxLungLivC        V_lnVMaxLungLivC        -3.297  3.297   );
Distrib(        lnKMClara       TruncNormal_v   M_lnKMClara     V_lnKMClara     -6.908  6.908   );
Distrib(        lnFracLungSysC  TruncNormal_v   M_lnFracLungSysC        V_lnFracLungSysC        -6.908  6.908   );


#Distrib(       lnVMaxTCOHC     TruncNormal_v   M_lnVMaxTCOHC   V_lnVMaxTCOHC   0       1       );
Distrib(        lnClTCOHC       TruncNormal_v   M_lnClTCOHC     V_lnClTCOHC     -11.513 6.908   );
Distrib(        lnKMTCOH        TruncNormal_v   M_lnKMTCOH      V_lnKMTCOH      -9.21   9.21    );
#Distrib(       lnVMaxGlucC     TruncNormal_v   M_lnVMaxGlucC   V_lnVMaxGlucC   0       1       );
Distrib(        lnClGlucC       TruncNormal_v   M_lnClGlucC     V_lnClGlucC     -9.21   4.605   );
Distrib(        lnKMGluc        TruncNormal_v   M_lnKMGluc      V_lnKMGluc      -6.908  6.908   );
Distrib(        lnkMetTCOHC     TruncNormal_v   M_lnkMetTCOHC   V_lnkMetTCOHC   -11.513 6.908   );


Distrib(        lnkUrnTCAC      TruncNormal_v   M_lnkUrnTCAC    V_lnkUrnTCAC    -4.605  4.605   );
```

```
Distrib(        lnkMetTCAC      TruncNormal_v   M_lnkMetTCAC    V_lnkMetTCAC    -9.21   4.605   );


Distrib(        lnkBileC        TruncNormal_v   M_lnkBileC      V_lnkBileC      -9.21   4.605   );
Distrib(        lnkEHRC TruncNormal_v   M_lnkEHRC        V_lnkEHRC        -9.21   4.605   );
Distrib(        lnkUrnTCOGC     TruncNormal_v   M_lnkUrnTCOGC   V_lnkUrnTCOGC   -6.908  6.908   );


####Distrib(    lnFracKidDCVCC  TruncNormal_v   M_lnFracKidDCVCC        V_lnFracKidDCVCC        -6.908  6.908   );
####Distrib(    lnkDCVGC        TruncNormal_v   M_lnkDCVGC      V_lnkDCVGC      -9.21   4.605   );


####Distrib(    lnkNATC TruncNormal_v   M_lnkNATC        V_lnkNATC        -9.21   4.605   );
####Distrib(    lnkKidBioactC   TruncNormal_v   M_lnkKidBioactC V_lnkKidBioactC -9.21   4.605   );

Level { # Subject A

 Experiment { # 45 ## Monster Subject A, lower dose
 # Data from Monster et al. (1976)
 #  Male
# CC= 0;


#       BW=     70      PctFat= 0.12
#       lnBW=   4.248495242     ;       VFatC=  0.560747664     ;
        BWmeas = 70.0;
        VFatCmeas = 0.12;

#       MV=     7.7
        Conc=   NDoses(2,       65      0,      0       4       );
        QPmeas= 210; # NDoses(2, 210 0, 0.0 4.0);

Print(  RetDose,        4);
Data(   RetDose,        320);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 210     );
        Print(  CAlvPPM,        4.5     6       23.75   48      72      );
        Data(   CAlvPPM,        3.766118721     1.842123288     0.122808219     0.034795662     0.020877397     );
        Print(  CVen,   3.5     6       23.75   );
        Data(   CVen,   1.2     0.13    0.01    );
        Print(  TotCTCOH,       3.5     6       23.75   );
        Data(   TotCTCOH,       4.3     4.4     1.1     );
        Print(  CBldTCA,        3.5     6       23.75   48      72      );
        Data(   CBldTCA,        3.6     5.7     10.1    11.4    11.8    );
        Print(  AUrnTCOGTCOH,   16      24      32      40      48      56      64      72      80      88      );
        Data(   AUrnTCOGTCOH,   31.5445 84.4675 119.4505        146.3605        157.573 163.553 169.0845        176.709 179.
        Print(  zAUrnTCA,       16      24      32      40      48      56      64      72      80      88      );
        Data(   zAUrnTCA,       1.1445  3.27    5.232   8.502   9.9735  10.791  12.099  14.388  15.5325 16.8405 );


 Print(CTCOH, 1);
 Data (CTCOH, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};

 Experiment { # 46 ## Monster Subject A, higher dose
 # Data from Monster et al. (1976)
 #  Male
# CC= 0;


#       BW=     70      PctFat= 0.12
```

```
#       lnBW=   4.248495242     ;       VFatC=  0.560747664     ;
        BWmeas = 70.0;
        VFatCmeas = 0.12;

#       MV=     8.9
        Conc=   NDoses(2,       140     0,      0       4       );
        QPmeas= 282; # NDoses(2, 282 0, 0.0 4.0);
Print(  RetDose,        4);
Data(   RetDose,        740);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 282     );
        Print(  CAlvPPM,        4.5     6.5     23.5    48      );
        Data(   CAlvPPM,        5.989968911     2.572163121     0.28188089      0.070470222     );
        Print(  CVen,   6.5     23.5    48      72      );
        Data(   CVen,   0.28    0.014   0.005   0.0025  );
        Print(  TotCTCOH,       3.99    6.5     23.5    48      72      );
        Data(   TotCTCOH,       6.1     7.2     2.9     0.72    0.15    );
        Print(  CBldTCA,        3.99    6.5     23.5    48      72      142     214     479     );
        Data(   CBldTCA,        5.2     9       15      20      17.5    12.5    7.4     1.5     );
        Print(  AUrnTCOGTCOH,   16      24      32      40      48      56      64      72      80      );
        Data(   AUrnTCOGTCOH,   58.305  164.5995        246.675 295.113 326.209 340.561 353.418 360.594 364.481 );
        Print(  zAUrnTCA,       16      24      32      40      48      56      64      72      80      );
        Data(   zAUrnTCA,       0.8175  3.597   5.559   9.81    13.8975 17.1675 22.563  26.9775 28.9395 );

 Print(CTCOH, 1);
 Data (CTCOH, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};

}

Level { # Subject B

 Experiment { # 47 ## Monster Subject B, lower dose
 # Data from Monster et al. (1976)
 #  Male
# CC= 0;


#       BW=     80      PctFat= 0.26
#       lnBW=   4.382026635     ;       VFatC=  1.214953271     ;
        BWmeas = 80.0;
        VFatCmeas = 0.26;

#       MV=     10.7
        Conc=   NDoses(2,       68      0,      0       4       );
        QPmeas= 390; # NDoses(2, 390 0, 0.0 4.0);
Print(  RetDose,        4);
Data(   RetDose,        430);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 390     );
        Print(  CAlvPPM,        4.083   4.5     22      48      80      );
        Data(   CAlvPPM,        3.675658588     1.531524412     0.245043906     0.110269758     0.076882525     );
        Print(  CVen,   3.5     6       22.83333333     47      72      );
        Data(   CVen,   1.5     0.16    0.0156  0.0065  0.0034  );
        Print(  TotCTCOH,       3.5     6       22.83333333     47      );
        Data(   TotCTCOH,       2.9     2.5     0.45    0.15    );
        Print(  CBldTCA,        3.5     6       22.83333333     47      72      142     214     );
        Data(   CBldTCA,        4       6.6     9.1     8.9     8.8     4.5     2.4     );
        Print(  AUrnTCOGTCOH,   16      24      32      40      48      56      64      72      80      88      );
        Data(   AUrnTCOGTCOH,   41.86   92.391  117.507 136.4935        148.1545        155.6295        162.5065        167.
        Print(  zAUrnTCA,       8       16      24      32      40      48      56      64      72      80      88      );
```

```
        Data(   zAUrnTCA,       0.4905  2.1255  7.0305  11.9355 19.7835 25.3425 29.103  34.989  41.856  46.2705 51.5025 );

 Print(CTCOH, 1);
 Data (CTCOH, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};

 Experiment { # 48 ## Monster Subject B, higher dose
 # Data from Monster et al. (1976)
 #  Male
# CC= 0;


#       BW=     80      PctFat= 0.26
#       lnBW=   4.382026635     ;       VFatC=  1.214953271     ;
        BWmeas = 80.0;
        VFatCmeas = 0.26;
#       MV=     10.4
        Conc=   NDoses(2,       138     0,      0       4       );
        QPmeas= 372; # NDoses(2, 372 0, 0.0 4.0);
Print(  RetDose,        4);
Data(   RetDose,        790);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 372     );
        Print(  CAlvPPM,        4.083   6       24      56      95      );
        Data(   CAlvPPM,        4.993960819     3.433348063     0.343334806     0.103000442     0.043697157     );
        Print(  CVen,   6.5     23      47.33333333     72.33333333     94.5    );
        Data(   CVen,   0.22    0.028   0.0085  0.0048  0.0011  );
        Print(  TotCTCOH,       3.99    6.5     23      47.33333333     72.33333333     94.5    );
        Data(   TotCTCOH,       4.5     3.9     1.2     0.35    0.11    0.03    );
        Print(  CBldTCA,        3.99    6.5     23      47.33333333     72.33333333     94.5    164     260     404     );
        Data(   CBldTCA,        4       6.6     12      13      11      10      5.4     1.6     0.04    );
        Print(  AUrnTCOGTCOH,   16      24      32      40      48      56      64      72      80      );
        Data(   AUrnTCOGTCOH,   74.75   181.493 232.7715        272.09  301.99  315.445 324.415 331.292 336.076 );
        Print(  zAUrnTCA,       16      24      32      40      48      56      64      72      80      );
        Data(   zAUrnTCA,       1.7985  8.829   14.715  26.487  39.24   47.415  55.59   64.419  71.1225 );

 Print(CTCOH, 1);
 Data (CTCOH, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
```

```
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};

}

Level { # Subject C

 Experiment { # 49 ## Monster Subject C, lower dose
 # Data from Monster et al. (1976)
 #  Male
# CC= 0;


#       BW=     62      PctFat= 0.14
#       lnBW=   4.127134385     ;       VFatC=  0.654205607     ;
        BWmeas = 62.0;
        VFatCmeas = 0.14;

#       MV=     8.5
        Conc=   NDoses(2,       70      0,      0       4       );
        QPmeas= 258; # NDoses(2, 258 0, 0.0 4.0);
Print(  RetDose,        4);
Data(   RetDose,        330);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 258     );
        Print(  CAlvPPM,        4.5     6       22.5    47.75   70.5    );
        Data(   CAlvPPM,        5.517282574     3.678188383     0.239082245     0.062529203     0.018390942     );
        Print(  CVen,   3.583333333     6       22.5    47.75   );
        Data(   CVen,   1.6     0.18    0.011   0.0023  );
        Print(  TotCTCOH,       3.583333333     6       22.5    );
        Data(   TotCTCOH,       2.8     2.7     0.51    );
        Print(  CBldTCA,        3.583333333     6       22.5    47.75   70.5    134     214     454     );
        Data(   CBldTCA,        3.1     5.2     7.8     8.1     6.2     4.1     2.1     0.04    );
        Print(  AUrnTCOGTCOH,   16      24      32      40      48      56      64      72      80      88      );
        Data(   AUrnTCOGTCOH,   35.88   91.6435 116.909 134.849 145.1645        149.6495        153.088 155.48  156.676 157.
        Print(  zAUrnTCA,       16      24      32      40      48      56      64      72      80      88      );
        Data(   zAUrnTCA,       1.4715  4.7415  7.521   14.715  20.4375 22.563  26.814  31.2285 33.354  36.1335 );

 Print(CTCOH, 1);
 Data (CTCOH, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};

