

## SUPPORTING INFORMATION

PrenDB: A substrate prediction database to enable biocatalytic use of prenyltransferases

**Jakub Gunera**<sup>‡†1</sup>, **Florian Kindinger**<sup>§1</sup>, **Shu-Ming Li**<sup>§†2</sup> and **Peter Kolb**<sup>‡†3</sup>

<sup>‡</sup> Department of Pharmaceutical Chemistry, Philipps-University, Marburg, Hesse, 35032, Germany

<sup>§</sup> Institute of Pharmaceutical Biology and Biotechnology, Philipps-University, Marburg, Hesse, 35032, Germany

<sup>†</sup> Synmikro, LOEWE Centre for Synthetic Microbiology, Philipps-University, Marburg, Hesse, 35043, Germany

<sup>1</sup>These authors contributed equally to this study.

<sup>2</sup>To whom correspondence should be addressed: [shuming.li@staff.uni-marburg.de](mailto:shuming.li@staff.uni-marburg.de)

<sup>3</sup>To whom correspondence should be addressed: [peter.kolb@uni-marburg.de](mailto:peter.kolb@uni-marburg.de)

**Table S1:** List of substrates with their PrenDB ID, SMILES string and cluster membership (C)

ID	PrenDB ID	SMILES	C
S1	PTDBSUB00695	<chem>O=C1NC(Cc2c[nH]c3ccccc23)C(=O)N2CCC[C@@H]12</chem>	1
S2	PTDBSUB00027	<chem>O=C1N[C@H](Cc2c[nH]c3ccccc23)C(=O)N2CCC[C@H]12</chem>	1
S3	PTDBSUB00022	<chem>O=C1N[C@H](Cc2c[nH]c3ccccc23)C(=O)N2CCC[C@@H]12</chem>	1
S4	PTDBSUB00001	<chem>O=C1N[C@@H](Cc2c[nH]c3ccccc23)C(=O)N2CCC[C@@H]12</chem>	1
S5	PTDBSUB00017	<chem>O=C1N[C@@H](Cc2c[nH]c3ccccc23)C(=O)N2CCC[C@H]12</chem>	1
S6	PTDBSUB00286	<chem>O=C1N[C@H](Cc2c[nH]c3ccccc23)C(=O)Nc2ccccc21</chem>	2
S7	PTDBSUB00392	<chem>O=C1N[C@@H](Cc2c[nH]c3ccccc23)C(=O)Nc2ccccc21</chem>	2
S8	PTDBSUB00049	<chem>C[C@@H]1NC(=O)[C@@H](Cc2c[nH]c3ccccc23)NC1=O</chem>	2
S9	PTDBSUB00044	<chem>C[C@H]1NC(=O)[C@@H](Cc2c[nH]c3ccccc23)NC1=O</chem>	2
S10	PTDBSUB00032	<chem>C[C@@H]1NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC1=O</chem>	2
S11	PTDBSUB00039	<chem>C[C@H]1NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC1=O</chem>	2
S12	PTDBSUB00012	<chem>O=C1N[C@@H](Cc2c[nH]c3ccccc23)C(=O)N[C@H]1Cc1ccccc1</chem>	2
S13	PTDBSUB00005	<chem>O=C1N[C@@H](Cc2c[nH]c3ccccc23)C(=O)N[C@H]1Cc1ccc(O)cc1</chem>	2
S14	PTDBSUB00412	<chem>O=C1N[C@H](Cc2c[nH]c3ccccc23)C(=O)N[C@H]1Cc1ccc(O)cc1</chem>	2
S15	PTDBSUB00059	<chem>O=C1CNC(=O)[C@H](Cc2c[nH]c3ccccc23)N1</chem>	2
S16	PTDBSUB00072	<chem>O=C1N[C@@H](Cc2c[nH]c3ccccc23)C(=O)N[C@H]1Cc1c[nH]c2ccccc12</chem>	2
S17	PTDBSUB00054	<chem>O=C1N[C@@H](Cc2c[nH]c3ccccc23)C(=O)N[C@H]1Cc1cnc[nH]1</chem>	2
S18	PTDBSUB00064	<chem>CC(C)[C@@H]1NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC1=O</chem>	2
S19	PTDBSUB00103	<chem>[NH3+][C@@H](Cc1c[nH]c2ccccc12)C(=O)[O-]</chem>	3
S20	PTDBSUB00173	<chem>[NH3+][C@H](Cc1c[nH]c2ccccc12)C(=O)[O-]</chem>	3
S21	PTDBSUB00186	<chem>C[C@@]([NH3+])(Cc1c[nH]c2ccccc12)C(=O)[O-]</chem>	3
S22	PTDBSUB00189	<chem>C[C@]([NH3+])(Cc1c[nH]c2ccccc12)C(=O)[O-]</chem>	3
S23	PTDBSUB00179	<chem>[NH3+]CCc1c[nH]c2ccccc12</chem>	3
S24	PTDBSUB00415	<chem>O=C([O-])Cc1c[nH]c2ccccc12</chem>	3
S25	PTDBSUB00491	<chem>O=C([O-])C(=O)Cc1c[nH]c2ccccc12</chem>	3
S26	PTDBSUB00297	<chem>O=C([O-])CCc1c[nH]c2ccccc12</chem>	3
S27	PTDBSUB00496	<chem>O=C([O-])CCCc1c[nH]c2ccccc12</chem>	3
S28	PTDBSUB00676	<chem>CC(=O)N[C@@H](Cc1c[nH]c2ccccc12)C(C)=O</chem>	3
S29	PTDBSUB00317	<chem>CC(=O)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)[O-]</chem>	3
S30	PTDBSUB00423	<chem>CC(=O)N[C@H](Cc1c[nH]c2ccccc12)C(=O)[O-]</chem>	3
S31	PTDBSUB00183	<chem>C[NH2+][C@@H](Cc1c[nH]c2ccccc12)C(=O)[O-]</chem>	3
S32	PTDBSUB00192	<chem>O=C([O-])[C@@H](O)Cc1c[nH]c2ccccc12</chem>	3
S33	PTDBSUB00195	<chem>O=C([O-])[C@H](O)Cc1c[nH]c2ccccc12</chem>	3
S34	PTDBSUB00176	<chem>[NH3+][C@H](CC(=O)[O-])Cc1c[nH]c2ccccc12</chem>	3
S35	PTDBSUB00418	<chem>[NH3+][C@@H](CC(=O)[O-])Cc1c[nH]c2ccccc12</chem>	3
S36	PTDBSUB00139	<chem>[NH3+][C@@H](Cc1c[nH]c2ccccc12)C(=O)NCC(=O)[O-]</chem>	3
S37	PTDBSUB00488	<chem>[NH3+][C@H](Cc1c[nH]c2ccccc12)C(=O)NO</chem>	3
S38	PTDBSUB00499	<chem>COC(=O)[C@H]([NH3+])Cc1c[nH]c2ccccc12</chem>	3
S39	PTDBSUB00593	<chem>[NH3+][C@@H](C(=O)[O-])[C@@H](O)c1ccc(O)c(O)c1</chem>	4
S40	PTDBSUB00722	<chem>[NH3+][C@@H](C(=O)[O-])C(O)c1ccc(O)c(O)c1</chem>	4

