Supplementary Information

The journey of HIV-1 non-nucleoside reverse transcriptase inhibitors (NNRTIs) from lab to clinic

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Table S1: Published X-ray Crystal Structures of HIV-1 Reverse Transcriptase (RT) with the approved NNRTI drugs

PDB ID	NNRTI	Resolution (Å)	HIV-1 RT	Release Year	Reference
3HVT	NVP	2.90	wild-type	1994	[1]
1VRT	NVP	2.20	wild-type	1996	[2]
1FKP	NVP	2.90	K103N	2000	[3]
1JLB	NVP	3.00	Y181C	2001	[4]
1JLF	NVP	2.60	Y188C	2001	[4]
1LW0	NVP	2.80	T215Y	2002	[5]
1LWC	NVP	2.62	M184V	2002	[5]
1LWE	NVP	2.81	M41L/T215Y	2002	[5]
1LWF	NVP	2.80	RTMQ+M184V M41L/D67N/K70R/ M184V/T215Y	2002	[5]
1S1U	NVP	3.00	L100I	2004	[6]
1S1X	NVP	2.80	V108I	2004	[6]
2HND	NVP	2.50	K101E	2006	[7]
2HNY	NVP	2.50	E138K	2006	[7]
3LP0	NVP	2.79	wild-type	2010	[8]
3LP1	NVP	2.23	wild-type	2010	[8]
3QIP	NVP	2.09	wild-type	2011	[9]
3V81	NVP	2.85	wild-type	2012	[10]
4B3Q	NVP	5.00	wild-type	2013	[11]
4PUO	NVP	2.90	wild-type	2014	[12]
4PWD	NVP	3.00	wild-type	2014	[12]
4Q0B	NVP	3.30	wild-type	2014	[12]
5HBM	NVP	3.04	wild-type	2016	unpublished
1KLM	DLV	2.65	wild-type	1998	[13]
1FK9	EFV	2.50	wild-type	2000	[3]
1FKO	EFV	2.90	K103N	2000	[3]
1IKV	EFV	3.00	K103N	2001	[4]
1IKW	EFV	3.00	wild-type	2001	[4]
1JKH	EFV	2.50	Y181C	2001	[4]
4B3O	EFV	3.30	wild-type	2013	[11]
6BSG	EFV	2.44	wild-type	2018	unpublished
6BSH	EFV	2.65	wild-type	2018	unpublished
6BSI	EFV	3.25	wild-type	2018	unpublished
6BSJ	EFV	2.89	wild-type	2018	unpublished
1SV5	ETV	2.90	K103N	2004	[14]
3M8P	ETV	2.67	wild-type	2010	[15]
3MEC	ETV	2.30	wild-type	2010	[16]

3MED	ETV	2.50	K103N	2010	[16]
2ZD1	RPV	1.80	wild-type	2008	[17]
2ZE2	RPV	2.90	L100I/K103N	2008	[17]
3BGR	RPV	2.10	K103N/Y181C	2008	[17]
3MEE	RPV	2.40	wild-type	2010	[18]
3MEG	RPV	2.80	K103N	2010	[18]
3QLH	RPV	2.70	wild-type	2011	[19]
4G1Q	RPV	1.51	wild-type	2013	[20]
4ICL	RPV	1.80	wild-type	2013	[20]
4ID5	RPV	1.95	wild-type	2013	[20]
4IDK	RPV	2.10	wild-type	2013	[20]
4IFV	RPV	2.05	wild-type	2013	[20]
4IFY	RPV	2.10	wild-type	2013	[20]
4IG3	RPV	1.95	wild-type	2013	[20]
4KFB	RPV	1.85	wild-type	2013	[20]

