

High-throughput functional screening of steroid substrates with wild-type and chimeric P450 enzymes

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## **Supplementary Materials**

**Table S1. Table of specific activities observed with the different enzymes when assayed for the different steroidal substrates of this work (in five parts).**

EOR, MOR, EFEE stands for 7-ethoxy-, 7-methoxy-resorufin, and 7-ethoxy-fluorescein ethyl ester, respectively. The different hydroxylated metabolites observed in LC/MS are designated by one or two letters, abbreviating the name of the steroid, and a number corresponding to the rank in elution time on the LC. RUNdM stands for the unique N-demethylation metabolite of mifepristone observed in LC/MS. Specific activities are expressed as pmol product per min per mg microsomal protein for EOR, MOR and EFEE. Specific activities are expressed as LC/MS peak area units per min per mg microsomal protein for all other activities.

ENZYME	TESTOSTERONE							MIFEPRISTONE					17-METHYL-TESTOSTERONE					
	EOR	MOR	EFEE	T1	T2	T3	T4	RU NdM	RU1	RU2	RU3	RU4	RU5	MT1	MT2	MT3	MT4	MT5
Human wt CYP1A1-1	4,739E+03	1,352E+04	3,331E+02	1,721E+03	1,013E+02	0,000E+00	0,000E+00	8,361E+00	5,865E+02	1,216E+03	0,000E+00	1,215E+03	1,090E+03	1,291E+03	1,265E+02	7,483E+02	2,458E+03	0,000E+00
Human wt CYP1A1-2	4,543E+03	1,361E+04	3,401E+02	1,436E+03	8,422E+01	0,000E+00	1,008E+03	1,355E+01	1,214E+03	8,811E+02	3,156E+04	2,292E+03	1,926E+03	2,159E+03	1,324E+02	4,353E+02	3,917E+03	0,000E+00
Human wt CYP1A2-1	8,065E+02	1,230E+04	1,921E-01	0,000E+00	1,480E+00	0,000E+00	0,000E+00	4,531E-01	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00
Human wt CYP1A2-2	8,473E+02	1,311E+04	3,842E-01	0,000E+00	2,600E+00	0,000E+00	0,000E+00	7,681E-01	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00
Mouse wt CYP1A1-1	1,026E+04	3,567E+04	1,028E+02	1,713E+02	4,778E+01	0,000E+00	2,523E+03	4,961E+01	0,000E+00	0,000E+00	0,000E+00	0,000E+00	2,656E+02	0,000E+00	9,093E+01	6,635E+02	7,452E+02	0,000E+00
Mouse wt CYP1A1-2	1,075E+04	3,888E+04	8,357E+01	9,606E+01	3,245E+01	0,000E+00	1,599E+03	6,963E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	5,992E+01	4,167E+02	1,277E+03	0,000E+00
Rabbit wt CYP1A2-1	2,408E+02	2,874E+04	3,202E+02	3,877E+02	5,880E+01	1,477E+02	0,000E+00	5,824E+01	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	7,068E+01	5,203E+02	4,353E+02	0,000E+00
Rabbit wt CYP1A2-2	2,771E+02	2,767E+04	2,776E+02	9,673E+01	1,988E+01	1,664E+02	0,000E+00	1,463E+01	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	4,067E+01	4,488E+02	5,436E+02	0,000E+00
Chim3	9,973E+03	3,055E+04	6,763E+01	0,000E+00	4,830E+01	3,442E+02	5,738E+03	1,057E+01	0,000E+00	0,000E+00	0,000E+00	0,000E+00	1,242E+02	0,000E+00	8,920E+01	6,494E+02	1,535E+03	0,000E+00
Chim4	1,552E+03	1,315E+04	1,153E+02	6,767E+02	6,487E+01	3,155E+02	0,000E+00	9,386E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	7,329E+01	2,625E+02	1,927E+03	0,000E+00
Chim5	1,352E+04	3,210E+04	2,445E+02	1,177E+03	3,274E+02	0,000E+00	6,305E+03	4,961E+01	0,000E+00	0,000E+00	0,000E+00	5,631E+02	5,295E+02	0,000E+00	4,853E+02	4,282E+03	3,676E+02	0,000E+00
Chim6	1,586E+03	1,295E+04	9,990E+01	6,932E+02	8,999E+01	3,792E+03	0,000E+00	8,518E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	9,163E+01	4,851E+02	2,856E+03	0,000E+00