 Experiment { # 50 ## Monster Subject C, higher dose
 # Data from Monster et al. (1976)
 #  Male
# CC= 0;


#       BW=     62      PctFat= 0.14
#       lnBW=   4.127134385     ;       VFatC=  0.654205607     ;
        BWmeas = 62.0;
        VFatCmeas = 0.14;
#       MV=     9.8
        Conc=   NDoses(2,       142     0,      0       4       );
        QPmeas= 336; # NDoses(2, 336 0, 0.0 4.0);
Print(  RetDose,        4);
```

```
Data(   RetDose,        710);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 336     );
        Print(  CAlvPPM,        4.5     6       23.33333333     48.16666667     71.5    );
        Data(   CAlvPPM,        4.884417808     2.767836758     0.325627854     0.11071347      0.035819064     );
        Print(  CVen,   6       23.33333333     48.16666667     71.5    );
        Data(   CVen,   0.25    0.022   0.0054  0.0025  );
        Print(  TotCTCOH,       3.99    6       23.33333333     48.16666667     71.5    );
        Data(   TotCTCOH,       5.2     5.1     1.6     0.34    0.06    );
        Print(  CBldTCA,        3.99    6       23.33333333     48.16666667     71.5    191     263     407     );
        Data(   CBldTCA,        3.6     6.5     12      11      10      5.8     3.8     1.5     );
        Print(  AUrnTCOGTCOH,   16      24      32      40      48      56      64      72      80      88      96      104
        Data(   AUrnTCOGTCOH,   49.933  132.457 178.204 210.3465        226.7915        239.499 242.19  247.871 250.861 251.
        Print(  zAUrnTCA,       16      24      32      40      48      56      64      72      80      88      96      104
        Data(   zAUrnTCA,       0.654   2.4525  4.251   11.118  15.696  22.7265 25.3425 31.2285 36.297  41.202  45.6165 48.0

 Print(CTCOH, 1);
 Data (CTCOH, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};

}

Level { # Subject D

 Experiment { # 51 ## Monster Subject D, lower dose
 # Data from Monster et al. (1976)
 #  Male
 #CC= 0;


#       BW=     67      PctFat= 0.09
#       lnBW=   4.204692619     ;       VFatC=  0.420560748     ;
        BWmeas = 67.;
        VFatCmeas = 0.09;
#       MV=     11.6
        Conc=   NDoses(2,       76      0,      0       4       );
        QPmeas= 444; # NDoses(2, 444 0, 0.0 4.0);
Print(  RetDose,        4);
Data(   RetDose,        470);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 444     );
        Print(  CAlvPPM,        4.5     6       24.08333333     48.16666667     72      );
        Data(   CAlvPPM,        4.666913489     2.10011107      0.204177465     0.06125324      0.020417747     );
        Print(  CVen,   6       24.08333333     48.16666667     );
        Data(   CVen,   0.175   0.0088  0.0025  );
        Print(  TotCTCOH,       3.416666667     6       24.08333333     48.16666667     );
        Data(   TotCTCOH,       3.2     3.2     0.6     0.11    );
        Print(  CBldTCA,        3.416666667     6       24.08333333     48.16666667     72      142     214     504     );
        Data(   CBldTCA,        2.4     4.5     9       11.6    9.8     5.4     2.6     0.25    );
        Print(  AUrnTCOGTCOH,   16      24      32      40      48      56      64      72      80      88      96      );
        Data(   AUrnTCOGTCOH,   49.7835 121.5435        153.088 179.5495        192.257 198.237 202.124 207.3565        209.
        Print(  zAUrnTCA,       16      24      32      40      48      56      64      72      80      88      96      );
        Data(   zAUrnTCA,       1.308   3.27    5.886   12.9165 21.582  25.6695 30.2475 35.316  39.4035 44.799  51.339  );

 Print(CTCOH, 1);
 Data (CTCOH, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
```

```
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};

 Experiment { # 52 ## Monster Subject D, higher dose
 # Data from Monster et al. (1976)
 #  Male
 #CC= 0;


#       BW=     67      PctFat= 0.09
#       lnBW=   4.204692619     ;       VFatC=  0.420560748     ;
        BWmeas = 67.0;
        VFatCmeas = 0.09;

#       MV=     12.3
        Conc=   NDoses(2,       140     0,      0       4       );
        QPmeas= 486; # NDoses(2, 486 0, 0.0 4.0);
Print(  RetDose,        4);
Data(   RetDose,        790);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 486     );
        Print(  CAlvPPM,        4.5     6.416666667     23.25   48.91666667     72.66666667     );
        Data(   CAlvPPM,        4.520886183     2.542998478     0.268427617     0.062162185     0.025429985     );
        Print(  CVen,   3.99    6.416666667     23.25   48.91666667     72.66666667     );
        Data(   CVen,   3.1     0.26    0.019   0.004   0.002   );
        Print(  TotCTCOH,       3.99    6.416666667     23.25   48.91666667     72.66666667     );
        Data(   TotCTCOH,       5       5.5     1.7     0.35    0.06    );
        Print(  CBldTCA,        3.99    6.416666667     23.25   48.91666667     72.66666667     144     216     );
        Data(   CBldTCA,        3.3     6.4     11      14      12.5    5.3     3.4     );
        Print(  AUrnTCOGTCOH,   16      24      32      40      48      56      64      72      80      88      96      104
        Data(   AUrnTCOGTCOH,   74.75   222.755 290.7775        332.6375        355.0625        366.1255        374.4975
        Print(  zAUrnTCA,       16      24      32      40      48      56      64      72      80      88      96      104
        Data(   zAUrnTCA,       1.635   8.829   17.004  25.6695 40.548  49.8675 60.168  74.229  80.9325 89.271  100.5525

 Print(CTCOH, 1);
 Data (CTCOH, -1);
 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};
```

```
}

}
############# END Monster et al. 1976 individual data #########

############# BEGIN CHIU et al. 2006 individual data ##########
Level { #Subject level
### FOR CHIU, NO DCVG OR DCVC PARAMETERS

Distrib(        lnQCC   TruncNormal_v   M_lnQCC V_lnQCC -0.8    0.8     );

Distrib(        lnVPRC  TruncNormal_v   M_lnVPRC        V_lnVPRC        -0.8    0.8     );

Distrib(        QFatC   TruncNormal_v   M_QFatC V_QFatC 0.08    1.92    );
Distrib(        QGutC   TruncNormal_v   M_QGutC V_QGutC 0.64    1.36    );
Distrib(        QLivC   TruncNormal_v   M_QLivC V_QLivC 0.1     1.9     );
Distrib(        QSlwC   TruncNormal_v   M_QSlwC V_QSlwC 0.36    1.64    );
Distrib(        lnDRespC        TruncNormal_v   M_lnDRespC      V_lnDRespC      -11.513 2.303   );
Distrib(        QKidC   TruncNormal_v   M_QKidC V_QKidC 0.76    1.24    );
Distrib(        FracPlasC       TruncNormal_v   M_FracPlasC     V_FracPlasC     0.85    1.15    );


Distrib(        VFatC   TruncNormal_v   M_VFatC V_VFatC 0.1     1.9     );
Distrib(        VGutC   TruncNormal_v   M_VGutC V_VGutC 0.84    1.16    );
Distrib(        VLivC   TruncNormal_v   M_VLivC V_VLivC 0.54    1.46    );
Distrib(        VRapC   TruncNormal_v   M_VRapC V_VRapC 0.84    1.16    );
Distrib(        VRespLumC       TruncNormal_v   M_VRespLumC     V_VRespLumC     0.6     1.4     );
Distrib(        VRespEffC       TruncNormal_v   M_VRespEffC     V_VRespEffC     0.6     1.4     );
Distrib(        VKidC   TruncNormal_v   M_VKidC V_VKidC 0.66    1.34    );
Distrib(        VBldC   TruncNormal_v   M_VBldC V_VBldC 0.76    1.24    );





Distrib(        lnPBC   TruncNormal_v   M_lnPBC V_lnPBC -0.6    0.6     );
Distrib(        lnPFatC TruncNormal_v   M_lnPFatC       V_lnPFatC       -0.6    0.6     );
Distrib(        lnPGutC TruncNormal_v   M_lnPGutC       V_lnPGutC       -1.2    1.2     );
Distrib(        lnPLivC TruncNormal_v   M_lnPLivC       V_lnPLivC       -1.2    1.2     );
Distrib(        lnPRapC TruncNormal_v   M_lnPRapC       V_lnPRapC       -1.2    1.2     );
Distrib(        lnPRespC        TruncNormal_v   M_lnPRespC      V_lnPRespC      -1.2    1.2     );
Distrib(        lnPKidC TruncNormal_v   M_lnPKidC       V_lnPKidC       -0.6    0.6     );
Distrib(        lnPSlwC TruncNormal_v   M_lnPSlwC       V_lnPSlwC       -0.9    0.9     );


Distrib(        lnPRBCPlasTCAC  TruncNormal_v   M_lnPRBCPlasTCAC        V_lnPRBCPlasTCAC        -4.605  4.605   );
Distrib(        lnPBodTCAC      TruncNormal_v   M_lnPBodTCAC    V_lnPBodTCAC    -1.008  1.008   );
Distrib(        lnPLivTCAC      TruncNormal_v   M_lnPLivTCAC    V_lnPLivTCAC    -1.008  1.008   );


Distrib(        lnkDissocC      TruncNormal_v   M_lnkDissocC    V_lnkDissocC    -0.18   0.18    );
Distrib(        lnBMaxkDC       TruncNormal_v   M_lnBMaxkDC     V_lnBMaxkDC     -0.546  0.546   );


Distrib(        lnPBodTCOHC     TruncNormal_v   M_lnPBodTCOHC   V_lnPBodTCOHC   -1.008  1.008   );
Distrib(        lnPLivTCOHC     TruncNormal_v   M_lnPLivTCOHC   V_lnPLivTCOHC   -1.008  1.008   );
Distrib(        lnPBodTCOGC     TruncNormal_v   M_lnPBodTCOGC   V_lnPBodTCOGC   -4.605  4.605   );
Distrib(        lnPLivTCOGC     TruncNormal_v   M_lnPLivTCOGC   V_lnPLivTCOGC   -4.605  4.605   );
####Distrib(    lnPeffDCVG      TruncNormal_v   M_lnPeffDCVG    V_lnPeffDCVG    -6.908  6.908   );


####Distrib(    lnkTSD  TruncNormal_v   M_lnkTSD        V_lnkTSD        -4.269  4.942   );
####Distrib(    lnkAS   TruncNormal_v   M_lnkAS V_lnkAS -6.571  7.244   );
####Distrib(    lnkTD   TruncNormal_v   M_lnkTD V_lnkTD -4.605  0       );
####Distrib(    lnkAD   TruncNormal_v   M_lnkAD V_lnkAD -7.195  6.62    );
####Distrib(    lnkASTCA        TruncNormal_v   M_lnkASTCA      V_lnkASTCA      -7.195  6.62    );
####Distrib(    lnkASTCOH       TruncNormal_v   M_lnkASTCOH     V_lnkASTCOH     -7.195  6.62    );


