

Supplementary Table S7. Comparison between observed and predicted PK parameters.

Comparison between observed (obs.) vs. predicted (pred.) PK parameters for the area under the curve (AUC) and the maximal concentration (Cmax) calculated during PBPK model development and validation. Information about the different studies can be found in Supplementary Table S5.

Study ID	Drug/ Metabolite	obs. AUC(0-t) [$\mu\text{mol}/\text{min}/\text{l}$]	pred. AUC(0-t) [$\mu\text{mol}/\text{min}/\text{l}$]	obs. Cmax [$\mu\text{mol}/\text{l}$]	pred. Cmax [$\mu\text{mol}/\text{l}$]
1	CAF	15352.03	18138.13	45.45	63.65
2	CAF	16454.46	16948.87	42.55	44.99
3	CAF	8801.67	8561.24	34.36	32.94
3	PX	3281.31	3064.54	8.3	7.44
3	TB	932.19	854.68	2.43	2.1
3	TP	333.45	327.64	0.97	0.95
4	CAF	20022.62	17521.79	84.74	66.65
4	PX	5910.42	6006.03	15.41	14.67
4	TB	1468.9	1646.02	3.75	4.09
4	TP	582.09	664.45	1.61	1.94
5	CAF	12575.88	15209.84	23.53	27.4
5	PX	8055.72	8032.27	8.62	7.8
5	TB	727.93	2348.92	1.64	2.22
5	TP	255.32	389.53	0.8	0.98
6	CAF	38045.37	26026.6	59.42	50.46
6	PX	22721.04	13927.44	18.36	15.31
6	TB	2008.78	4540.18	1.59	4.31
6	TP	2434.37	3137.84	1.58	2.07
7	CAF	3136.22	2822.1	6.41	5.79
8	CAF	18331.09	17405.76	34.67	35.15
9	CAF	38934.18	29637.11	66.48	59.05
10	CAF	48814.04	45627.33	83.73	89.42
11	APAP	20525.83	15740.6	114.33	94.66
11	APAPG	8039.71	5894.59	30.6	19.51
11	APAPS	4206.66	3004.43	15.55	13.44
11	APAPC	2106.23	1744.3	7.73	6.18
12	APAP	26802.18	23210.7	122.72	142.35
12	APAPG	12478.09	10453.6	38.58	28
12	APAPS	8145.02	6386.79	26.84	26.42
13	APAP	4856.58	6896.4	27.42	40.66
14	APAP	13396.63	14059.81	88.1	84.48
15	APAP	26806.68	28897.79	131.9	176.04
16	APAP	17493.32	16807.26	97.74	101.09
17	APAP	8674.87	20003.71	106.85	114.8
18	APAP	4459.37	8709.99	22.95	46.3
19	APAP	6290.79	10400.37	27.25	53.63