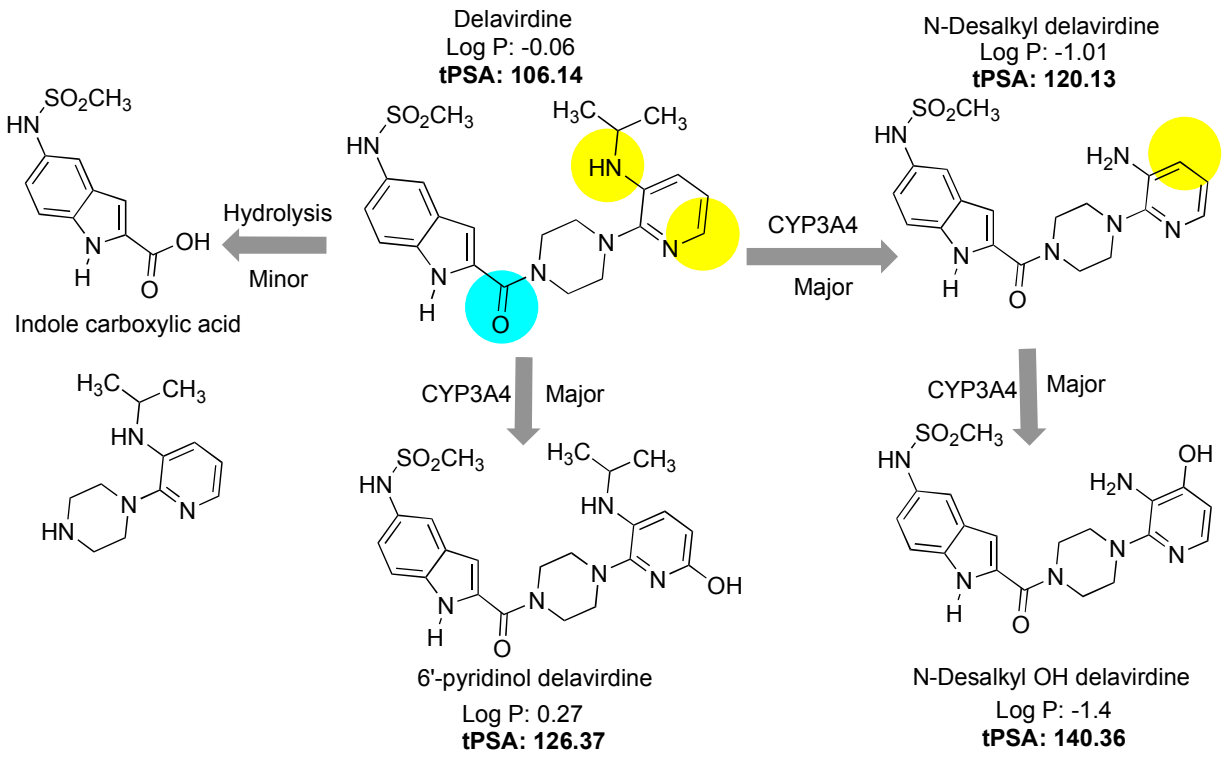

Figure S1: Metabolic pathway of DLV and various key metabolic sites are highlighted are in yellow and cyan colors.