Distrib(        lnVMaxC TruncNormal_v   M_lnVMaxC        V_lnVMaxC       -2.079  2.079   );
#Distrib(       lnKMC   TruncNormal_v   M_lnKMC V_lnKMC 0       1       );
Distrib(        lnClC   TruncNormal_v   M_lnClC V_lnClC -4.158  4.158   );
Distrib(        lnFracOtherC    TruncNormal_v   M_lnFracOtherC  V_lnFracOtherC  -6.908  6.908   );
Distrib(        lnFracTCAC      TruncNormal_v   M_lnFracTCAC    V_lnFracTCAC    -3.489  3.489   );
#Distrib(       lnVMaxDCVGC     TruncNormal_v   M_lnVMaxDCVGC   V_lnVMaxDCVGC   0       1       );
Distrib(        lnClDCVGC       TruncNormal_v   M_lnClDCVGC     V_lnClDCVGC     -13.815 13.815  );
Distrib(        lnKMDCVGC       TruncNormal_v   M_lnKMDCVGC     V_lnKMDCVGC     -4.158  4.158   );
#Distrib(       lnVMaxKidDCVGC  TruncNormal_v   M_lnVMaxKidDCVGC        V_lnVMaxKidDCVGC        0       1       );
Distrib(        lnClKidDCVGC    TruncNormal_v   M_lnClKidDCVGC  V_lnClKidDCVGC  -13.815 13.815  );
Distrib(        lnKMKidDCVGC    TruncNormal_v   M_lnKMKidDCVGC  V_lnKMKidDCVGC  -4.158  4.158   );
Distrib(        lnVMaxLungLivC  TruncNormal_v   M_lnVMaxLungLivC        V_lnVMaxLungLivC        -3.297  3.297   );
Distrib(        lnKMClara       TruncNormal_v   M_lnKMClara     V_lnKMClara     -6.908  6.908   );
Distrib(        lnFracLungSysC  TruncNormal_v   M_lnFracLungSysC        V_lnFracLungSysC        -6.908  6.908   );


#Distrib(       lnVMaxTCOHC     TruncNormal_v   M_lnVMaxTCOHC   V_lnVMaxTCOHC   0       1       );
Distrib(        lnClTCOHC       TruncNormal_v   M_lnClTCOHC     V_lnClTCOHC     -11.513 6.908   );
Distrib(        lnKMTCOH        TruncNormal_v   M_lnKMTCOH      V_lnKMTCOH      -9.21   9.21    );
#Distrib(       lnVMaxGlucC     TruncNormal_v   M_lnVMaxGlucC   V_lnVMaxGlucC   0       1       );
```

```
Distrib(        lnClGlucC       TruncNormal_v   M_lnClGlucC     V_lnClGlucC     -9.21   4.605   );
Distrib(        lnKMGluc        TruncNormal_v   M_lnKMGluc      V_lnKMGluc      -6.908  6.908   );
Distrib(        lnkMetTCOHC     TruncNormal_v   M_lnkMetTCOHC   V_lnkMetTCOHC   -11.513 6.908   );


Distrib(        lnkUrnTCAC      TruncNormal_v   M_lnkUrnTCAC    V_lnkUrnTCAC    -4.605  4.605   );
Distrib(        lnkMetTCAC      TruncNormal_v   M_lnkMetTCAC    V_lnkMetTCAC    -9.21   4.605   );


Distrib(        lnkBileC        TruncNormal_v   M_lnkBileC      V_lnkBileC      -9.21   4.605   );
Distrib(        lnkEHRC TruncNormal_v   M_lnkEHRC       V_lnkEHRC       -9.21   4.605   );
Distrib(        lnkUrnTCOGC     TruncNormal_v   M_lnkUrnTCOGC   V_lnkUrnTCOGC   -6.908  6.908   );


####Distrib(    lnFracKidDCVCC  TruncNormal_v   M_lnFracKidDCVCC        V_lnFracKidDCVCC        -6.908  6.908   );
####Distrib(    lnkDCVGC        TruncNormal_v   M_lnkDCVGC      V_lnkDCVGC      -9.21   4.605   );


####Distrib(    lnkNATC TruncNormal_v   M_lnkNATC       V_lnkNATC       -9.21   4.605   );
####Distrib(    lnkKidBioactC   TruncNormal_v   M_lnkKidBioactC V_lnkKidBioactC -9.21   4.605   );

#### Chiu et al. 2006 data

Level { # Subject A

Experiment { # 61 # Experiment A-TRI-1
#CC=0;

BWmeas= 70.5;   VFatCmeas=      0.11;
#lnBW=  4.25561271      ;       VFatC=  0.514018692     ;

QPmeas= 310.8; # NDoses(2, 310.8 0, 0.0 6.0);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 310.8   );

Conc =  NDoses( 17      1.155   1.185   1.322   1.262   1.357   1.282   1.339   1.330   1.284   1.248   1.077   1.257   1.18
        0.000   0.283   0.617   1.117   1.367   1.867   2.117   2.367   2.783   2.950   3.700   4.117   4.533   4.950   5.53

Print(  CAlvPPM,        0.3333  0.3343  0.6667  0.6677  1  1.001        1.3333  1.3343  1.6667  1.6677  1.6687  1.6697  2  2
Data(   CAlvPPM,        0.259221  0.26847       0.34737  0.389423       0.351313  0.417967      0.495419  0.424781      0.43

Print(  CVen,   1       2       4       5.7833  6.1167  7.0333  8.0333  );
Data(   CVen,   0.0045  0.0045  0.005   0.004   0.002   0.002   0.001   );
Print(  CBldTCA,        1       2       4       5.7833  6.1167  7.0333  8.0333  40.7833 98.2833 122.55  );
Data(   CBldTCA,        0.002   0.004   0.01    0.019   0.0265  0.0275  0.0375  0.047   0.024   0.0175  );
Print(  TotCTCOH,       1       2       4       5.7833  6.1167  7.0333  8.0333  40.7833 77.6167 98.2833 );
Data(   TotCTCOH,       0.007   0.048   0.066   0.0995  0.088   0.104   0.037   0.0035  0.0015  0.003   );
Print(  CTCOH,  1       2       4       5.7833  6.1167  7.0333  8.0333  40.7833 );
Data(   CTCOH,  0.005   0.007   0.011   0.027   0.0165  0.0195  0.02    0.002   );

#TCAUrnSat=     NDoses( 18      1       1       1       1       1       0       1       0       0       1       1       1
#       0   6.2833      7.6167  14.45   22.9167 29.7    31.2333 36.3667 38.6167 39.4    46.4167 65.7167 75.5667 86.7333 94.7
#       );
UrnMissing=     NDoses( 18      0       0       0       0       0       0       0       0       0       0       1       0
        0   6.2833      7.6167  14.45   22.9167 29.7    31.2333 36.3667 38.6167 39.4    46.4167 65.7167 75.5667 86.7333 94.7
        );
#Print( zAUrnTCA_sat,   6.2833  7.6167  14.45   22.9167 29.7    36.3667 46.4167 75.5667 94.7333
#); Data(       zAUrnTCA_sat,   0.0167  0.0234  0.0259  0.0449  0.0617  0.0878  0.1053  0.1321  0.1478
#       );
Print(  zAUrnTCA_collect,       31.2333 38.6167 39.4    121.4
); Data(        zAUrnTCA_collect,       0.0101  0.0165  0.0277  0.0465
        );
#TCOGUrnSat=    NDoses( 18      1       1       1       0       0       0       0       0       0       0       0       0
#       0   6.2833      7.6167  14.45   22.9167 29.7    31.2333 36.3667 38.6167 39.4    46.4167 65.7167 75.5667 86.7333 94.7
#       );

#Print( AUrnTCOGTCOH_sat,       6.2833  7.6167  14.45
#); Data(       AUrnTCOGTCOH_sat,       0.6353  0.8059  0.8711
#       );

Print(  AUrnTCOGTCOH_collect,   22.9167 29.7    31.2333 36.3667 38.6167 39.4    46.4167 75.5667 94.7333 121.4
); Data(        AUrnTCOGTCOH_collect,   0.5003  0.6866  0.7662  1.0048  1.0342  1.0736  1.1472  1.1793  1.1995  1.2039
        );

Print(  AUrnTCOGTCOH,   1);
Data(   AUrnTCOGTCOH,   -1);
Print(  zAUrnTCA,       1);
Data(   zAUrnTCA,       -1);

 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);
```

```
 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
}

Experiment { # 62 # Experiment A-TRI-2
#CC=0;

BWmeas= 70.5;   VFatCmeas=      0.11    ;
#lnBW=  4.25561271      ;       VFatC=  0.514018692     ;

QPmeas= 310.8; # NDoses(2, 310.8 0, 0.0 6.0);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 310.8   );

Conc =  NDoses( 21      1.019   0.932   1.085   1.031   1.035   1.165   1.238   1.194   1.200   1.171   1.249   1.194   1.14
        0.000   0.300   0.717   1.050   1.383   1.717   2.050   2.383   2.633   3.050   3.383   3.800   4.300   4.467   4.80

Print(  CAlvPPM,        0.3333  0.3343  0.6667  0.6677  1  1.001        1.3333  1.3343  1.6667  1.6677  2  2.001        2.33
Data(   CAlvPPM,        0.249519  0.262734      0.378056  0.382217      0.350707  0.385927      0.354557  0.314386      0.30

Print(  CVen,   0.8     2.05    5.8833  6.2167  8.05    122.9667        );
Data(   CVen,   0.003   0.003   0.006   0.0015  0.0005  0.001   );
Print(  CBldTCA,        0.8     2.05    5.8833  6.2167  8.05    25.6333 73.8    98.7167 122.9667        122.9677        );
Data(   CBldTCA,        0.001   0.002   0.0105  0.0115  0.0125  0.0205  0.0325  0.024   0.0285  0.024   );
Print(  TotCTCOH,       0.8     2.05    4.05    5.8833  6.2167  8.05    25.6333 );
Data(   TotCTCOH,       0.007   0.011   0.041   0.057   0.0595  0.044   0.01    );
Print(  CTCOH,  5.8833  6.2167  8.05    122.9667        );
Data(   CTCOH,  0.0025  0.003   0.0025  0.0055  );

#TCAUrnSat=     NDoses( 19      0       1       0       1       0       0       1       1       0       1       0       0
#       0   6.2167      10.3    14.3667 23.7167 27.4667 31.4667 37.2167 39.0667 42.0167 47.6333 63.9333 69.5167 92.45   96.8
#       );
UrnMissing=     NDoses( 19      0       0       0       0       0       0       0       0       0       0       1       0
        0   6.2167      10.3    14.3667 23.7167 27.4667 31.4667 37.2167 39.0667 42.0167 47.6333 63.9333 69.5167 92.45   96.8
        );
#Print( zAUrnTCA_sat,   10.3    23.7167 37.2167 39.0667 47.6333
#); Data(       zAUrnTCA_sat,   0.0043  0.0225  0.0288  0.0391  0.0478
#       );
Print(  zAUrnTCA_collect,       6.2167  14.3667 31.4667 42.0167 69.5167 96.85   120.85  142.5
); Data(        zAUrnTCA_collect,       0.017   0.0336  0.039   0.0491  0.062   0.0709  0.0847  0.0962
        );

#TCOGUrnSat=    NDoses( 19      0       0       0       0       0       0       0       0       0       0       1       0
#       0   6.2167      10.3    14.3667 23.7167 27.4667 31.4667 37.2167 39.0667 42.0167 47.6333 63.9333 69.5167 92.45   96.8
#       );
#Print( AUrnTCOGTCOH_sat,       6.2167  10.3
#); Data(       AUrnTCOGTCOH_sat,       0.778   0.9838
#       );
Print(  AUrnTCOGTCOH_collect,   14.3667 23.7167 31.4667 37.2167 39.0667 42.0167 47.6333 69.5167 96.85   120.85  142.5
); Data(        AUrnTCOGTCOH_collect,   0.5175  0.9178  0.9796  1.0985  1.1677  1.2565  1.3254  1.3535  1.3605  1.365   1.36
        );


Print(  AUrnTCOGTCOH,   1);
Data(   AUrnTCOGTCOH,   -1);
Print(  zAUrnTCA,       1);
Data(   zAUrnTCA,       -1);

 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
```

```
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
}

}

Level { # Subject B

Experiment { # 63 # Experiment B-TRI-1
#CC=0;