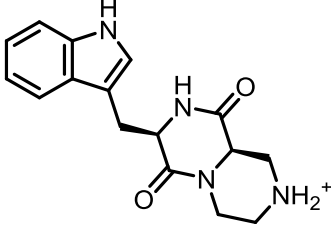
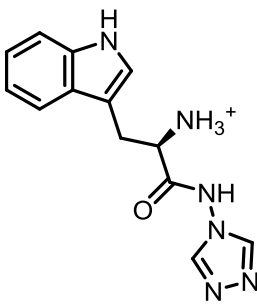
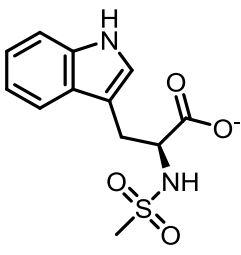
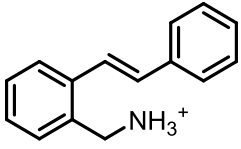
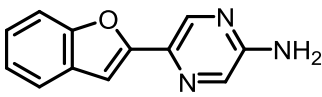
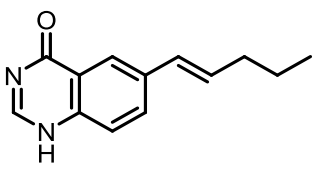
S41	PTDBSUB00689	Cc1ccc(C[C@@H]2NC(=O)[C@H](Cc3ccc(O)cc3)NC2=O)cc1	5
S42	PTDBSUB00571	O=C([O-])[C@@H](O)Cc1ccc(O)cc1	5
S43	PTDBSUB00574	O=C([O-])[C@H](O)Cc1ccc(O)cc1	5
S44	PTDBSUB00554	[NH3+][C@@H](C(=O)[O-])c1ccc(O)cc1	5
S45	PTDBSUB00551	[NH3+][C@H](CC(=O)[O-])c1ccc(O)cc1	5
S46	PTDBSUB00718	[NH3+][C](CC(=O)[O-])c1ccc(O)cc1	5
S47	PTDBSUB00376	CC([NH3+])(Cc1ccc(O)cc1)C(=O)[O-]	5
S48	PTDBSUB00578	C[C@@]([NH3+])(Cc1ccc(O)cc1)C(=O)[O-]	5
S49	PTDBSUB00467	O=C(CCc1ccc(O)cc1)c1c(O)cc(O)cc1O	5
S50	PTDBSUB00079	O=C([O-])C(=O)Cc1ccc(O)cc1	5
S51	PTDBSUB00568	O=C([O-])CCc1ccc(O)cc1	5
S52	PTDBSUB00666	Oc1cc2ccccc2cc1O	6
S53	PTDBSUB00652	Oc1ccc2ccccc2c1	6
S54	PTDBSUB00289	Oc1ccc2ccc(O)cc2c1	6
S55	PTDBSUB00613	Oc1ccc2cc(O)ccc2c1	6
S56	PTDBSUB00647	Nc1cccc2ccc(O)cc12	6
S57	PTDBSUB00448	COc1cccc2ccc(O)cc12	6
S58	PTDBSUB00451	CCOc1cccc2ccc(O)cc12	6
S59	PTDBSUB00656	Oc1ccc(O)c2ccccc12	6
S60	PTDBSUB00661	Oc1cccc2c(O)cccc12	6
S61	PTDBSUB00399	Oc1ccc2c(O)cccc2c1	6
S62	PTDBSUB00596	Oc1cccc2ccccc12	6
S63	PTDBSUB00445	Cc1ccc2ccccc(O)c2c1	6
S64	PTDBSUB00601	Oc1ccc2ccccc(O)c2c1	6
S65	PTDBSUB00088	COc1ccc2c3c4n(c2c1)[C@@H](C=C(C)C)OOC(C)(C)C[C@@H]4N1C(=O)[C@@H]2CCC N2C(=O)[C@]1(O)[C@H]3O	6
S66	PTDBSUB00082	COc1ccc2c3c([nH]c2c1)[C@H](C=C(C)C)N1C(=O)[C@@H]2CCCN2C(=O)[C@]1(O)[C@ H]3O	6
S67	PTDBSUB00085	COc1ccc2c3c(n(CC=C(C)C)c2c1)[C@H](C=C(C)C)N1C(=O)[C@@H]2CCCN2C(=O)[C@] 1(O)[C@H]3O	6
S68	PTDBSUB00094	Cc1cc2oc3ccccc(=O)c-3c([O-])c2cc1O	6
S69	PTDBSUB00100	Cc1c([O-])c(C)c2c(O)c3c(=O)cccc-3oc2c1C	6
S70	PTDBSUB00091	Cc1cc2oc3ccccc(=O)c-3c(O)c2c(CO)c1[O-]	6
S71	PTDBSUB00097	Cc1cc2oc3ccccc(=O)c-3c(O)c2c(C)c1[O-]	6
S72	PTDBSUB00479	COc1ccc(-c2coc3ccc(=O)cc(O)c-3c2[O-])cc1	6
S73	PTDBSUB00472	O=c1cc2oc(-c3ccc(O)cc3)cc([O-])c-2c(O)c1	6
S74	PTDBSUB00343	O=c1cc2oc3cc(O)cc([O-])c3c([O-])c-2c(O)c1	6
S75	PTDBSUB00339	O=c1cc2oc3ccc(O)cc3c([O-])c-2c(O)c1	6
S76	PTDBSUB00351	O=c1cc2oc3cc(O)ccc3c([O-])c-2c(O)c1	6
S77	PTDBSUB00292	O=C1C=C([O-])c2c([O-])cc(O)cc2C1=O	6
S78	PTDBSUB00606	O=C(O)c1cc2ccccc([O-])c2cc1O	6
S79	PTDBSUB00610	O=C(O)c1cc2cc(O)ccc2cc1[O-]	6
S80	PTDBSUB00483	O=C1C[C@H](c2ccccc2)Oc2cc(O)ccc21	6
S81	PTDBSUB00454	Cc1cc([O-])c2c(c1)O[C@H](c1ccc(O)cc1)CC2=O	6
S82	PTDBSUB00460	COc1ccc([C@@H]2CC(=O)c3c([O-])cc(C)cc3O2)cc1O	6

