Table S2. 4-OH-MPT putative metabolites predicted with GLORYx freeware and their prediction score (adjusted score for second-generation metabolites)

ID	Transformation	Elemental composition	Score	SMILES	Comment
P1	*O*-Sulfation	$C_{14}H_{20}N_2O_4S$	93.0%	O=S(=O)(O)Oc1cccc2[NH]cc(CCN(C)CCC)c21	
P1-1	+ Hydroxylation (propyl chain)	$C_{14}H_{20}N_2O_5S$	44.6%	CCC(O)N(C)CCc1c[NH]c2cccc(OS(=O)(=O)O)c21	= P4-2
P1-2	+ Hydroxylation (propyl chain)	$C_{14}H_{20}N_2O_5S$	44.6%	CC(O)CN(C)CCc1c[NH]c2cccc(OS(=O)(=O)O)c21	= P5-3
P1-3	+ Hydroxylation (propyl chain)	$C_{14}H_{20}N_2O_5S$	44.6%	O=S(=O)(O)Oc1cccc2[NH]cc(CCN(C)CCCO)c21	= P6-2
P1-4	+ *N*-Oxidation (alkyl chain)	$C_{14}H_{20}N_2O_5S$	44.6%	O=S(=O)(O)Oc1cccc2[NH]cc(CC[N+]([O-])(C)CCC)c21	= P7-1
P1-5	+ Carboxylation (propyl chain)	$C_{14}H_{18}N_2O_6S$	44.6%	O=C(O)CCN(C)CCc1c[NH]c2cccc(OS(=O)(=O)O)c21	
P1-6	+ *N*-Demethylation	$C_{13}H_{18}N_2O_4S$	44.6%	O=S(=O)(O)Oc1cccc2[NH]cc(CCNCCC)c21	= P9-1
P1-7	+ *N*-Depropylation	$C_{11}H_{14}N_2O_4S$	44.6%	O=S(=O)(O)Oc1cccc2[NH]cc(CCNC)c21	= P10-1
P1-8	+ Desulfation	$C_{14}H_{20}N_2O$	39.1%	CCCN(C)CCc1c[NH]c2cccc(O)c21	= parent
P2	*O*-Glucuronidation	$C_{20}H_{28}N_2O_7$	84.0%	CCCN(C)CCc1c[NH]c2cccc(OC3OC(C(O)C(O)C3O)C(=O)O)c21	
P2-1	+ Glucuronide opening	$C_{20}H_{28}N_2O_8$	41.2%	O=C(O)C(O)C(O)C(O)C(O)C(=O)Oc1cccc2[NH]cc(CCN(C)CCC)c21	
P2-2	+ Glucuronide opening	$C_{20}H_{28}N_2O_8$	41.2%	O=C(O)C(=O)C(O)C(O)C(O)C(O)Oc1cccc2[NH]cc(CCN(C)CCC)c21	
P2-3	+ Deglucuronidation	$C_{14}H_{20}N_2O$	41.2%	CCCN(C)CCc1c[NH]c2cccc(O)c21	= parent
P2-4	+ Hydroxylation (glucuronide)	$C_{20}H_{28}N_2O_8$	41.2%	CCCN(C)CCc1c[NH]c2cccc(OC3(O)OC(C(O)C(O)C3O)C(=O)O)c21	
P2-5	+ Hydroxylation (propyl chain)	$C_{20}H_{28}N_2O_8$	40.3%	CCC(O)N(C)CCc1c[NH]c2cccc(OC3OC(C(O)C(O)C3O)C(=O)O)c21	= P4-3
P2-6	+ Hydroxylation (propyl chain)	$C_{20}H_{28}N_2O_8$	40.3%	CC(O)CN(C)CCc1c[NH]c2cccc(OC3OC(C(O)C(O)C3O)C(=O)O)c21	= P5-4
P2-7	+ Hydroxylation (propyl chain)	$C_{20}H_{28}N_2O_8$	40.3%	OCCCN(C)CCc1c[NH]c2cccc(OC3OC(C(O)C(O)C3O)C(=O)O)c21	= P6-4