BWmeas= 75.6;   VFatCmeas=      0.204   ;
#lnBW=  4.325456283     ;       VFatC=  0.953271028     ;

QPmeas= 319.2; # NDoses(2, 319.2 0, 0.0 6.0);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 319.2   );

Conc =  NDoses( 23      1.117   1.080   1.107   1.060   1.011   1.067   1.114   1.142   1.153   1.116   1.133   1.122   1.19
        0.000   0.150   0.317   0.983   1.150   1.483   1.733   2.233   2.483   2.900   3.150   3.400   3.567   3.900   4.15


Print(  CAlvPPM,        0.3333  0.3343  0.3353  0.6667  0.6677  0.6687  1  1.001        1.3667  1.3677  1.6667  2.3333  2.33
Data(   CAlvPPM,        0.297425  0.284702  0.27631     0.280924  0.269558  0.28923     0.254859  0.28093       0.29746  0.3

Print(  CVen,   1       2       4       5.8333  7       8       );
Data(   CVen,   0.002   0.0045  0.003   0.004   0.001   0.001   );
Print(  CBldTCA,        1       2       4       5.8333  7       8       26.5    47.75   72.8333 );
Data(   CBldTCA,        0.002   0.005   0.12    0.031   0.035   0.0425  0.0725  0.0685  0.0485  );
Print(  TotCTCOH,       1       2       4       6.1667  7       8       26.5    47.75   72.8333 98.5    );
Data(   TotCTCOH,       0.0055  0.011   0.034   0.053   0.04    0.04    0.007   0.0025  0.001   0.0015  );
Print(  CTCOH,  1       2       4       5.8333  7       8       26.5    47.75   );
Data(   CTCOH,  0.003   0.006   0.008   0.011   0.026   0.0135  0.0055  0.0025  );

#TCAUrnSat=     NDoses( 18      1       1       1       1       1       1       1       1       1       1       1       1
#       0   6.4833      11.4833 14.2333 20.4833 22.9833 26.2333 29.4833 34.4833 39.4833 47.2333 62.9833 71.4833 84.4833 91.4
#       );
UrnMissing=     NDoses( 18      0       0       0       0       0       0       0       0       0       0       1       0
        0   6.4833      11.4833 14.2333 20.4833 22.9833 26.2333 29.4833 34.4833 39.4833 47.2333 62.9833 71.4833 84.4833 91.4
        );
#Print( zAUrnTCA_sat,   6.4833  11.4833 14.2333 20.4833 22.9833 26.2333 29.4833 34.4833 39.4833 47.2333 71.4833
#); Data(       zAUrnTCA_sat,   0.0204  0.0361  0.0444  0.072   0.0888  0.0994  0.1234  0.1334  0.1481  0.1703  0.1778
#       );
Print(  zAUrnTCA_collect,       0
); Data(        zAUrnTCA_collect,       -1
        );

#TCOGUrnSat=    NDoses( 18      0       1       1       0       0       0       0       0       0       0       0       0
#       0   6.4833      11.4833 14.2333 20.4833 22.9833 26.2333 29.4833 34.4833 39.4833 47.2333 62.9833 71.4833 84.4833 91.4
#       );

#Print( AUrnTCOGTCOH_sat,       11.4833 14.2333
#); Data(       AUrnTCOGTCOH_sat,       0.4522  0.6758
#       );
Print(  AUrnTCOGTCOH_collect,   6.4833  20.4833 22.9833 26.2333 29.4833 34.4833 39.4833 47.2333 71.4833 91.4833 116.4833
); Data(        AUrnTCOGTCOH_collect,   0.6936  1.1404  1.3606  1.4823  1.6973  1.8812  2.0137  2.1577  2.1792  2.2126  2.23
        );

Print(  AUrnTCOGTCOH,   1);
Data(   AUrnTCOGTCOH,   -1);
Print(  zAUrnTCA,       1);
Data(   zAUrnTCA,       -1);

 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
```

```
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
}


Experiment { # 64 # Experiment B-TRI-2
#CC=0;

BWmeas= 75.6;   VFatCmeas=      0.204   ;
#lnBW=  4.325456283     ;       VFatC=  0.953271028     ;

QPmeas= 319.2; # NDoses(2, 319.2 0, 0.0 6.0);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 319.2   );

Conc =  NDoses( 31      1.424   1.305   1.367   1.341   1.353   0.492   0.248   0.302   1.594   1.876   1.642   1.583   1.46
        0.000   0.133   0.300   0.467   0.717   1.050   1.300   1.383   1.550   1.633   1.717   1.800   1.883   1.967   2.10

Print(  CAlvPPM,        0.3333  0.3343  0.6667  0.6677  1  1.001        1.3333  1.6667  1.6677  2.3333  2.3343  2.6667  2.66
Data(   CAlvPPM,        0.292512  0.230086      0.25225  0.233197       0.195014  0.249061      0.073272        0.0486764  0

Print(  CVen,   0.95    5.7833  6.1167  6.95    7.95    );
Data(   CVen,   0.0025  0.006   0.003   0.001   0.001   );
Print(  CBldTCA,        0.95    5.7833  6.1167  6.95    7.95    26.4667 50.2167 74.1333 144.6667        );
Data(   CBldTCA,        0.002   0.041   0.034   0.0325  0.042   0.057   0.06    0.068   0.0405  );
Print(  TotCTCOH,       5.7833  6.1167  6.95    7.95    26.4667 50.2167 74.1333 99.6333 );
Data(   TotCTCOH,       0.0425  0.037   0.036   0.0325  0.011   0.004   0.0025  0.001   );
Print(  CTCOH,  5.7833  6.1167  6.95    7.95    );
Data(   CTCOH,  0.011   0.0075  0.0065  0.008   );
#TCAUrnSat=     NDoses( 17      1       1       1       1       1       1       1       1       1       0       1       1
#       0   6.3 9.1333  11.6333 15.1333 26.1333 32.1333 36.1333 41.6333 50.1333 65.1333 73.1333 87.3833 94.6333 111.3833
#       );
UrnMissing=     NDoses( 17      0       0       0       0       0       0       0       0       0       1       0       1
        0   6.3 9.1333  11.6333 15.1333 26.1333 32.1333 36.1333 41.6333 50.1333 65.1333 73.1333 87.3833 94.6333 111.3833
        );
#Print( zAUrnTCA_sat,   6.3     9.1333  11.6333 15.1333 26.1333 32.1333 36.1333 41.6333 50.1333 73.1333 94.6333 117.9667
#); Data(       zAUrnTCA_sat,   0.0143  0.0228  0.0304  0.0425  0.0659  0.073   0.0846  0.0917  0.1043  0.1149  0.1227  0.13
#       );
Print(  zAUrnTCA_collect,       0
); Data(        zAUrnTCA_collect,       -1
        );
#TCOGUrnSat=    NDoses( 17      1       1       1       0       0       0       0       0       0       0       0       0
#       0   6.3 9.1333  11.6333 15.1333 26.1333 32.1333 36.1333 41.6333 50.1333 65.1333 73.1333 87.3833 94.6333 111.3833
#       );
#Print( AUrnTCOGTCOH_sat,       6.3     9.1333  11.6333
#); Data(       AUrnTCOGTCOH_sat,       0.7941  1.3632  1.6546
#       );
Print(  AUrnTCOGTCOH_collect,   15.1333 26.1333 32.1333 36.1333 41.6333 50.1333 73.1333 94.6333 117.9667
); Data(        AUrnTCOGTCOH_collect,   0.2776  0.8985  1.1068  1.3213  1.4584  1.6555  1.7119  1.7378  1.7532
        );


Print(  AUrnTCOGTCOH,   1);
Data(   AUrnTCOGTCOH,   -1);
Print(  zAUrnTCA,       1);
Data(   zAUrnTCA,       -1);

 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);

}

}
```

```
Level { # Subject C

Experiment { # 65 # Experiment C-TRI-1
#CC=0;

BWmeas= 75.2;   VFatCmeas=      0.204   ;
#lnBW=  4.320151231     ;       VFatC=  0.953271028     ;

QPmeas= 310.8; # NDoses(2, 310.8 0, 0.0 6.0);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 310.8   );

Conc =  NDoses( 18      1.218   1.155   1.185   1.322   1.262   1.357   1.282   1.339   1.330   1.284   1.248   1.077   1.25
        0.000   0.050   0.550   0.883   1.383   1.633   2.133   2.383   2.633   3.050   3.217   3.967   4.383   4.800   5.21

Print(  CAlvPPM,        0.3333  0.3343  0.6667  0.6677  1  1.001        1.3333  1.3343  1.6667  1.6677  2  2.001        2.33
Data(   CAlvPPM,        0.401675  0.330756      0.377474  0.356618      0.403155  0.375551      0.331179  0.328483      0.30

Print(  CVen,   1       2       4       5.8333  7.05    51.8833 );
Data(   CVen,   0.001   0.004   0.004   0.0025  0.001   0.0005  );
Print(  CBldTCA,        1       2       4       5.8333  7.05    28.55   51.8833 74.9667 98.6    120.8833        );
Data(   CBldTCA,        0.001   0.004   0.014   0.015   0.035   0.055   0.053   0.045   0.033   0.027   );
Print(  TotCTCOH,       1       2       4       5.8333  6.1667  7.05    8.3833  28.55   51.8833 74.9667 120.8833        );
Data(   TotCTCOH,       0.005   0.0165  0.213   0.094   0.095   0.088   0.075   0.012   0.014   0.012   0.001   );
Print(  CTCOH,  1       2       4       5.8333  7.05    28.55   51.8833 74.9667 );
Data(   CTCOH,  0.003   0.006   0.02    0.016   0.024   0.006   0.0015  0.001   );

#TCAUrnSat=     NDoses( 16      0       1       1       0       0       1       0       1       0       1       0       1
#       0   7.2167      14.1333 22.3833 28.3833 32.8833 38.3833 45.6333 62.3833 69.8833 86.2167 94.4667 110.3833        118.
#       );
UrnMissing=     NDoses( 16      0       0       0       0       0       0       0       1       0       1       0       1
        0   7.2167      14.1333 22.3833 28.3833 32.8833 38.3833 45.6333 62.3833 69.8833 86.2167 94.4667 110.3833        118.
        );
#Print( zAUrnTCA_sat,   14.1333 22.3833 38.3833
#); Data(       zAUrnTCA_sat,   0.0114  0.0237  0.0317
#       );
Print(  zAUrnTCA_collect,       7.2167  28.3833 45.6333 69.8833 94.4667 118.3833        141.3833
); Data(        zAUrnTCA_collect,       0.0106  0.0213  0.0333  0.0527  0.067   0.0823  0.0951
        );
#TCOGUrnSat=    NDoses( 16      0       1       1       0       0       0       0       0       0       0       0       0
#       0   7.2167      14.1333 22.3833 28.3833 32.8833 38.3833 45.6333 62.3833 69.8833 86.2167 94.4667 110.3833        118.
#       );
#Print( AUrnTCOGTCOH_sat,       14.1333 22.3833
#); Data(       AUrnTCOGTCOH_sat,       0.6721  1.2857
#       );
Print(  AUrnTCOGTCOH_collect,   7.2167  28.3833 38.3833 45.6333 69.8833 94.4667 118.3833        141.3833
); Data(        AUrnTCOGTCOH_collect,   0.5381  0.9118  1.1632  1.3584  1.4847  1.5212  1.5427  1.5485
        );

Print(  AUrnTCOGTCOH,   1);
Data(   AUrnTCOGTCOH,   -1);
Print(  zAUrnTCA,       1);
Data(   zAUrnTCA,       -1);