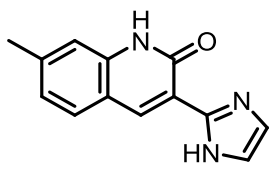
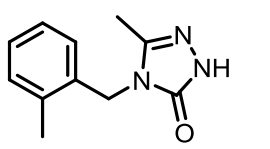
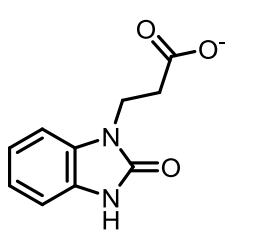
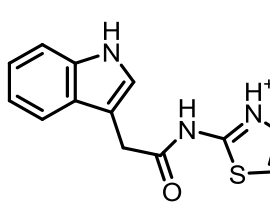
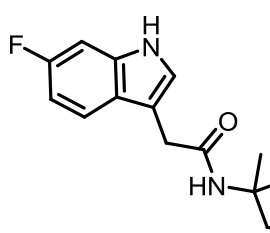
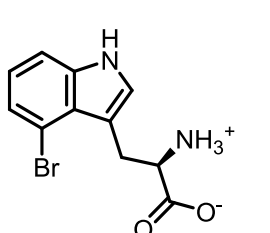
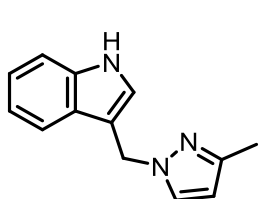
S83	PTDBSUB00464	<chem>COc1cc([C@H]2Oc3cc([C@H]4Oc5cc(O)cc([O-])c5C(=O)[C@@H]4O)ccc3O[C@@H]2CO)ccc1O</chem>	6
S84	PTDBSUB00457	<chem>Cc1cc(O)c2c(c1)O[C@H](c1ccc(O)c(O)c1)CC2O</chem>	6
S85	PTDBSUB00475	<chem>Oc1ccc(C2=COc3cc(O)cc(O)c3C2O)cc1</chem>	6
S86	PTDBSUB00367	<chem>Cn1c(O)c2c3c(c4c(c2c1O)=c1cccc1=N4)N=c1cccc1=3</chem>	6
S87	PTDBSUB00144	<chem>COc1c(O)c(=C2C=Nc3cccc32)c(OC)c(O)c1=C1C=Nc2cccc21</chem>	6
S88	PTDBSUB00396	<chem>O=C([O-])c1cccc2c1Nc1cccc1N2</chem>	6
S89	PTDBSUB00385	<chem>CC(=O)O[C@H]1[C@@H](C)C[NH+](C)[C@@H]2Cc3c[nH]c4cccc(c34)[C@@H]12</chem>	7
S90	PTDBSUB00388	<chem>CC(=O)O[C@H]1[C@H](C)C[NH+](C)[C@@H]2Cc3c[nH]c4cccc(c34)[C@@H]12</chem>	7
S91	PTDBSUB00136	<chem>CC(=O)/C=C/c1c[nH]c2cccc12</chem>	8
S92	PTDBSUB00300	<chem>O=C([O-])/C=C/c1c[nH]c2cccc12</chem>	8
S93	PTDBSUB00359	<chem>O=C1NCc2c1c1c3cccc3[nH]c1c1[nH]c3cccc3c21</chem>	8
S94	PTDBSUB00364	<chem>O=C1N[C@@H](O)c2c1c1c3cccc3[nH]c1c1[nH]c3cccc3c21</chem>	8
S95	PTDBSUB00148	<chem>C=c1c(OC)c(-c2c(CC=C(C)C)[nH]c3cccc23)c(=C)c(OC)c1-c1c[nH]c2cccc12</chem>	8
S96	PTDBSUB00151	<chem>C=CC(C)(C)n1cc(C2=C(OC)C(=O)C(c3c[nH]c4cccc34)=C(OC)C2=O)c2cccc21</chem>	8
S97	PTDBSUB00703	<chem>[NH3+][C@H](Cc1cc(l)c([O-])c(l)c1)C(=O)[O-]</chem>	9
S98	PTDBSUB00370	<chem>[NH3+][C@@H](Cc1cc(Br)c([O-])c(Br)c1)C(=O)[O-]</chem>	9
S99	PTDBSUB00373	<chem>[NH3+][C@@H](Cc1cc(l)c([O-])c(l)c1)C(=O)[O-]</chem>	9
S100	PTDBSUB00548	<chem>[NH3+][C@@H](Cc1ccc([O-])c([N+](=O)[O-])c1)C(=O)[O-]</chem>	9
S101	PTDBSUB00706	<chem>[NH3+][C@H](Cc1ccc([O-])c([N+](=O)[O-])c1)C(=O)[O-]</chem>	9
S102	PTDBSUB00106	<chem>[NH3+][C@@H](Cc1ccc(O)cc1)C(=O)[O-]</chem>	9
S103	PTDBSUB00542	<chem>[NH3+][C@H](Cc1ccc(O)cc1)C(=O)[O-]</chem>	9
S104	PTDBSUB00321	<chem>Nc1ccc(C[C@H]([NH3+])C(=O)[O-])cc1</chem>	9
S105	PTDBSUB00545	<chem>Nc1ccc(C[C@@H]([NH3+])C(=O)[O-])cc1</chem>	9
S106	PTDBSUB00587	<chem>[NH3+][C@H](Cc1ccc(O)c(l)c1)C(=O)[O-]</chem>	9
S107	PTDBSUB00584	<chem>[NH3+][C@@H](Cc1ccc(O)c(F)c1)C(=O)[O-]</chem>	9
S108	PTDBSUB00382	<chem>[NH3+][C@@H](Cc1ccc(O)c(l)c1)C(=O)[O-]</chem>	9
S109	PTDBSUB00581	<chem>[NH3+][C@H](Cc1ccc(O)c(F)c1)C(=O)[O-]</chem>	9
S110	PTDBSUB00112	<chem>[NH3+][C@@H](Cc1cccc(O)c1)C(=O)[O-]</chem>	9
S111	PTDBSUB00565	<chem>[NH3+][C@H](Cc1cccc(O)c1)C(=O)[O-]</chem>	9
S112	PTDBSUB00562	<chem>Nc1cc(C[C@@H]([NH3+])C(=O)[O-])ccc1O</chem>	9
S113	PTDBSUB00379	<chem>[NH3+][C@@H](Cc1ccc(O)c(O)c1)C(=O)[O-]</chem>	9
S114	PTDBSUB00590	<chem>[NH3+][C@H](Cc1ccc(O)c(O)c1)C(=O)[O-]</chem>	9
S115	PTDBSUB00161	<chem>Cc1ccc2c(C[C@H]([NH3+])C(=O)[O-])c[nH]c2c1</chem>	10
S116	PTDBSUB00164	<chem>Cc1ccc2c(C[C@@H]([NH3+])C(=O)[O-])c[nH]c2c1</chem>	10
S117	PTDBSUB00310	<chem>[NH3+][C@H](Cc1c[nH]c2cc(F)ccc12)C(=O)[O-]</chem>	10
S118	PTDBSUB00441	<chem>[NH3+][C@@H](Cc1c[nH]c2cc(F)ccc12)C(=O)[O-]</chem>	10
S119	PTDBSUB00516	<chem>[NH3+][C@H](Cc1c[nH]c2ccc(F)cc12)C(=O)[O-]</chem>	10
S120	PTDBSUB00438	<chem>[NH3+][C@@H](Cc1c[nH]c2ccc(F)cc12)C(=O)[O-]</chem>	10
S121	PTDBSUB00432	<chem>[NH3+][C@@H](Cc1c[nH]c2ccc(Br)cc12)C(=O)[O-]</chem>	10
S122	PTDBSUB00435	<chem>[NH3+][C@H](Cc1c[nH]c2ccc(Br)cc12)C(=O)[O-]</chem>	10
S123	PTDBSUB00167	<chem>COc1ccc2[nH]cc(C[C@H]([NH3+])C(=O)[O-])c2c1</chem>	10
S124	PTDBSUB00170	<chem>COc1ccc2[nH]cc(C[C@@H]([NH3+])C(=O)[O-])c2c1</chem>	10

