Message

From: Schlosser, Paul [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=121CF759D94E4F08AFDE0CEB646E711B-SCHLOSSER, PAUL]
Sent: 11/14/2019 4:44:27 PM
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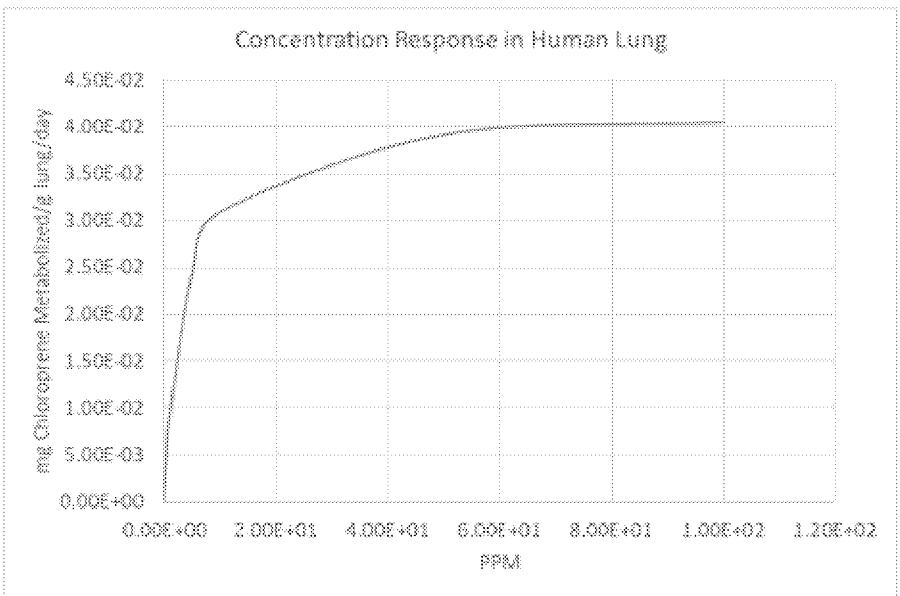
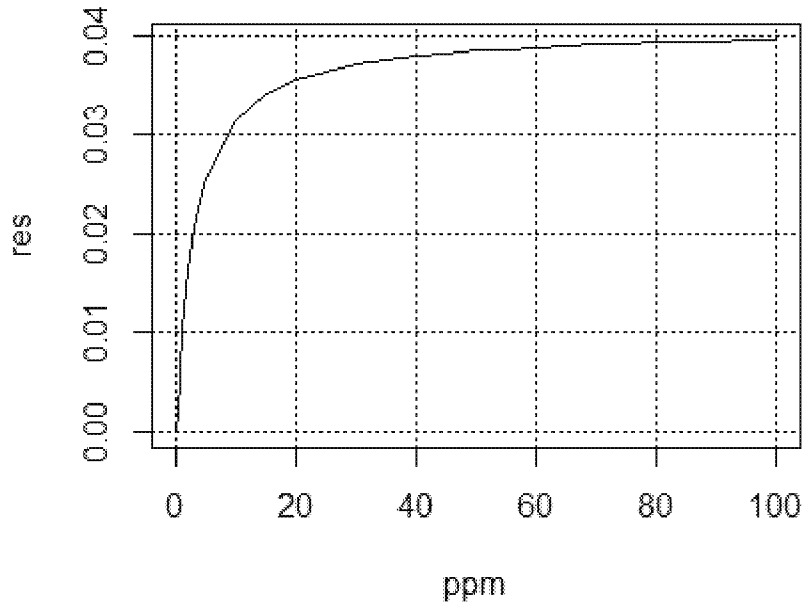
Subject: RE: Chloroprene PBPK: sensitivity analysis scripts

P.S. First below is the figure from the report, 2nd is what I get… I think the apparent sharp bends in the report figure are just from only having a few points. But note that the value I get at 100 ppm is slightly lower too.

-Paul





From: Schlosser, Paul
Sent: Thursday, November 14, 2019 10:22 AM
To: 'Jerry Campbell' <JCampbell@ramboll.com>; Harvey Clewell <HClewell@ramboll.com>
Cc: Walsh, Patrick <patrick-walsh@denka-pe.com>; Thayer, Kris <thayer.kris@epa.gov>; Cascio, Wayne <Cascio.Wayne@epa.gov>; Jones, Samantha <Jones.Samantha@epa.gov>; Lavoie, Emma <Lavoie.Emma@epa.gov>; Bahadori, Tina <Bahadori.Tina@epa.gov>; Kirby, Kevin <KIRBY.KEVIN@EPA.GOV>; Vandenberg, John <Vandenberg.John@epa.gov>; Morozov, Viktor <Morozov.Viktor@epa.gov>; Davis, Allen <Davis.Allen@epa.gov>; White, Paul <White.Paul@epa.gov>; Hawkins, Belinda <Hawkins.Belinda@epa.gov>
Subject: Chloroprene PBPK: sensitivity analysis scripts

Jerry,

In the Fmouse_Metric_SA.R and Human_continuous_SA.R scripts, the output variable being captured, # 23, is the liver metabolic intensity, AMP, not the lung (# 24, AMPLU).

```
> out[1,]<-1:28
> out[1,]
  time     AI     AX     AM   AMLU    AMK    ALU     AL     AK     AS     AR     AF
     1      2      3      4      5      6      7      8      9     10     11     12
MASBAL    CLU     CL     CK     CS     CR     CF     CV  CVLUM    ppm    AMP  AMPLU
    13     14     15     16     17     18     19     20     21     22     23     24
  AMPK    cvl  qcbal   vbal
    25     26     27     28
```

I assume the values in the spreadsheet (with plots) where from the acslX version, as once I make this correction in the SA scripts the resulting SC values are almost the same, only off by 0.01 in a few cases, and are identical for the human SC values.

Similar to what I did for the mouse_inviv_SA script, I've condensed these SA scripts and put the human metabolic parameters into params/Human.R file, to facilitate the QA.

?? Do you have a spreadsheet where Figure 8 is created?

-Paul

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