 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
}

Experiment { # 66 # Experiment C-TRI-2
#CC=0;
BWmeas= 75.2;   VFatCmeas=      0.204   ;
#lnBW=  4.320151231     ;       VFatC=  0.953271028     ;

QPmeas= 310.8; # NDoses(2, 310.8 0, 0.0 6.0);
#       Print(  QPsamp, 1       );
```

```
#       Data(   QPsamp, 310.8   );

Conc =  NDoses( 21      0.965   1.019   0.932   1.085   1.031   1.035   1.165   1.238   1.194   1.200   1.171   1.249   1.19
        0.000   0.133   0.467   0.883   1.217   1.550   1.883   2.217   2.550   2.800   3.217   3.550   3.967   4.467   4.63

Print(  CAlvPPM,        0.3833  0.3843  0.6667  0.6677  0.95  0.951     1.3667  1.3677  1.65  1.651     2  2.001        2.33
Data(   CAlvPPM,        0.253178  0.257009      0.254465  0.29185       0.301115  0.312384      0.340338  0.287822      0.37

Print(  CVen,   1       1.9     3.9833  5.8833  6.2167  7.0667  8.0667  );
Data(   CVen,   0.002   0.002   0.003   0.003   0.001   0.0005  0.001   );
Print(  CBldTCA,        1       1.9     3.9833  5.8833  6.2167  7.0667  8.0667  25.6333 52.6333 74.8    97.8    124.1333
Data(   CBldTCA,        0.001   0.004   0.0065  0.012   0.0135  0.018   0.0155  0.048   0.058   0.051   0.038   0.036   );
Print(  TotCTCOH,       1       1.9     3.9833  5.8833  6.2167  7.0667  8.0667  25.6333 52.6333 74.8    );
Data(   TotCTCOH,       0.006   0.013   0.055   0.097   0.066   0.069   0.079   0.013   0.0095  0.004   );
Print(  CTCOH,  3.9833  5.8833  6.2167  7.0667  8.0667  25.6333 );
Data(   CTCOH,  0.002   0.003   0.004   0.003   0.003   0.002   );
#TCAUrnSat=     NDoses( 17      0       1       1       0       1       0       1       0       0       1       1       0
#       0   7.9667      13.6333 22.1333 29.1333 33.4667 37.6333 46.1333 50.8    63.8    70.1333 86.55   94.1333 110.1333
#       );
UrnMissing=     NDoses( 17      0       0       0       0       0       0       0       0       1       0       1       0
        0   7.9667      13.6333 22.1333 29.1333 33.4667 37.6333 46.1333 50.8    63.8    70.1333 86.55   94.1333 110.1333
        );
#Print( zAUrnTCA_sat,   13.6333 22.1333 33.4667 46.1333 70.1333
#); Data(       zAUrnTCA_sat,   0.0103  0.0233  0.032   0.0465  0.0542
#       );
Print(  zAUrnTCA_collect,       7.9667  29.1333 37.6333 50.8    94.1333 141.6333
); Data(        zAUrnTCA_collect,       0.0133  0.0232  0.0315  0.0454  0.0542  0.0575
        );
#TCOGUrnSat=    NDoses( 17      1       1       0       0       0       0       0       0       0       0       0       0
#       0   7.9667      13.6333 22.1333 29.1333 33.4667 37.6333 46.1333 50.8    63.8    70.1333 86.55   94.1333 110.1333
#       );
#Print( AUrnTCOGTCOH_sat,       7.9667  13.6333
#); Data(       AUrnTCOGTCOH_sat,       0.8675  1.6259
#       );
Print(  AUrnTCOGTCOH_collect,   22.1333 29.1333 33.4667 37.6333 46.1333 50.8    70.1333 94.1333 141.6333
); Data(        AUrnTCOGTCOH_collect,   0.5968  0.9005  1.0882  1.2845  1.556   1.6346  1.6844  1.706   1.7109
        );

Print(  AUrnTCOGTCOH,   1);
Data(   AUrnTCOGTCOH,   -1);
Print(  zAUrnTCA,       1);
Data(   zAUrnTCA,       -1);

 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
}

}

Level { # Subject D

Experiment { # 67 # Experiment D-TRI-1
#CC=0;

BWmeas= 70.5;   VFatCmeas=      0.129   ;
#lnBW=  4.25561271      ;       VFatC=  0.602803738     ;

QPmeas= 298.2; # NDoses(2, 298.2 0, 0.0 6.0);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 298.2   );

Conc =  NDoses( 22      1.080   1.117   1.080   1.107   1.060   1.011   1.067   1.114   1.142   1.153   1.116   1.133   1.12
        0.000   0.050   0.550   0.717   1.383   1.550   1.883   2.133   2.633   2.883   3.300   3.550   3.800   3.967   4.30
Print(  CAlvPPM,        0.3333  0.3343  0.6667  0.6677  1  1.001        1.3333  1.3343  1.6667  1.6677  2  2.001        2.33
Data(   CAlvPPM,        0.339106  0.340422      0.424221  0.398335      0.393694  0.396775      0.309778  0.348686      0.30
```

```
Print(  CVen,   1       4       5.8333  6.1667  8       );
Data(   CVen,   0.004   0.0035  0.007   0.0025  0.001   );
Print(  CBldTCA,        1       4       5.8333  6.1667  8       25.2167 49.8833 73.7333 );
Data(   CBldTCA,        0.003   0.032   0.056   0.047   0.072   0.0595  0.0875  0.052   );
Print(  TotCTCOH,       1       2       4       5.8333  6.1667  7       8       25.2167 73.7333 99.6333 );
Data(   TotCTCOH,       0.006   0.011   0.035   0.073   0.104   0.366   0.133   0.01    0.0025  0.001   );
Print(  CTCOH,  1       4       5.8333  6.1667  8       25.2167 49.8833 );
Data(   CTCOH,  0.0025  0.016   0.022   0.014   0.0095  0.005   0.003   );

#TCAUrnSat=     NDoses( 19      0       1       1       1       1       1       1       1       0       1       1       1
#       0   6.3 8.7167  12.6333 22.7167 25.9667 31.8833 33.3833 35.55   40.4167 48.55   61.3    72.3833 84.5    93.55   108.
#       );
UrnMissing=     NDoses( 19      0       0       0       0       0       0       0       0       0       0       1       0
        0   6.3 8.7167  12.6333 22.7167 25.9667 31.8833 33.3833 35.55   40.4167 48.55   61.3    72.3833 84.5    93.55   108.
        );
#Print( zAUrnTCA_sat,   8.7167  12.6333 22.7167 25.9667 31.8833 33.3833 35.55   48.55   72.3833
#); Data(       zAUrnTCA_sat,   0.0117  0.0168  0.0313  0.041   0.05    0.0511  0.0568  0.0782  0.0972
#       );
Print(  zAUrnTCA_collect,       6.3     40.4167
); Data(        zAUrnTCA_collect,       0.0141  0.0171
        );
#TCOGUrnSat=    NDoses( 19      1       1       1       1       0       0       0       0       0       0       0       0
#       0   6.3 8.7167  12.6333 22.7167 25.9667 31.8833 33.3833 35.55   40.4167 48.55   61.3    72.3833 84.5    93.55   108.
#       );



#Print( AUrnTCOGTCOH_sat,       6.3     8.7167  12.6333 22.7167
#); Data(       AUrnTCOGTCOH_sat,       0.7557  1.1772  1.4037  2.0733
#       );
Print(  AUrnTCOGTCOH_collect,   25.9667 31.8833 33.3833 35.55   40.4167 48.55   72.3833 93.55   118.1333        132.8833
); Data(        AUrnTCOGTCOH_collect,   0.2368  0.3721  0.3835  0.4405  0.4633  0.6079  0.6947  0.7139  0.728   0.7312
        );

Print(  AUrnTCOGTCOH,   1);
Data(   AUrnTCOGTCOH,   -1);
Print(  zAUrnTCA,       1);
Data(   zAUrnTCA,       -1);

 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
}

}


Level { # Subject F

Experiment { # 68 # Experiment F-TRI-1
#CC=0;

BWmeas= 69.5;   VFatCmeas=      0.18    ;
#lnBW=  4.241326753     ;       VFatC=  0.841121495     ;

QPmeas= 327.6; # NDoses(2, 327.6 0, 0.0 6.0);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 327.6   );

Conc =  NDoses( 18      1.308   1.218   1.155   1.185   1.322   1.262   1.357   1.282   1.339   1.330   1.284   1.248   1.07
        0.000   0.083   0.333   0.833   1.167   1.667   1.917   2.417   2.667   2.917   3.333   3.500   4.250   4.667   5.08
Print(  CAlvPPM,        0.3333  0.3343  0.6667  0.6677  1  1.001        1.3333  1.3343  1.6667  1.6677  2  2.001        2.33
Data(   CAlvPPM,        0.214147  0.446694      0.166763  0.188716      0.43794  0.41233        0.330501  0.20073       0.31

Print(  CVen,   1       4       5.8333  6.1667  7       8       49.8333 );
Data(   CVen,   0.0025  0.004   0.005   0.002   0.001   0.001   0.0005  );
Print(  CBldTCA,        1       4       5.8333  6.1667  7       8       25.6667 49.8333 73.8333 100.9667        122.6333
```

```
Data(   CBldTCA,        0.002   0.018   0.029   0.0445  0.041   0.048   0.067   0.073   0.07    0.0505  0.039   );
Print(  TotCTCOH,       1       2       4       5.8333  6.1667  7       8       25.6667 73.8333 122.6333        );
Data(   TotCTCOH,       0.014   0.0115  0.022   0.05    0.05    0.141   0.044   0.0075  0.003   0.001   );
Print(  CTCOH,  1       4       5.8333  6.1667  7       8       25.6667 49.8333 73.8333 );
Data(   CTCOH,  0.002   0.008   0.0095  0.0175  0.01    0.01    0.003   0.001   0.001   );

#TCAUrnSat=     NDoses( 21      1       1       1       1       1       1       1       0       1       1       1       1
#       0   6.3 8.1667  9.1667  12.6667 14.6667 24.6667 29.6667 31.6667 36.6667 39.1667 41.6667 48.4167 62.6667 72.1667 88.6
#       );
UrnMissing=     NDoses( 21      0       0       0       0       0       0       0       0       0       0       0       0
        0   6.3 8.1667  9.1667  12.6667 14.6667 24.6667 29.6667 31.6667 36.6667 39.1667 41.6667 48.4167 62.6667 72.1667 88.6
        );
#Print( zAUrnTCA_sat,   6.3     8.1667  9.1667  12.6667 14.6667 24.6667 29.6667 36.6667 39.1667 41.6667 48.4167 72.1667 97.6
#); Data(       zAUrnTCA_sat,   0.0002  0.0094  0.01    0.0201  0.0249  0.0378  0.0515  0.0691  0.0936  0.1106  0.1211  0.13
#       );
Print(  zAUrnTCA_collect,       31.6667
); Data(        zAUrnTCA_collect,       0.0088
        );
#TCOGUrnSat=    NDoses( 21      0       0       1       0       0       0       0       0       0       0       0       0
#       0   6.3 8.1667  9.1667  12.6667 14.6667 24.6667 29.6667 31.6667 36.6667 39.1667 41.6667 48.4167 62.6667 72.1667 88.6
#       );



#Print( AUrnTCOGTCOH_sat,       9.1667
#); Data(       AUrnTCOGTCOH_sat,       0.0788
#       );
Print(  AUrnTCOGTCOH_collect,   6.3     8.1667  12.6667 14.6667 24.6667 29.6667 31.6667 36.6667 39.1667 41.6667 48.4167 72.1
); Data(        AUrnTCOGTCOH_collect,   0.0063  0.2254  0.4775  0.6152  0.9452  1.0952  1.143   1.2548  1.3098  1.3584  1.37
        );