S125	PTDBSUB00155	Cc1ccc2[nH]cc(C[C@H]([NH3+])C(=O)[O-])c2c1	10
S126	PTDBSUB00158	Cc1ccc2[nH]cc(C[C@@H]([NH3+])C(=O)[O-])c2c1	10
S127	PTDBSUB00429	[NH3+][C@@H](Cc1c[nH]c2ccc(O)cc12)C(=O)[O-]	10
S128	PTDBSUB00511	[NH3+][C@H](Cc1c[nH]c2ccc(O)cc12)C(=O)[O-]	10
S129	PTDBSUB00303	Cn1cc(C[C@@H]([NH3+])C(=O)[O-])c2ccccc21	11
S130	PTDBSUB00109	[NH3+][C@@H](Cc1ccccc1O)C(=O)[O-]	11
S131	PTDBSUB00558	[NH3+][C@H](Cc1ccccc1O)C(=O)[O-]	11
S132	PTDBSUB00313	Cc1cccc2c(C[C@@H]([NH3+])C(=O)[O-])c[nH]c12	11
S133	PTDBSUB00407	Cc1cccc2c(C[C@H]([NH3+])C(=O)[O-])c[nH]c12	11
S134	PTDBSUB00120	Cc1cccc2[nH]cc(C[C@H]([NH3+])C(=O)[O-])c12	11
S135	PTDBSUB00306	Cc1cccc2[nH]cc(C[C@@H]([NH3+])C(=O)[O-])c12	11
S136	PTDBSUB00123	COc1cccc2[nH]cc(C[C@H]([NH3+])C(=O)[O-])c12	11
S137	PTDBSUB00126	Nc1cccc2[nH]cc(C[C@H]([NH3+])C(=O)[O-])c12	11
S138	PTDBSUB00274	CC(C)=CCc1cc(C)cc2[nH]cc(C[C@H]([NH3+])C(=O)[O-])c12	12
S139	PTDBSUB00276	CC(C)=CCc1cc(C)cc2[nH]cc(C[C@@H]([NH3+])C(=O)[O-])c12	12
S140	PTDBSUB00270	CC(C)=CCc1c(C)ccc2[nH]cc(C[C@H]([NH3+])C(=O)[O-])c12	12
S141	PTDBSUB00272	CC(C)=CCc1c(C)ccc2[nH]cc(C[C@@H]([NH3+])C(=O)[O-])c12	12
S142	PTDBSUB00278	COc1ccc2[nH]cc(C[C@H]([NH3+])C(=O)[O-])c2c1CC=C(C)C	12
S143	PTDBSUB00281	COc1ccc2[nH]cc(C[C@@H]([NH3+])C(=O)[O-])c2c1CC=C(C)C	12
S144	PTDBSUB00239	CC(C)=CCc1c(C)ccc2c(C[C@H]([NH3+])C(=O)[O-])c[nH]c12	12
S145	PTDBSUB00242	CC(C)=CCc1c(C)ccc2c(C[C@@H]([NH3+])C(=O)[O-])c[nH]c12	12
S146	PTDBSUB00233	CC(C)=CCc1cc(C)cc2c(C[C@H]([NH3+])C(=O)[O-])c[nH]c12	12
S147	PTDBSUB00236	CC(C)=CCc1cc(C)cc2c(C[C@@H]([NH3+])C(=O)[O-])c[nH]c12	12
S148	PTDBSUB00245	COc1cc(CC=C(C)C)c2[nH]cc(C[C@H]([NH3+])C(=O)[O-])c2c1	12
S149	PTDBSUB00248	COc1cc(CC=C(C)C)c2[nH]cc(C[C@@H]([NH3+])C(=O)[O-])c2c1	12
S150	PTDBSUB00251	CC(C)=CCc1cccc2[nH]cc(C[C@H]([NH3+])C(=O)[O-])c12	13
S151	PTDBSUB00253	CC(C)=CCc1cccc2[nH]cc(C[C@@H]([NH3+])C(=O)[O-])c12	13
S152	PTDBSUB00266	CC(C)=CCc1cccc2[nH]cc(C[C@H](O)C(=O)[O-])c12	13
S153	PTDBSUB00268	CC(C)=CCc1cccc2[nH]cc(C[C@@H](O)C(=O)[O-])c12	13
S154	PTDBSUB00255	CC(C)=CCc1cccc2[nH]cc(C[C@H]([NH3+])CC(=O)[O-])c12	13
S155	PTDBSUB00260	C[NH2+][C@@H](Cc1c[nH]c2ccc(CC=C(C)C)c12)C(=O)[O-]	13
S156	PTDBSUB00257	CC(C)=CCc1cccc2[nH]cc(CC[NH3+])c12	13
S157	PTDBSUB00262	CC(C)=CCc1cccc2[nH]cc(C[C@@](C)([NH3+])C(=O)[O-])c12	13
S158	PTDBSUB00264	CC(C)=CCc1cccc2[nH]cc(C[C@](C)([NH3+])C(=O)[O-])c12	13
S159	PTDBSUB00205	CC(C)=CCc1cccc2c(C[C@H]([NH3+])C(=O)[O-])c[nH]c12	14
S160	PTDBSUB00208	CC(C)=CCc1cccc2c(C[C@@H]([NH3+])C(=O)[O-])c[nH]c12	14
S161	PTDBSUB00226	CC(C)=CCc1cccc2c(C[C@H](O)C(=O)[O-])c[nH]c12	14
S162	PTDBSUB00229	CC(C)=CCc1cccc2c(C[C@@H](O)C(=O)[O-])c[nH]c12	14
S163	PTDBSUB00211	CC(C)=CCc1cccc2c(C[C@H]([NH3+])CC(=O)[O-])c[nH]c12	14
S164	PTDBSUB00217	C[NH2+][C@@H](Cc1c[nH]c2c(CC=C(C)C)ccc12)C(=O)[O-]	14
S165	PTDBSUB00214	CC(C)=CCc1cccc2c(CC[NH3+])c[nH]c12	14
S166	PTDBSUB00220	CC(C)=CCc1cccc2c(C[C@@](C)([NH3+])C(=O)[O-])c[nH]c12	14
S167	PTDBSUB00223	CC(C)=CCc1cccc2c(C[C@](C)([NH3+])C(=O)[O-])c[nH]c12	14

