

Appendix 5: Summary of Analytical Data and Toxicity Study Matches Used in Developing Predictive Models

The following table indicates which analytical data were matched with a specific toxicity study in order to develop predictive models. The green highlights indicate the Analytical Report -Toxicity study pairings that included Method 2 compositional (ring classes 1-7) results that were used in the development of the final models.

Table 5A-1. Analytical Data to Toxicity Studies Matches for Use in Developing Predictive Models

Sample	Analytical Method	Analytical Report No.	Repeat-Dose Study to Match Analytical to	Developmental Study to Match Analytical to	
				Prenatal	Postnatal
8281	Method 2	53201	20535	50511	-
8281	Method 1	62780	20535	50511	-
82191	Method 2	50152	30327	-	-
83366	Method 1	62779	50391	50431	-
83366	Method 2	64348 ZQ	50391	50431	-
85244	Method 1	62778	61590	61801	-
85244	Method 2	64348 ZV	61590	61801	-
86001	Method 1	60711	20525	50541	-
86001	Method 2	64348 ZA	20525	50541	-
86045	Method 1	62781	-	50341	-
86045	Method 2	64349ZW	-	50341	-
86181	Method 1	61525 ZA	64165	64168	-
86181	Method 2	64348 ZO	64165	64168	-
86187	Method 1	61740 ZA	61737	62884	62884
86187	Method 2	64349 ZA	61737	62884	62884
86192	Method 1	61530 ZB	64002	-	-
86193	Method 1	61528 ZA	63237	64643	-
86193	Method 2	64348 ZT	63237	64643	-
86268	Method 1	Avg of 63402 & 63898 ZC ^a	62724	-	-
86270	Method 2	63806 ZF	62326	62328	62328
86271	Method 1	61741 ZD	63456	64146	64146
86271	Method 2	63803 ZD	63456	64146	64146
86272	Method 1	61525 ZC	64184	-	-
86272	Method 2	64348 ZR	64184	-	-
86484	Method 1	61807	62710	62934	-
86484	Method 2	64348 ZM	62710	62934	-
86525	Method 1	62783	62260	-	-
87058	Method 1	62777	62262	-	-
87213	Method 1	62775	61996	61998	61998
87213	Method 2	64348 ZN	61996	61998	61998

Table 5A-1 (cont.). Analytical Data to Toxicity Studies Matches for Use in Developing Predictive Models

Sample	Analytical Method	Analytical Report No.	Repeat-Dose Study to Match Analytical to	Developmental Study to Match Analytical to	
				Prenatal	Postnatal
87293	Method 1	62776	62261	-	-
88614	Method 2	63057	63036	63239	-
89040	Method 1	63898 ZB	1451-81	51841	-
89106	Method 1	63786	63266	63264	-
89106	Method 2	63263	63266	63264	-
89645	Method 2	63837	63834	63836	63836 64282
89646	Method 1	64180	63846	63848	63848 64283
89646	Method 2	63849	63846	63848	63848 64283
90062	Method 1	Avg of 63402 & 63898 ZC ^a	62724	-	-
F-179	Method 2	65726-ZA-ZR	ATX-910012	ATX-910042	ATX-910155
F-179	Method 1	65726-ZA-ZR	ATX-910012	ATX-910042	ATX-910155
F-193	Method 2	65726-ZA-ZR	-	ATX-920011	ATX-910127
F-193	Method 1	65726-ZA-ZR	-	ATX-920011	ATX-910127
F-194	Method 2	65726-ZA-ZR	-	-	ATX-910128
F-194	Method 1	65726-ZA-ZR	-	-	ATX-910128
F-195	Method 2	65726-ZA-ZR	-	ATX-920156	ATX-910129
F-195	Method 1	65726-ZA-ZR	-	ATX-920156	ATX-910129
F-196	Method 2	65726-ZA-ZR	-	ATX-920012	ATX-910130
F-196	Method 1	65726-ZA-ZR	-	ATX-920012	ATX-910130
F-197	Method 2	65726-ZA-ZR	-	ATX-920154	ATX-910131
F-197	Method 1	65726-ZA-ZR	-	ATX-920154	ATX-910131
F-199	Method 2	65726-ZA-ZR	-	ATX-920013	ATX-910133
F-199	Method 1	65726-ZA-ZR	-	ATX-920013	ATX-910133
F-200	Method 2	65726-ZA-ZR	-	-	ATX-910134
F-200	Method 1	65726-ZA-ZR	-	-	ATX-910134
F-201	Method 2	65726-ZA-ZR	-	-	ATX-910135
F-201	Method 1	65726-ZA-ZR	-	-	ATX-910135
F-213	Method 2	65726-ZA-ZR	-	-	ATX-910262
F-213	Method 1	65726-ZA-ZR	-	-	ATX-910262
F-215	Method 2	65726-ZA-ZR	-	ATX-920155	ATX-910263
F-215	Method 1	65726-ZA-ZR	-	ATX-920155	ATX-910263
F-220	Method 2	65726-ZA-ZR	-	-	ATX-910290
F-220	Method 1	65726-ZA-ZR	-	-	ATX-910290
F-221	Method 2	65726-ZA-ZR	-	-	ATX-910269
F-221	Method 1	65726-ZA-ZR	-	-	ATX-910269
F-222	Method 2	65726-ZA-ZR	-	-	ATX-910270