Print(  AUrnTCOGTCOH,   1);
Data(   AUrnTCOGTCOH,   -1);
Print(  zAUrnTCA,       1);
Data(   zAUrnTCA,       -1);

 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
}

Experiment { # 69 # Experiment F-TRI-2
#CC=0;

BWmeas= 69.5;   VFatCmeas=      0.18    ;
#lnBW=  4.241326753     ;       VFatC=  0.841121495     ;

QPmeas= 327.6; # NDoses(2, 327.6 0, 0.0 6.0);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 327.6   );

Conc =  NDoses( 32      1.344   1.252   1.424   1.305   1.367   1.341   1.353   0.492   0.248   0.302   1.594   1.876   1.64
        0.000   0.300   0.383   0.633   0.800   0.967   1.217   1.550   1.800   1.883   2.050   2.133   2.217   2.300   2.38
Print(  CAlvPPM,        0.3333  0.3343  0.6667  0.6677  1  1.001        1.3333  1.3343  1.6667  1.6677  2  2.001        2.33
Data(   CAlvPPM,        0.42561  0.351669       0.416291  0.294322      0.39137  0.543459       0.347941  0.392029      0.07

Print(  CVen,   1       2       4       5.8333  6.2333  8       );
Data(   CVen,   0.0035  0.001   0.005   0.006   0.002   0.001   );
Print(  CBldTCA,        1       2       4       5.8333  6.2333  8       26.6333 73.3833 94.3833 128.6333        );
Data(   CBldTCA,        0.002   0.0035  0.02    0.039   0.0425  0.048   0.074   0.067   0.0545  0.036   );
Print(  TotCTCOH,       1       2       4       5.8333  6.2333  7       8       26.6333 50.55   73.3833 );
Data(   TotCTCOH,       0.0065  0.018   0.038   0.065   0.043   0.041   0.036   0.012   0.0025  0.001   );
Print(  CTCOH,  4       5.8333  6.2333  8       26.6333 );
Data(   CTCOH,  0.008   0.009   0.009   0.007   0.002   );

#TCAUrnSat=     NDoses( 20      0       1       0       1       1       1       1       1       1       0       1       0
#       0   6.1333      8.1333  9.6333  15.6333 22.8    26.6333 30.3833 34.1333 39.3833 40.6333 48.6333 63.6333 72.1333 86.6
```

```
#       );
UrnMissing=     NDoses( 20      0       0       0       0       0       0       0       0       0       0       0       1
        0   6.1333      8.1333  9.6333  15.6333 22.8    26.6333 30.3833 34.1333 39.3833 40.6333 48.6333 63.6333 72.1333 86.6
        );
#Print( zAUrnTCA_sat,   8.1333  15.6333 22.8    26.6333 30.3833 34.1333 39.3833 48.6333 72.1333 93.6333 143.1333
#); Data(       zAUrnTCA_sat,   0.0115  0.028   0.049   0.0561  0.0688  0.0897  0.0959  0.1072  0.1216  0.1282  0.133
#       );
Print(  zAUrnTCA_collect,       40.6333 118.6333
); Data(        zAUrnTCA_collect,       0.0198  0.024
        );
#TCOGUrnSat=    NDoses( 20      0       1       0       0       0       0       0       0       0       0       0       0
#       0   6.1333      8.1333  9.6333  15.6333 22.8    26.6333 30.3833 34.1333 39.3833 40.6333 48.6333 63.6333 72.1333 86.6
#       );



#Print( AUrnTCOGTCOH_sat,       8.1333
#); Data(       AUrnTCOGTCOH_sat,       0.635
#       );
Print(  AUrnTCOGTCOH_collect,   6.1333  9.6333  15.6333 22.8    26.6333 30.3833 34.1333 39.3833 40.6333 48.6333 72.1333 93.6
); Data(        AUrnTCOGTCOH_collect,   0.5917  1.0628  1.4811  1.9016  2.0542  2.1926  2.3728  2.4387  2.4618  2.5126  2.55
        );

Print(  AUrnTCOGTCOH,   1);
Data(   AUrnTCOGTCOH,   -1);
Print(  zAUrnTCA,       1);
Data(   zAUrnTCA,       -1);

 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
}

}

Level { # Subject G

Experiment { # 70 # Experiment G-TRI-2
#CC=0;

BWmeas= 71;     VFatCmeas=      0.096   ;
#lnBW=  4.262679877     ;       VFatC=  0.448598131     ;

QPmeas= 302.4; # NDoses(2, 302.4 0, 0.0 6.0);
#       Print(  QPsamp, 1       );
#       Data(   QPsamp, 302.4   );

Conc =  NDoses( 32      1.344   1.252   1.424   1.305   1.367   1.341   1.353   0.492   0.248   0.302   1.594   1.876   1.64
        0.000   0.050   0.133   0.383   0.550   0.717   0.967   1.300   1.550   1.633   1.800   1.883   1.967   2.050   2.13
Print(  CAlvPPM,        0.3333  0.3343  0.6667  0.6677  1  1.001        1.3333  1.3343  1.6667  1.6677  2  2.001        2.33
Data(   CAlvPPM,        0.313836  0.289407      0.358654  0.330007      0.286794  0.351549      0.098419  0.111763      0.05

Print(  CVen,   1       2       4       5.8333  6.2     );
Data(   CVen,   0.002   0.004   0.004   0.005   0.001   );
Print(  CBldTCA,        1       2       4       5.8333  6.2     51.1333 71.8833 98.55   143.75  );
Data(   CBldTCA,        0.001   0.002   0.0135  0.0255  0.027   0.0665  0.0635  0.0445  0.0385  );
Print(  TotCTCOH,       1       4       5.8333  6.2     7       8.05    27.3833 51.1333 );
Data(   TotCTCOH,       0.008   0.024   0.0455  0.049   0.049   0.041   0.009   0.006   );
Print(  CTCOH,  4       5.8333  6.2     );
Data(   CTCOH,  0.008   0.011   0.013   );

#TCAUrnSat=     NDoses( 16      1       1       0       1       1       1       1       1       1       1       1       1
#       0   6.2167      10.8833 13.3833 24.3833 29.8833 33.3833 36.8833 48.3833 62.8833 71.1333 88.8833 96.3833 108.3833
#       );
UrnMissing=     NDoses( 16      0       0       0       0       0       1       1       1       1       0       1       0
        0   6.2167      10.8833 13.3833 24.3833 29.8833 33.3833 36.8833 48.3833 62.8833 71.1333 88.8833 96.3833 108.3833
        );
```

```
#Print( zAUrnTCA_sat,   6.2167  10.8833 24.3833 29.8833 71.1333 96.3833
#); Data(       zAUrnTCA_sat,   0.0085  0.0176  0.0381  0.0463  0.0563  0.0641
#       );
Print(  zAUrnTCA_collect,       13.3833
); Data(        zAUrnTCA_collect,       0.0037
        );

#TCOGUrnSat=    NDoses( 16      1       1       1       0       0       0       0       0       0       0       0       0
#       0   6.2167      10.8833 13.3833 24.3833 29.8833 33.3833 36.8833 48.3833 62.8833 71.1333 88.8833 96.3833 108.3833
#       );



#Print( AUrnTCOGTCOH_sat,       6.2167  10.8833 13.3833
#); Data(       AUrnTCOGTCOH_sat,       0.7646  1.2333  1.4698
#       );
Print(  AUrnTCOGTCOH_collect,   24.3833 29.8833 71.1333 96.3833
); Data(        AUrnTCOGTCOH_collect,   0.778   0.9906  1.0389  1.0529
        );

Print(  AUrnTCOGTCOH,   1);
Data(   AUrnTCOGTCOH,   -1);
Print(  zAUrnTCA,       1);
Data(   zAUrnTCA,       -1);

 Data (CPlasTCA, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(CPlasTCA, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
}

}

}
############# END CHIU et al. 2006 individual data ##########

################### END Individual Data ########################

########### BEGIN GROUPED DATA THAT ARE UNIQUE #################

###### BEGIN BERNAUER ET AL DATA ########
Level { #Subject level
### FOR BERNAUER, ALL PARAMETERS

Distrib(        lnQCC   TruncNormal_v   M_lnQCC V_lnQCC -0.8    0.8     );

Distrib(        lnVPRC  TruncNormal_v   M_lnVPRC        V_lnVPRC        -0.8    0.8     );

Distrib(        QFatC   TruncNormal_v   M_QFatC V_QFatC 0.08    1.92    );
Distrib(        QGutC   TruncNormal_v   M_QGutC V_QGutC 0.64    1.36    );
Distrib(        QLivC   TruncNormal_v   M_QLivC V_QLivC 0.1     1.9     );
Distrib(        QSlwC   TruncNormal_v   M_QSlwC V_QSlwC 0.36    1.64    );
Distrib(        lnDRespC        TruncNormal_v   M_lnDRespC      V_lnDRespC      -11.513 2.303   );
Distrib(        QKidC   TruncNormal_v   M_QKidC V_QKidC 0.76    1.24    );
Distrib(        FracPlasC       TruncNormal_v   M_FracPlasC     V_FracPlasC     0.85    1.15    );


Distrib(        VFatC   TruncNormal_v   M_VFatC V_VFatC 0.1     1.9     );
Distrib(        VGutC   TruncNormal_v   M_VGutC V_VGutC 0.84    1.16    );
Distrib(        VLivC   TruncNormal_v   M_VLivC V_VLivC 0.54    1.46    );
Distrib(        VRapC   TruncNormal_v   M_VRapC V_VRapC 0.84    1.16    );
Distrib(        VRespLumC       TruncNormal_v   M_VRespLumC     V_VRespLumC     0.6     1.4     );
Distrib(        VRespEffC       TruncNormal_v   M_VRespEffC     V_VRespEffC     0.6     1.4     );
Distrib(        VKidC   TruncNormal_v   M_VKidC V_VKidC 0.66    1.34    );
Distrib(        VBldC   TruncNormal_v   M_VBldC V_VBldC 0.76    1.24    );
```

```
Distrib(        lnPBC   TruncNormal_v   M_lnPBC V_lnPBC -0.6    0.6     );
Distrib(        lnPFatC TruncNormal_v   M_lnPFatC       V_lnPFatC       -0.6    0.6     );
Distrib(        lnPGutC TruncNormal_v   M_lnPGutC       V_lnPGutC       -1.2    1.2     );
Distrib(        lnPLivC TruncNormal_v   M_lnPLivC       V_lnPLivC       -1.2    1.2     );
Distrib(        lnPRapC TruncNormal_v   M_lnPRapC       V_lnPRapC       -1.2    1.2     );
Distrib(        lnPRespC        TruncNormal_v   M_lnPRespC      V_lnPRespC      -1.2    1.2     );
Distrib(        lnPKidC TruncNormal_v   M_lnPKidC       V_lnPKidC       -0.6    0.6     );
Distrib(        lnPSlwC TruncNormal_v   M_lnPSlwC       V_lnPSlwC       -0.9    0.9     );


Distrib(        lnPRBCPlasTCAC  TruncNormal_v   M_lnPRBCPlasTCAC        V_lnPRBCPlasTCAC        -4.605  4.605   );
Distrib(        lnPBodTCAC      TruncNormal_v   M_lnPBodTCAC    V_lnPBodTCAC    -1.008  1.008   );
Distrib(        lnPLivTCAC      TruncNormal_v   M_lnPLivTCAC    V_lnPLivTCAC    -1.008  1.008   );


Distrib(        lnkDissocC      TruncNormal_v   M_lnkDissocC    V_lnkDissocC    -0.18   0.18    );
Distrib(        lnBMaxkDC       TruncNormal_v   M_lnBMaxkDC     V_lnBMaxkDC     -0.546  0.546   );