P2-8	+ *N*-Oxidation (alkyl chain)	$C_{20}H_{28}N_2O_8$	40.3%	[O-][N+](C)(CCC)CCc1c[NH]c2cccc(OC3OC(C(O)C(O)C3O)C(=O)O)c21	= P7-2
P2-9	+ Carboxylation (propyl chain)	$C_{20}H_{26}N_2O_9$	40.3%	O=C(O)CCN(C)CCc1c[NH]c2cccc(OC3OC(C(O)C(O)C3O)C(=O)O)c21	
P2-10	+ *N*-Demethylation	$C_{19}H_{26}N_2O_7$	40.3%	O=C(O)C1OC(Oc2cccc3[NH]cc(CCNCCC)c23)C(O)C(O)C1O	= P9-2
P2-11	+ *N*-Depropylation	$C_{17}H_{22}N_2O_7$	40.3%	O=C(O)C1OC(Oc2cccc3[NH]cc(CCNC)c23)C(O)C(O)C1O	= P10-2
P3	*O*-Methylation	$C_{15}H_{22}N_2O$	47.0%	CCCN(C)CCc1c[NH]c2cccc(OC)c21	
P4	Hydroxylation (propyl chain)	$C_{14}H_{20}N_2O_2$	43.0%	CCC(O)N(C)CCc1c[NH]c2cccc(O)c21	
P4-1	+ *O*-Sulfation (propyl chain)	$C_{14}H_{20}N_2O_5S$	40.4%	O=S(=O)(O)OC(CC)N(C)CCc1c[NH]c2cccc(O)c21	
P4-2	+ *O*-Sulfation (indole)	$C_{14}H_{20}N_2O_5S$	40.0%	CCC(O)N(C)CCc1c[NH]c2cccc(OS(=O)(=O)O)c21	= P1-1
P4-3	+ *O*-Glucuronidation (indole)	$C_{20}H_{28}N_2O_8$	36.1%	CCC(O)N(C)CCc1c[NH]c2cccc(OC3OC(C(O)C(O)C3O)C(=O)O)c21	= P2-5
P4-4	+ *O*-Glucuronidation (propyl chain)	$C_{20}H_{28}N_2O_8$	28.0%	Oc1cccc2[NH]cc(CCN(C)C(OC3OC(C(O)C(O)C3O)C(=O)O)CC)c12	
P5	Hydroxylation (propyl chain)	$C_{14}H_{20}N_2O_2$	43.0%	CC(O)CN(C)CCc1c[NH]c2cccc(O)c21	
P5-1	+ *O*-Sulfation (propyl chain)	$C_{14}H_{20}N_2O_5S$	42.6%	O=S(=O)(O)OC(C)CN(C)CCc1c[NH]c2cccc(O)c21	
P5-2	+ *O*-Glucuronidation (propyl chain)	$C_{20}H_{28}N_2O_8$	41.3%	Oc1cccc2[NH]cc(CCN(C)CC(C)OC3OC(C(O)C(O)C3O)C(=O)O)c12	
P5-3	+ *O*-Sulfation (indole)	$C_{14}H_{20}N_2O_5S$	40.0%	CC(O)CN(C)CCc1c[NH]c2cccc(OS(=O)(=O)O)c21	= P1-2
P5-4	+ *O*-Glucuronidation (indole)	$C_{20}H_{28}N_2O_8$	36.1%	CC(O)CN(C)CCc1c[NH]c2cccc(OC3OC(C(O)C(O)C3O)C(=O)O)c21	= P2-6
P6	Hydroxylation (propyl chain)	$C_{14}H_{20}N_2O_2$	43.0%	OCCCN(C)CCc1c[NH]c2cccc(O)c21	
P6-1	+ *O*-Sulfation (propyl chain)	$C_{14}H_{20}N_2O_5S$	40.9%	O=S(=O)(O)OCCCN(C)CCc1c[NH]c2cccc(O)c21	
P6-2	+ *O*-Sulfation (indole)	$C_{14}H_{20}N_2O_5S$	40.0%	O=S(=O)(O)Oc1cccc2[NH]cc(CCN(C)CCCO)c21	= P1-3