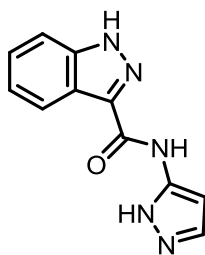
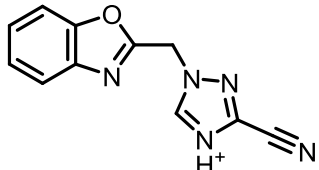
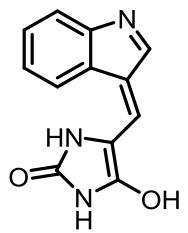
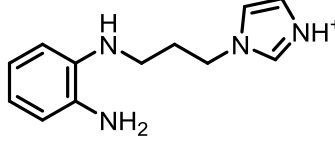
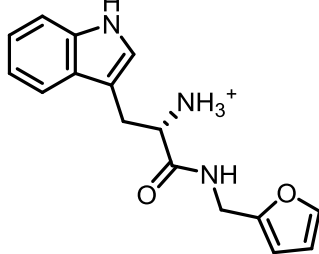
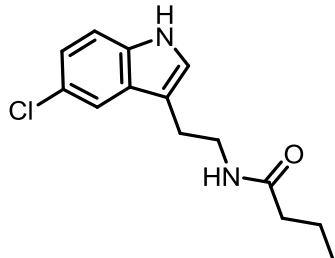