Distrib(        lnPBodTCOHC     TruncNormal_v   M_lnPBodTCOHC   V_lnPBodTCOHC   -1.008  1.008   );
Distrib(        lnPLivTCOHC     TruncNormal_v   M_lnPLivTCOHC    V_lnPLivTCOHC   -1.008  1.008   );
Distrib(        lnPBodTCOGC     TruncNormal_v   M_lnPBodTCOGC   V_lnPBodTCOGC   -4.605  4.605   );
Distrib(        lnPLivTCOGC     TruncNormal_v   M_lnPLivTCOGC   V_lnPLivTCOGC   -4.605  4.605   );
Distrib(        lnPeffDCVG      TruncNormal_v   M_lnPeffDCVG    V_lnPeffDCVG    -6.908  6.908   );


####Distrib(    lnkTSD  TruncNormal_v   M_lnkTSD        V_lnkTSD        -4.269  4.942   );
####Distrib(    lnkAS   TruncNormal_v   M_lnkAS V_lnkAS -6.571  7.244   );
####Distrib(    lnkTD   TruncNormal_v   M_lnkTD V_lnkTD -4.605  0       );
####Distrib(    lnkAD   TruncNormal_v   M_lnkAD V_lnkAD -7.195  6.62    );
####Distrib(    lnkASTCA        TruncNormal_v   M_lnkASTCA      V_lnkASTCA      -7.195  6.62    );
####Distrib(    lnkASTCOH       TruncNormal_v   M_lnkASTCOH     V_lnkASTCOH     -7.195  6.62    );


Distrib(        lnVMaxC TruncNormal_v   M_lnVMaxC        V_lnVMaxC       -2.079  2.079   );
#Distrib(       lnKMC   TruncNormal_v   M_lnKMC V_lnKMC 0       1       );
Distrib(        lnClC   TruncNormal_v   M_lnClC V_lnClC -4.158  4.158   );
Distrib(        lnFracOtherC    TruncNormal_v   M_lnFracOtherC  V_lnFracOtherC  -6.908  6.908   );
Distrib(        lnFracTCAC      TruncNormal_v   M_lnFracTCAC    V_lnFracTCAC    -3.489  3.489   );
#Distrib(       lnVMaxDCVGC     TruncNormal_v   M_lnVMaxDCVGC   V_lnVMaxDCVGC   0       1       );
Distrib(        lnClDCVGC       TruncNormal_v   M_lnClDCVGC     V_lnClDCVGC     -13.815 13.815  );
Distrib(        lnKMDCVGC       TruncNormal_v   M_lnKMDCVGC     V_lnKMDCVGC     -4.158  4.158   );
#Distrib(       lnVMaxKidDCVGC  TruncNormal_v   M_lnVMaxKidDCVGC        V_lnVMaxKidDCVGC        0       1       );
Distrib(        lnClKidDCVGC    TruncNormal_v   M_lnClKidDCVGC  V_lnClKidDCVGC  -13.815 13.815  );
Distrib(        lnKMKidDCVGC    TruncNormal_v   M_lnKMKidDCVGC  V_lnKMKidDCVGC  -4.158  4.158   );
Distrib(        lnVMaxLungLivC  TruncNormal_v   M_lnVMaxLungLivC        V_lnVMaxLungLivC        -3.297  3.297   );
Distrib(        lnKMClara       TruncNormal_v   M_lnKMClara     V_lnKMClara     -6.908  6.908   );
Distrib(        lnFracLungSysC  TruncNormal_v   M_lnFracLungSysC        V_lnFracLungSysC        -6.908  6.908   );


#Distrib(       lnVMaxTCOHC     TruncNormal_v   M_lnVMaxTCOHC   V_lnVMaxTCOHC   0       1       );
Distrib(        lnClTCOHC       TruncNormal_v   M_lnClTCOHC     V_lnClTCOHC     -11.513 6.908   );
Distrib(        lnKMTCOH        TruncNormal_v   M_lnKMTCOH      V_lnKMTCOH      -9.21   9.21    );
#Distrib(       lnVMaxGlucC     TruncNormal_v   M_lnVMaxGlucC   V_lnVMaxGlucC   0       1       );
Distrib(        lnClGlucC       TruncNormal_v   M_lnClGlucC     V_lnClGlucC     -9.21   4.605   );
Distrib(        lnKMGluc        TruncNormal_v   M_lnKMGluc      V_lnKMGluc      -6.908  6.908   );
Distrib(        lnkMetTCOHC     TruncNormal_v   M_lnkMetTCOHC   V_lnkMetTCOHC   -11.513 6.908   );


Distrib(        lnkUrnTCAC      TruncNormal_v   M_lnkUrnTCAC    V_lnkUrnTCAC    -4.605  4.605   );
Distrib(        lnkMetTCAC      TruncNormal_v   M_lnkMetTCAC    V_lnkMetTCAC    -9.21   4.605   );


Distrib(        lnkBileC        TruncNormal_v   M_lnkBileC      V_lnkBileC      -9.21   4.605   );
Distrib(        lnkEHRC TruncNormal_v   M_lnkEHRC       V_lnkEHRC       -9.21   4.605   );
Distrib(        lnkUrnTCOGC     TruncNormal_v   M_lnkUrnTCOGC   V_lnkUrnTCOGC   -6.908  6.908   );


##Distrib(      lnFracKidDCVCC  TruncNormal_v   M_lnFracKidDCVCC        V_lnFracKidDCVCC        -6.908  6.908   );
Distrib(        lnkDCVGC        TruncNormal_v   M_lnkDCVGC      V_lnkDCVGC      -9.21   4.605   );


Distrib(        lnkNATC TruncNormal_v   M_lnkNATC        V_lnkNATC       -9.21   4.605   );
Distrib(        lnkKidBioactC   TruncNormal_v   M_lnkKidBioactC V_lnkKidBioactC -9.21   4.605   );

Level {# Bernauer et al. (1996) - Urinary mercapturates from GSH conjugation

 Experiment { # 85
#         Subject=1;
 #PROCED BernH
 #! Data from Bernauer et al. (1996) -- Human
 #! From procedure BernH in TCENew.cmd
 #! Human -- 40, 80, 160 ppm TCE for 6 hours
#  CC=0;
  Conc=NDoses(2, 40.0 0, 0.0 6.0);
# Revised for consistency with molar data, and for 1,1+1,2 isomers for DCVC
Print (AUrnTCTotMole, 0);
```

```
Data (AUrnTCTotMole, -1);
Print (zAUrnTCA,
6       11      16      23      30      35      40      47      54
);
Data (zAUrnTCA,
1.557452405     3.14839841      5.681351918     8.719500561     11.70391989     14.45667515     16.84309415     19.6760945
);
Print (AUrnTCOGTCOH,
6       11      16      23      30      35      40      47      54
);
Data (AUrnTCOGTCOH,
13.63675325     33.61944879     51.78263372     61.25685742     71.08859899     81.97374145     91.93316798     98.27911027
);
Print (zAUrnNDCVC,
6       11      16      23      30      35      40      47      54
);
Data (zAUrnNDCVC,
0.005309749     0.012434097     0.019694974     0.025776734     0.035646562     0.042820557     0.05376152      0.060468832
);

 Data (CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (CVen, -1);
 Data (CTCOH, -1);
 Data (TotCTCOH, -1);
 Data (CAlvPPM, -1);
 Print(CBldTCA, 1);
 Print(CPlasTCA, 1);
 Print(CVen, 1);
 Print(CTCOH, 1);
 Print(TotCTCOH, 1);
 Print(CAlvPPM, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};

 Experiment { # 86
         #Subject=2;
#  CC=0;
  Conc=NDoses(2, 80.0 0, 0.0 6.0);
 # Conc=80.0;
# Revised for consistency with molar data, and for 1,1+1,2 isomers for DCVC
Print (AUrnTCTotMole, 0);
Data (AUrnTCTotMole, -1);
Print (zAUrnTCA,
6       11      16      23      30      35      40      47      54
);
Data (zAUrnTCA,
1.941365664     4.874486405     7.841594641     11.14857782     16.28748693     21.28364856     27.26544753     31.66206976
);
Print (AUrnTCOGTCOH,
6       11      16      23      30      35      40      47      54
);
Data (AUrnTCOGTCOH,
36.6438435      86.08691135     124.9572477     151.426392      174.630428      192.4174939     208.1833023     220.8519223
);
Print (zAUrnNDCVC,
6       11      16      23      30      35      40      47      54
);
Data (zAUrnNDCVC,
0.007553303     0.013224905     0.027986974     0.036437397     0.057308365     0.068022128     0.078623254     0.088400143
);

 Data (CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (CVen, -1);
 Data (CTCOH, -1);
```

```
 Data (TotCTCOH, -1);
 Data (CAlvPPM, -1);
 Print(CBldTCA, 1);
 Print(CPlasTCA, 1);
 Print(CVen, 1);
 Print(CTCOH, 1);
 Print(TotCTCOH, 1);
 Print(CAlvPPM, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};
 Experiment{ # 87
         #Subject=3;
#  CC=0;
  Conc=NDoses(2, 160.0 0, 0.0 6.0);
# Revised for consistency with molar data, and for 1,1+1,2 isomers for DCVC
Print (AUrnTCTotMole, 0);
Data (AUrnTCTotMole, -1);
Print (zAUrnTCA,
6       11      16      23      30      35      40      47      54
);
Data (zAUrnTCA,
2.838297949     8.369594126     16.2537551      24.5176767      35.0353951      44.90091589     55.13794165     63.40186326
);
Print (AUrnTCOGTCOH,
6       11      16      23      30      35      40      47      54
);
Data (AUrnTCOGTCOH,
62.99517723     150.9920375     229.5471746     284.5357705     305.7381042     334.9696792     359.5181595     375.6974964
);
Print (zAUrnNDCVC,
6       11      16      23      30      35      40      47      54
);
Data (zAUrnNDCVC,
0.01122279      0.026161736     0.053723225     0.064310553     0.073536529     0.078057851     0.091739498     0.102725693
);
 Data (CBldTCA, -1);
 Data (CPlasTCA, -1);
 Data (CVen, -1);
 Data (CTCOH, -1);
 Data (TotCTCOH, -1);
 Data (CAlvPPM, -1);
 Print(CBldTCA, 1);
 Print(CPlasTCA, 1);
 Print(CVen, 1);
 Print(CTCOH, 1);
 Print(TotCTCOH, 1);
 Print(CAlvPPM, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
```

```
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};

} # Bernauer

}
###### END BERNAUER ET AL DATA ########

################## BEGIN Muller et al. 1974 (TCA, TCOH dosing)
Level { #Subject level
### FOR MULLER, ONLY PHYSIOLOGICAL, TCA, TCOH, and TCOG PARAMETERS

Distrib(        lnQCC   TruncNormal_v   M_lnQCC V_lnQCC -0.8    0.8     );

Distrib(        lnVPRC  TruncNormal_v   M_lnVPRC        V_lnVPRC        -0.8    0.8     );

Distrib(        QFatC   TruncNormal_v   M_QFatC V_QFatC 0.08    1.92    );
Distrib(        QGutC   TruncNormal_v   M_QGutC V_QGutC 0.64    1.36    );
Distrib(        QLivC   TruncNormal_v   M_QLivC V_QLivC 0.1     1.9     );
Distrib(        QSlwC   TruncNormal_v   M_QSlwC V_QSlwC 0.36    1.64    );
####Distrib(    lnDRespC        TruncNormal_v   M_lnDRespC      V_lnDRespC      -11.513 2.303   );
Distrib(        QKidC   TruncNormal_v   M_QKidC V_QKidC 0.76    1.24    );
Distrib(        FracPlasC       TruncNormal_v   M_FracPlasC     V_FracPlasC     0.85    1.15    );