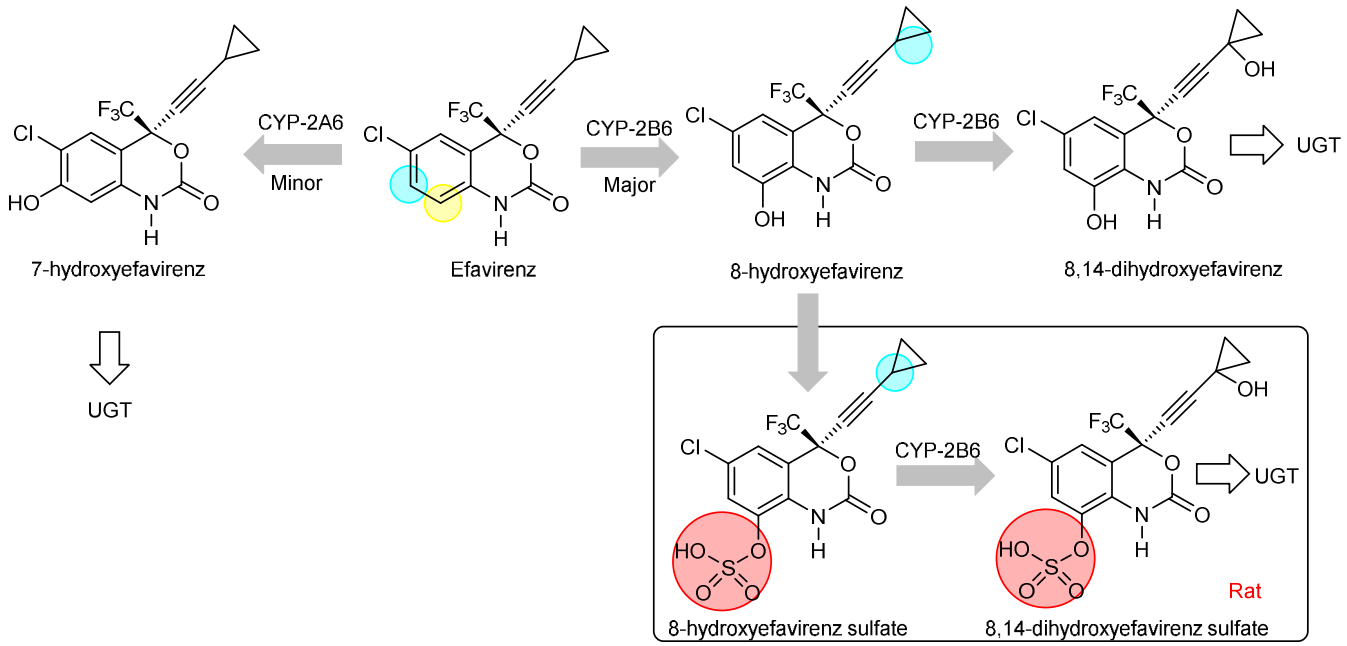

Figure S2: Metabolic pathway of EFV and various key metabolic sites are highlighted are in yellow and cyan colors.

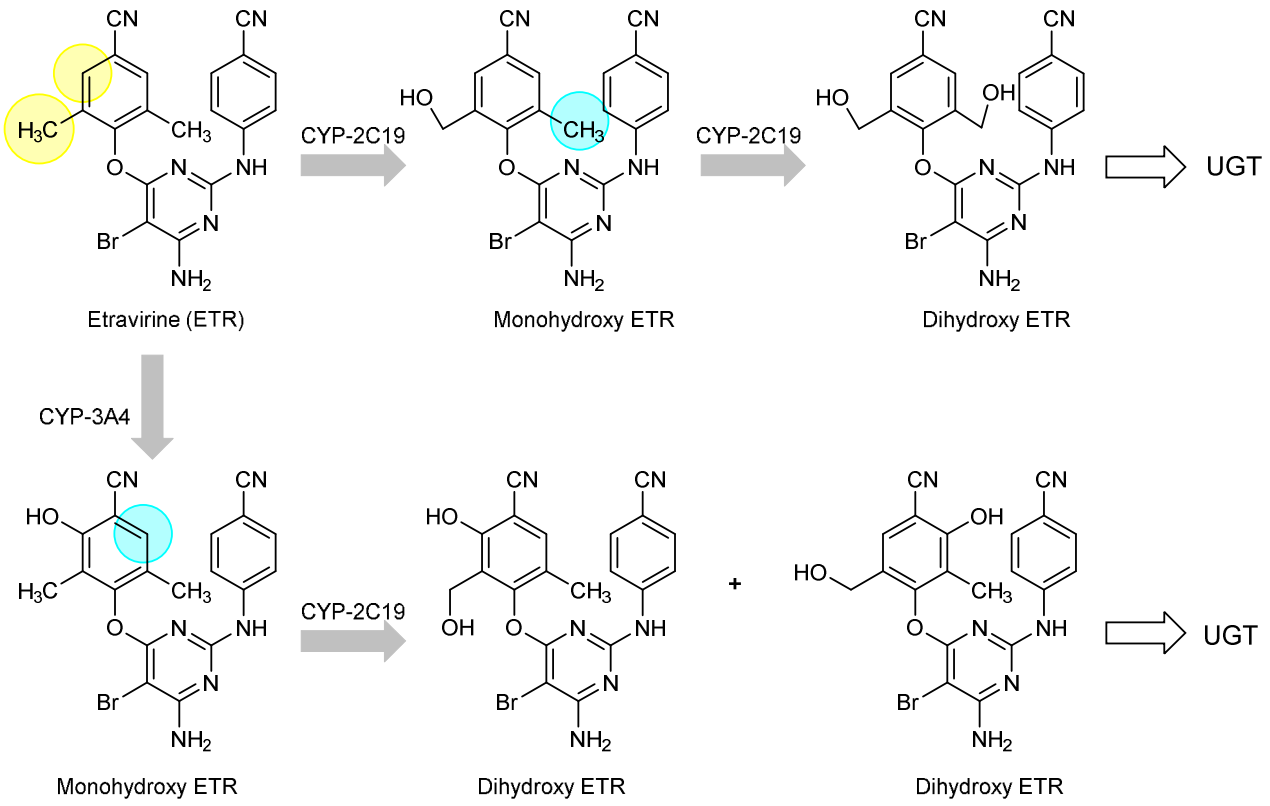

Figure S3: Metabolic pathway of ETR and various key metabolic sites are highlighted are in yellow and cyan colors