Chim7	3,228E+03	1,622E+04	3,485E+02	0,000E+00	8,165E+01	0,000E+00	0,000E+00	9,632E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	1,309E+02	1,814E+02	0,000E+00	0,000E+00
Chim8	8,114E+03	1,450E+04	1,298E+02	0,000E+00	7,778E+01	0,000E+00	3,870E+03	3,220E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	6,963E+01	8,440E+02	1,725E+03	0,000E+00
Chim9	1,276E+04	4,494E+04	1,233E+02	0,000E+00	5,757E+01	0,000E+00	2,571E+03	1,943E+01	0,000E+00	0,000E+00	0,000E+00	0,000E+00	2,217E+02	0,000E+00	1,321E+02	1,201E+03	2,463E+03	0,000E+00
Chim11	4,714E+03	2,401E+04	3,605E+02	1,629E+02	1,373E+01	0,000E+00	0,000E+00	5,190E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	1,645E+01	0,000E+00	2,825E+02	0,000E+00
Chim12	1,586E+03	1,295E+04	9,990E+01	6,932E+02	8,999E+01	4,131E+02	0,000E+00	8,518E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	9,163E+01	4,851E+02	2,856E+03	0,000E+00
Chim13	2,967E+03	9,834E+03	2,033E+02	0,000E+00	2,747E+01	7,882E+02	1,657E+03	2,837E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	3,134E+01	6,238E+02	3,943E+02	0,000E+00
Chim14	2,953E+02	3,439E+04	3,940E+02	0,000E+00	8,961E+00	0,000E+00	0,000E+00	8,564E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	2,834E+01	3,284E+02	2,533E+02	0,000E+00
ChiMo1	2,383E+03	1,188E+04	3,775E+01	1,966E+02	9,186E+00	0,000E+00	0,000E+00	9,133E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	1,775E+01	0,000E+00	7,470E+02	0,000E+00
ChiMo2	3,680E+02	1,461E+03	0,000E+00	0,000E+00	1,314E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	3,021E+00	0,000E+00	0,000E+00	0,000E+00
ChiMo3	4,089E+01	5,233E+02	9,702E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	2,218E-01	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00
ChiMo4	3,862E+01	2,835E+02	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	3,213E+00	0,000E+00	0,000E+00	0,000E+00
ChiMo5	1,703E+04	5,059E+04	3,202E+02	2,581E+03	2,749E+02	2,462E+03	6,448E+03	1,563E+01	0,000E+00	0,000E+00	0,000E+00	4,633E+03	1,139E+03	9,220E+02	1,612E+02	1,618E+03	1,692E+03	0,000E+00
ChiMo6-1	2,163E+03	1,167E+04	1,443E+02	0,000E+00	1,208E+01	0,000E+00	0,000E+00	9,175E-01	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	7,163E+00	0,000E+00	0,000E+00	3,087E+04
ChiMo6-2	2,163E+03	1,167E+04	1,443E+02	1,396E+02	1,178E+01	1,705E+02	1,164E+03	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	6,698E+00	0,000E+00	0,000E+00	5,306E+04
ChiMo7	1,054E+04	5,526E+04	1,402E+02	0,000E+00	5,895E+01	2,138E+02	0,000E+00	3,661E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	2,460E+01	8,690E+01	2,515E+02	0,000E+00
ChiMo8	9,134E+03	3,399E+04	4,330E+02	1,455E+02	1,766E+02	9,471E+02	0,000E+00	5,355E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	8,061E+01	2,853E+02	8,150E+02	0,000E+00
ChiMo9	1,640E+03	9,943E+03	2,459E+01	1,227E+02	1,830E+01	8,479E+01	0,000E+00	5,128E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	2,144E+01	2,975E+02	0,000E+00	0,000E+00
ChiMo10	8,701E+02	5,102E+03	1,787E+01	0,000E+00	5,082E+00	7,008E+03	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00
ChiMo11	7,269E+01	1,047E+03	7,685E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	0,000E+00	1,983E+03	1,173E+03	0,000E+00	0,000E+00	0,000E+00	0,000E+00	5,288E+00	0,000E+00	0,000E+00	0,000E+00