Table 5A-1 (cont.). Analytical Data to Toxicity Studies Matches for Use in Developing Predictive Models

Sample	Analytical Method	Analytical Report No.	Repeat- Dose Study to Match Analytical to	Developmental Study to Match Analytical to	
				Prenatal	Postnatal
F-222	Method 1	65726-ZA-ZR	-	-	ATX-910270
F-225	Method 2	65726-ZA-ZR	-	-	ATX-910264
F-225	Method 1	65726-ZA-ZR	-	-	ATX-910264
F-227	Method 2	65726-ZA-ZR	-	-	ATX-910266
F-227	Method 1	65726-ZA-ZR	-	-	ATX-910266
F-228	Method 2	65726-ZA-ZR	-	-	ATX-910267
F-228	Method 1	65726-ZA-ZR	-	-	ATX-910267
F-229	Method 2	65726-ZA-ZR	-	-	ATX-910268
F-229	Method 1	65726-ZA-ZR	-	-	ATX-910268
F-233	Method 2	66149	ATX-910233	-	ATX-930021
F-233	Method 1	66149	ATX-910233	-	ATX-930021
F-236	Method 2	66149	ATX-910257	-	ATX-930023
F-236	Method 1	66149	ATX-910257	-	ATX-930023
F-250	Method 2	66149	ATX-920056	-	ATX-930024
F-250	Method 1	66149	ATX-920056	-	ATX-930024
F-251	Method 2	66149	ATX-920064	-	ATX-930025
F-251	Method 1	66149	ATX-920064	-	ATX-930025
F-274	Method 2	66149	-	-	ATX-930069
F-274	Method 1	66149	-	-	ATX-930069
F-275	Method 2	66149	-	-	ATX-930071
F-275	Method 1	66149	-	-	ATX-930071
F-276	Method 2	66149	-	-	ATX-930073
F-276	Method 1	66149	-	-	ATX-930073
F-277	Method 2	66149	-	-	ATX-930075
F-277	Method 1	66149	-	-	ATX-930075

^a Two sets of analytical data on the sample were provided to the Task Group. The Task Group decided to average the two sets, since there were no attributes which allowed one set to be selected over the other.

Following the identification of the reports to be used for comparison (**Table 5A-1**, above), data were reviewed to ensure that they were sufficiently robust. Although all the available data from the repeat-dose studies were used for statistical modeling, some of the developmental toxicity data were excluded. The details of the data points that were excluded and the reasons for their exclusion are described in detail in **Appendix 2**.