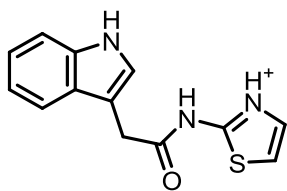
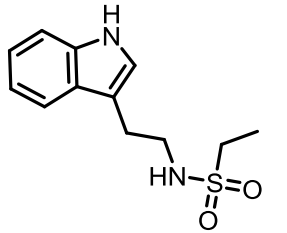
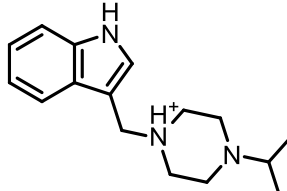
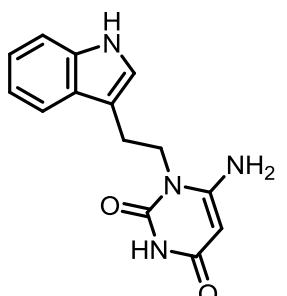
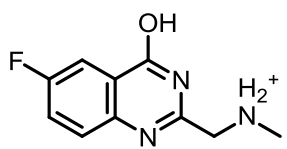
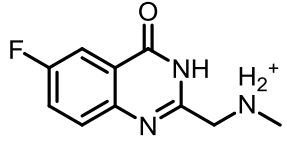
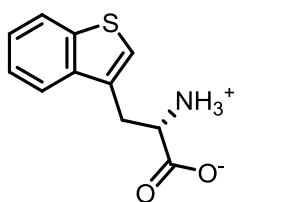
**Table S2:** Structures, IDs, enzyme-related yields and number of matched PrenDB reactions.