P6-3	+ *O*-Glucuronidation (propyl chain)	$C_{20}H_{28}N_2O_8$	40.0%	Oc1cccc2[NH]cc(CCN(C)CCCOC3OC(C(O)C(O)C3O)C(=O)O)c12	
P6-4	+ *O*-Glucuronidation (indole)	$C_{20}H_{28}N_2O_8$	35.3%	OCCCN(C)CCc1c[NH]c2cccc(OC3OC(C(O)C(O)C3O)C(=O)O)c21	= P2-7
P7	*N*-Oxidation (alkyl chain)	$C_{14}H_{20}N_2O_2$	43.0%	[O-][N+](C)(CCC)CCc1c[NH]c2cccc(O)c21	
P7-1	+ *O*-Sulfation (indole)	$C_{14}H_{20}N_2O_5S$	40.0%	O=S(=O)(O)Oc1cccc2[NH]cc(CC[N+]([O-])(C)CCC)c21	= P1-4
P7-2	+ *O*-Glucuronidation (indole)	$C_{20}H_{28}N_2O_8$	36.1%	[O-][N+](C)(CCC)CCc1c[NH]c2cccc(OC3OC(C(O)C(O)C3O)C(=O)O)c21	= P2-8
P7-3	+ *O*-Methylation (indole)	$C_{15}H_{22}N_2O_2$	33.5%	[O-][N+](C)(CCC)CCc1c[NH]c2cccc(OC)c21	
P8	Carboxylation (propyl chain)	$C_{14}H_{18}N_2O_3$	43.0%	O=C(O)CCN(C)CCc1c[NH]c2cccc(O)c21	
P8-1	+ *O*-Glucuronidation (carboxyl group)	$C_{20}H_{26}N_2O_9$	40.9%	O=C(OC1OC(C(O)C(O)C1O)C(=O)O)CCN(C)CCc1c[NH]c2cccc(O)c21	
P8-2	+ *O*-Sulfation (indole)	$C_{14}H_{18}N_2O_6S$	40.0%	O=C(O)CCN(C)CCc1c[NH]c2cccc(OS(=O)(=O)O)c21	
P8-3	+ *O*-Glucuronidation (indole)	$C_{20}H_{26}N_2O_9$	35.3%	O=C(O)CCN(C)CCc1c[NH]c2cccc(OC3OC(C(O)C(O)C3O)C(=O)O)c21	
P9	*N*-Demethylation	$C_{13}H_{18}N_2O$	43.0%	Oc1cccc2[NH]cc(CCNCCC)c21	
P9-1	+ *O*-Sulfation	$C_{13}H_{18}N_2O_4S$	40.0%	O=S(=O)(O)Oc1cccc2[NH]cc(CCNCCC)c21	= P1-6
P9-2	+ *O*-Glucuronidation	$C_{19}H_{26}N_2O_7$	36.1%	O=C(O)C1OC(Oc2cccc3[NH]cc(CCNCCC)c23)C(O)C(O)C1O	= P2-10
P10	*N*-Depropylation	$C_{11}H_{14}N_2O$	43.0%	Oc1cccc2[NH]cc(CCNC)c21	
P10-1	+ *O*-Sulfation	$C_{11}H_{14}N_2O_4S$	40.4%	O=S(=O)(O)Oc1cccc2[NH]cc(CCNC)c21	= P1-7
P10-2	+ *O*-Glucuronidation	$C_{17}H_{22}N_2O_7$	36.6%	O=C(O)C1OC(Oc2cccc3[NH]cc(CCNC)c23)C(O)C(O)C1O	= P2-11
P10-3	+ *N*-Acetylation (alkyl chain)	$C_{13}H_{16}N_2O_2$	34.8%	CC(=O)N(C)CCc1c[NH]c2cccc(O)c21	
P11	Hydroxylation (indole)	$C_{14}H_{20}N_2O_2$	31.0%	CCCN(C)CCc1c2c(cccc2O)[NH]c1O	
P12	Hydroxylation (methyl chain)	$C_{14}H_{20}N_2O_2$	25.0%	CCCN(CO)CCc1c[NH]c2cccc(O)c21	