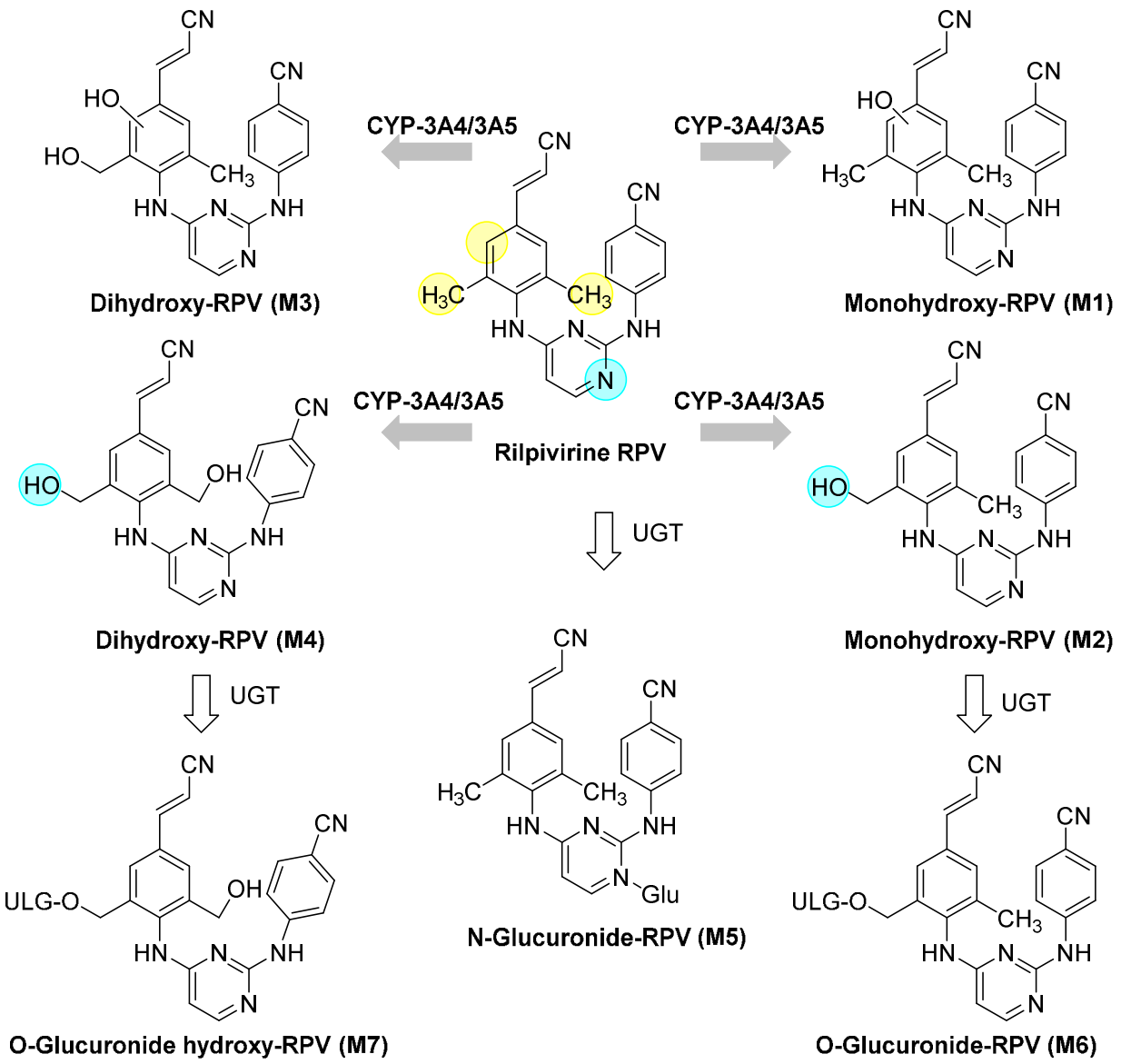

Figure S4: Metabolic pathways of RPV and key metabolic sites are highlighted are in yellow and cyan colors

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