Distrib(        VFatC   TruncNormal_v   M_VFatC V_VFatC 0.1     1.9     );
Distrib(        VGutC   TruncNormal_v   M_VGutC V_VGutC 0.84    1.16    );
Distrib(        VLivC   TruncNormal_v   M_VLivC V_VLivC 0.54    1.46    );
Distrib(        VRapC   TruncNormal_v   M_VRapC V_VRapC 0.84    1.16    );
Distrib(        VRespLumC       TruncNormal_v   M_VRespLumC     V_VRespLumC     0.6     1.4     );
Distrib(        VRespEffC       TruncNormal_v   M_VRespEffC     V_VRespEffC     0.6     1.4     );
Distrib(        VKidC   TruncNormal_v   M_VKidC V_VKidC 0.66    1.34    );
Distrib(        VBldC   TruncNormal_v   M_VBldC V_VBldC 0.76    1.24    );





####Distrib(    lnPBC   TruncNormal_v   M_lnPBC V_lnPBC -0.6    0.6     );
####Distrib(    lnPFatC TruncNormal_v   M_lnPFatC       V_lnPFatC       -0.6    0.6     );
####Distrib(    lnPGutC TruncNormal_v   M_lnPGutC       V_lnPGutC       -1.2    1.2     );
####Distrib(    lnPLivC TruncNormal_v   M_lnPLivC       V_lnPLivC       -1.2    1.2     );
####Distrib(    lnPRapC TruncNormal_v   M_lnPRapC       V_lnPRapC       -1.2    1.2     );
####Distrib(    lnPRespC        TruncNormal_v   M_lnPRespC      V_lnPRespC      -1.2    1.2     );
####Distrib(    lnPKidC TruncNormal_v   M_lnPKidC       V_lnPKidC       -0.6    0.6     );
####Distrib(    lnPSlwC TruncNormal_v   M_lnPSlwC       V_lnPSlwC       -0.9    0.9     );


Distrib(        lnPRBCPlasTCAC  TruncNormal_v   M_lnPRBCPlasTCAC        V_lnPRBCPlasTCAC        -4.605  4.605   );
Distrib(        lnPBodTCAC      TruncNormal_v   M_lnPBodTCAC    V_lnPBodTCAC    -1.008  1.008   );
Distrib(        lnPLivTCAC      TruncNormal_v   M_lnPLivTCAC    V_lnPLivTCAC    -1.008  1.008   );


Distrib(        lnkDissocC      TruncNormal_v   M_lnkDissocC    V_lnkDissocC    -0.18   0.18    );
Distrib(        lnBMaxkDC       TruncNormal_v   M_lnBMaxkDC     V_lnBMaxkDC     -0.546  0.546   );


Distrib(        lnPBodTCOHC     TruncNormal_v   M_lnPBodTCOHC   V_lnPBodTCOHC   -1.008  1.008   );
Distrib(        lnPLivTCOHC     TruncNormal_v   M_lnPLivTCOHC   V_lnPLivTCOHC   -1.008  1.008   );
Distrib(        lnPBodTCOGC     TruncNormal_v   M_lnPBodTCOGC   V_lnPBodTCOGC   -4.605  4.605   );
Distrib(        lnPLivTCOGC     TruncNormal_v   M_lnPLivTCOGC   V_lnPLivTCOGC   -4.605  4.605   );
####Distrib(    lnPeffDCVG      TruncNormal_v   M_lnPeffDCVG    V_lnPeffDCVG    -6.908  6.908   );


####Distrib(    lnkTSD  TruncNormal_v   M_lnkTSD        V_lnkTSD        -4.269  4.942   );
####Distrib(    lnkAS   TruncNormal_v   M_lnkAS V_lnkAS -6.571  7.244   );
####Distrib(    lnkTD   TruncNormal_v   M_lnkTD V_lnkTD -4.605  0       );
####Distrib(    lnkAD   TruncNormal_v   M_lnkAD V_lnkAD -7.195  6.62    );
Distrib(        lnkASTCA        TruncNormal_v   M_lnkASTCA      V_lnkASTCA      -7.195  6.62    );
Distrib(        lnkASTCOH       TruncNormal_v   M_lnkASTCOH     V_lnkASTCOH     -7.195  6.62    );


####Distrib(    lnVMaxC TruncNormal_v   M_lnVMaxC       V_lnVMaxC       -2.079  2.079   );
#####Distrib(   lnKMC   TruncNormal_v   M_lnKMC V_lnKMC 0       1       );
####Distrib(    lnClC   TruncNormal_v   M_lnClC V_lnClC -4.158  4.158   );
####Distrib(    lnFracOtherC    TruncNormal_v   M_lnFracOtherC  V_lnFracOtherC  -6.908  6.908   );
####Distrib(    lnFracTCAC      TruncNormal_v   M_lnFracTCAC    V_lnFracTCAC    -3.489  3.489   );
#####Distrib(   lnVMaxDCVGC     TruncNormal_v   M_lnVMaxDCVGC   V_lnVMaxDCVGC   0       1       );
####Distrib(    lnClDCVGC       TruncNormal_v   M_lnClDCVGC     V_lnClDCVGC     -13.815 13.815  );
####Distrib(    lnKMDCVGC       TruncNormal_v   M_lnKMDCVGC     V_lnKMDCVGC     -4.158  4.158   );
#####Distrib(   lnVMaxKidDCVGC  TruncNormal_v   M_lnVMaxKidDCVGC        V_lnVMaxKidDCVGC        0       1       );
####Distrib(    lnClKidDCVGC    TruncNormal_v   M_lnClKidDCVGC  V_lnClKidDCVGC  -13.815 13.815  );
####Distrib(    lnKMKidDCVGC    TruncNormal_v   M_lnKMKidDCVGC  V_lnKMKidDCVGC  -4.158  4.158   );
####Distrib(    lnVMaxLungLivC  TruncNormal_v   M_lnVMaxLungLivC        V_lnVMaxLungLivC        -3.297  3.297   );
```

```
####Distrib(    lnKMClara       TruncNormal_v   M_lnKMClara     V_lnKMClara     -6.908  6.908   );
####Distrib(    lnFracLungSysC  TruncNormal_v   M_lnFracLungSysC        V_lnFracLungSysC        -6.908  6.908   );


#Distrib(       lnVMaxTCOHC     TruncNormal_v   M_lnVMaxTCOHC   V_lnVMaxTCOHC   0       1       );
Distrib(        lnClTCOHC       TruncNormal_v   M_lnClTCOHC     V_lnClTCOHC     -11.513 6.908   );
Distrib(        lnKMTCOH        TruncNormal_v   M_lnKMTCOH      V_lnKMTCOH      -9.21   9.21    );
#Distrib(       lnVMaxGlucC     TruncNormal_v   M_lnVMaxGlucC   V_lnVMaxGlucC   0       1       );
Distrib(        lnClGlucC       TruncNormal_v   M_lnClGlucC     V_lnClGlucC     -9.21   4.605   );
Distrib(        lnKMGluc        TruncNormal_v   M_lnKMGluc      V_lnKMGluc      -6.908  6.908   );
Distrib(        lnkMetTCOHC     TruncNormal_v   M_lnkMetTCOHC   V_lnkMetTCOHC   -11.513 6.908   );


Distrib(        lnkUrnTCAC      TruncNormal_v   M_lnkUrnTCAC    V_lnkUrnTCAC    -4.605  4.605   );
Distrib(        lnkMetTCAC      TruncNormal_v   M_lnkMetTCAC    V_lnkMetTCAC    -9.21   4.605   );


Distrib(        lnkBileC        TruncNormal_v   M_lnkBileC      V_lnkBileC      -9.21   4.605   );
Distrib(        lnkEHRC TruncNormal_v   M_lnkEHRC       V_lnkEHRC       -9.21   4.605   );
Distrib(        lnkUrnTCOGC     TruncNormal_v   M_lnkUrnTCOGC   V_lnkUrnTCOGC   -6.908  6.908   );


####Distrib(    lnFracKidDCVCC  TruncNormal_v   M_lnFracKidDCVCC        V_lnFracKidDCVCC        -6.908  6.908   );
####Distrib(    lnkDCVGC        TruncNormal_v   M_lnkDCVGC      V_lnkDCVGC      -9.21   4.605   );


####Distrib(    lnkNATC TruncNormal_v   M_lnkNATC       V_lnkNATC       -9.21   4.605   );
####Distrib(    lnkKidBioactC   TruncNormal_v   M_lnkKidBioactC V_lnkKidBioactC -9.21   4.605   );

Level {

 Experiment { # 88      # Muller et al. 1974
              # TCA Dosing (3 mg/kg NaTCA = 2.646 mg/kg TCA)
 # NaTCA MW = 185.4
 # TCA MW = 163.5
 # 1 mg NaTCA equiv to  0.8819 mg TCA


# CC= 0;
# Conc=0;

PODoseTCA = NDoses(2, 2.646 0,0 0.01); # Drink over 0.01 hr = 36 seconds

 Print(CPlasTCA, 0.496  0.993   2.98    5.46    9.93    23.8    34.2    48.9    58.8    72      81.6    95.8    106     120
);
 Data (CPlasTCA, 22.7   29.4    23      24.4    21.8    17.2    15.6    14      11.4    8.95    8.48    5.4     5.82    5
);

 Print(zAUrnTCA, 24     48      72      96      120     144     168
);
 Data (zAUrnTCA, 43.4   59.7    75      88.7    98.58   107.98  113.03
);

 Print (CAlvPPM, 0);
 Data (CAlvPPM, -1);

 Print(AUrnTCOGTCOH, 0);
 Data (AUrnTCOGTCOH, -1);

 Print (CVen,   0);
 Data (CVen,    -1);

 Print (CTCOH, 0);
 Data (CTCOH, -1);

 Print (CBldTCA, 0);
 Data (CBldTCA, -1);

 Data (TotCTCOH, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(TotCTCOH, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
```

```
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};

 Experiment { # 89      # Muller et al. 1974
                # TCOH Dosing (10 mg/kg)

# CC= 0;
# Conc=0;

PODoseTCOH = NDoses(2,10 0 ,0 0.01); # Drink over 0.01 hr = 36 seconds

 Print (CTCOH, 0.402    0.415   0.807   1.57    3.11    5.97    10.9    24      35.2    47.9    72.2    96.2
);
 Data (CTCOH, 5.79      4.93    4.1     3.76    2.58    1.91    1.22    0.498   0.276   0.163   0.0487  0.0196
);

 Print(AUrnTCOGTCOH, 24 48      72      96      120
);
 Data (AUrnTCOGTCOH, 84.2       100.9   109.26  113.16  115.39
);

 Print(CPlasTCA, 0.496  0.993   1.49    3.47    5.96    10.9    23.8    34.7    47.6    71.7    95.5    122     146     170
);
 Data (CPlasTCA, 4.8    3.88    6.57    6.86    11.5    18.7    24.2    20.8    17.1    12.1    9.28    8.72    5.73    5.3
);

 Print(zAUrnTCA, 24     48      72      96      120     144     168
);
 Data (zAUrnTCA, 27.8   70.2    101     125.8   147.9   156.74  161.23
);


 Print (CAlvPPM, 0);
 Data (CAlvPPM, -1);


 Print (CVen,   0);
 Data (CVen,    -1);

 Print (CBldTCA, 0);
 Data (CBldTCA, -1);

 Data (TotCTCOH, -1);
 Data (AUrnTCTotMole, -1);
 Data (zAUrnNDCVC, -1);
 Print(TotCTCOH, 1);
 Print(AUrnTCTotMole, 1);
 Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

 #Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
 #Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
 #Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
 #Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect,-1);

};

}

}
################## END Muller et al. 1974 (TCA, TCOH dosing)
}
#### END STUDIES
}
```

```
#### END POPULATION
End.
```