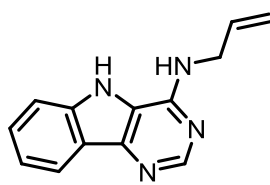
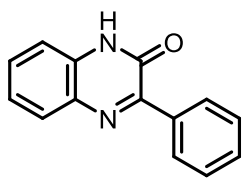
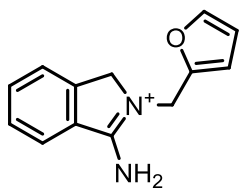
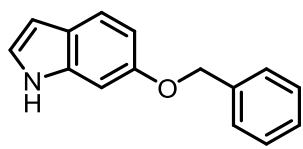
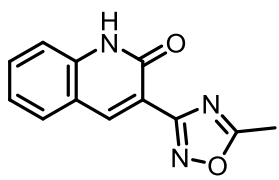
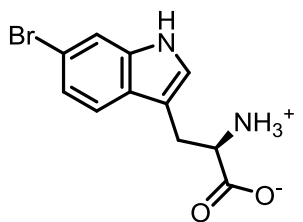
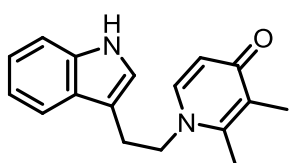
Substrate	ID	Product yield [%]			Matched reactions
		FtmPT1	FgaPT2	CdpNPT	
	1	94.1	18.2	41.3	299
	2	81.3	80.1	29.5	299
	3	-	3.2	22.1	299
	4	-	-	-	6
	5	-	-	0.9	33
	6	-	-	-	57

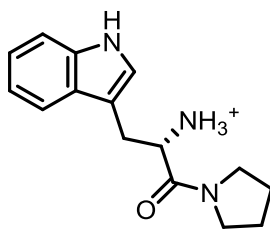
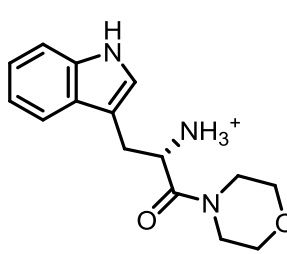
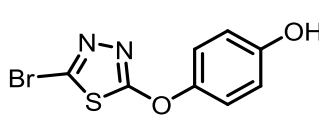
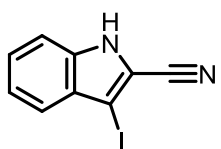
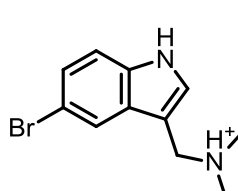
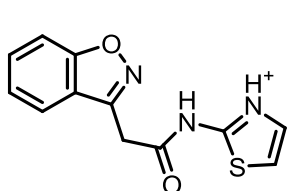
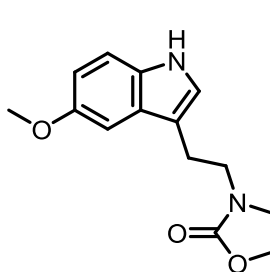
	7	7.0	-	10.1	57
	8	-	-	-	6
	9	-	5.3	-	17
	10	40.8	28.9	99.7	233
	11	48.1	17.1	88.1	238
	12	8.5	-	14.4	299
	13	71.0	31.7	47.2	231

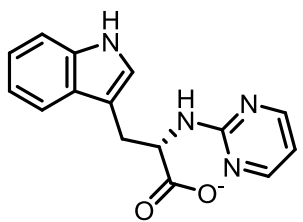
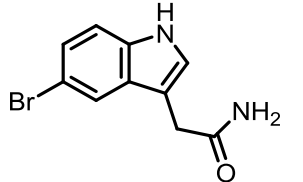


	14	2.0	-	2.6	50
	15	-	-	-	58
	16	68.8	34.8	29.7	20
	17	-	-	-	14
	18	89.1	84.9	62.0	299
	19	76.4	6.2	46.9	233

	20	76.0	37.4	97.4	233
	21	98.6	99.2	99.3	233
	22	-	-	-	231
	23	64.8	75.0	65.2	233
	24 <sup>a</sup>	-	-	-	50
	25	-	-	-	50
	26	-	-	-	33

	27	8.7	82.9	11.8	137
	28	-	-	-	23
	29 <sup>b</sup>	-	-	-	6
	30	60.1	59.4	96.1	229
	31	-	-	-	50
	32	47.5	44.7	-	299
	33	99.5	99.1	87.2	233

	34	44.4	19.9	94.8	299
	35	35.5	16.3	94.1	299
	36 <sup>b</sup>	-	-	-	77
	37	-	-	-	137
	38	-	-	-	235
	39 <sup>b</sup>	3.8	-	2.8	33
	40	51.5	4.4	9.2	237

	41	9.9	22.5	13.5	325
	42	-	14.9	38.1	299

<sup>a</sup> Compound **24** is the imidic acid tautomer of **25** and was thus excluded from further consideration in this work. Total and relative numbers throughout the manuscript reflect the number of unique compounds, i.e. 38.

<sup>b</sup> These compounds could not be obtained as ordered and were excluded from further consideration in this work