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CORRECTION

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Correction to: A potential implication of UDP-glucuronosyltransferase 2B10 in the detoxification of drugs used in pediatric hematopoietic stem cell transplantation setting: an in silico investigation

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Following publication of the original article [1], the following typesetting error was noticed:

1) The equal contribution note has been updated.
2) Table 1, column 4 (InterPro-Protein Family), row 3 "ransferase" should be "transferase"
3) The footnote for Table 3 was mistakenly added to the body text (last para in pg 10 [1], continued as para 1 in pg.12 i.e. "Results are presented as the mean±SD……...to compare our results with other putative ligands" The correct Table 3 and footnote are supplied below.
4) The footnote for Table 5 was mistakenly added to the body text. The correct Table 5 and footnote are supplied below.
5) In the section *Molecular dynamics simulations with GROMACS* "Eight compounds showing ΔG value of ≤ −1.0 kcal/mol predicted by AutoDock Vina", should be "Eight compounds showing ΔG value of ≤ −0.1 kcal/mol predicted by AutoDock Vina"

The original article can be found online at https://doi.org/10.1186/s12860-021-00402-5.

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Table 3 Estimated binding free energy and dissociation constant between putative substrates and human UGT2B10

Model	Substrate	Ligand	*ΔG*[Kcal/mol ± SD]	Kd[mM]
UGT2B10 with UDPGlcA	**Controls**	**Amitriptyline**	**−1.9 ± 0.2**	**39.0**
		Itraconazole	19.0 ± 0.5	1.1×10^{17}
	Putative ligands	**4-hydroxy voriconazole**	**−1.0 ± 0.0**	**184.7**
		Acetaminophen	**−5.5 ± 0.0**	**0.1**
		Cyclosporine A	154.9 ± 2.9	1.8×10^{118}
		Bilirubine	6.9 **± 0.0**	1.2×10^{15}
		Dihydroxy voriconazole	−0.6 ± 0.0	363.0
		Hydroxy voriconazole	**−1.2 ± 0.1**	**125.0**
		Lorazepam	**−2.6 ± 0.0**	**12.4**
		Methotrexate	−0.5 ± 0.5	567.3
		Methylprednisolone	5.2 ± 0.1	6.2×10^{6}
		Mycophenolic acid	**−5.1 ± 0.1**	**0.2**
		Posaconazole	17.6 ± 0.3	8.8×10^{15}
		UDCA-G1	2.2 ± 0.1	4.4×10^{4}
		UDCA-G2	1.2 ± 0.1	8053.6
		Ursodeoxycholic acid	2.2 ± 0.1	4.4×10^{4}
		Voriconazole	**−1.0 ± 0.1**	**197.8**
		Voriconazole N-oxide	**−2.3 ± 0.1**	**2.1×10^{4}**
		Voriconazole N-oxide intermediate UK-215,364 [35]	**−6.4 ± 0.1**	**0.02**

Results are presented as the mean ± SD of three different replicates. *Kd* dissociation constant, *UDCA-G1 and UDCA-G2* ursodeoxycholic acid glucuronide conjugate 1 and 2 [44], *UDPGlcA* UDP-glucuronic acid. Molecules with ΔG of < −0.1 and with an SD of ≤0.1 Kcal/mol were selected for further for MD simulations (methotrexate was not selected as it has an SD 0.5). SD is calculated from 8 docking poses or models (default option). The ligand binding pose was selected for further analyses is the pose with the lowest free binding energy (Kcal/mol). Bilirubin was selected for further molecular docking simulations as an endogenous negative control to compare our results with other putative ligands

Reference

1. Robin S, Hassine KB, Muthukumaran J, et al. A potential implication of UDP-glucuronosyltransferase 2B10 in the detoxification of drugs used in pediatric hematopoietic stem cell transplantation setting: an in silico investigation. BMC Mol Cell Biol. 2022;23:5. https://doi.org/10.1186/s12860-021-00402-5.

Table 5 Average values of hydrogen bonds, RMSD, RMSF, RoG, SASA, trace of the covariance matrix values and MM/PBSA binding free energy values of the different UGT2B10 with putative substrates

Complex	Average number of intramolecular hydrogen bonds± SD	Average number of intermolecular hydrogen bonds± SD	Average RMSD[nm ± SD]	Average RoG[nm]	Average RMSF[nm ± SD]	Average SASA[nm^2 ± SD]	Trace of the covariance matrix[nm^2]	MMPBSAbinding free energy[kcal/mol]
UGT2B10 apo form	302.73 ± 9.60	N/A	0.39 ± 0.05	2.26 ± 1.38*10^{-2}	0.20 ± 0.08	216.39 ± 4.74	42.08	NA
UGT2B10-UDPGlcA	305.29 ± 11.70	7.54 ± 2.01	0.43 ± 0.05	2.28 ± 9.57*10^{-4}	0.19 ± 0.09	221.01 ± 5.74	38.82	NC
UGT2B10-UDPGlcA-AMT	290.12 ± 10.25	0.21 ± 0.41	0.49 ± 0.05	2.29 ± 1.16*10^{-2}	0.21 ± 0.12	227.45 ± 4.47	55.6	− 160.85 ± 10.99
UGT2B10-UDPGlcA-APAP	304.67 ± 8.96	1.16 ± 0.68	0.47 ± 0.08	2.24 ± 2.84*10^{-2}	0.25 ± 0.11	224.61 ± 4.02	76.97	− 174.24 ± 13.38
UGT2B10-UDPGlcA-BIL	292.97 ± 11.69	0.00 ± 0.00	0.39 ± 0.07	2.31 ± 1.88*10^{-2}	0.21 ± 0.13	234.64 ± 3.93	65.10	−104.00 ± 11.06
UGT2B10-UDPGlcA-ITZ	310.11 ± 10.43	0.24 ± 0.44	0.51 ± 0.05	2.33 ± 1.29*10^{-2}	0.23 ± 0.14	244.84 ± 6.86	60.70	− 127.79 ± 15.25
UGT2B10-UDPGlcA-LOR	300.25 ± 8.69	0.65 ± 0.79	0.42 ± 0.06	2.28 ± 1.14*10^{-2}	0.20 ± 0.10	230.58 ± 3.67	48.81	− 162.07 ± 19.30
UGT2B10-UDPGlcA-MPA	303.7 ± 9.09	2.48 ± 1.33	0.47 ± 0.05	2.33 ± 1.21*10^{-2}	0.22 ± 0.16	230.48 ± 6.97	60.23	− 158.46 ± 11.95
UGT2B10-UDPGlcA-VCZ	301.51 ± 9.69	0.76 ± 0.96	0.49 ± 0.07	2.31 ± 2.16*10^{-2}	0.24 ± 0.16	234.23 ± 5.28	87.61	−59.56 ± 17.13
UGT2B10-UDPGlcA-HVCZ	311.18 ± 9.89	0.87 ± 0.66	0.46 ± 0.05	2.27 ± 1.13*10^{-2}	0.19 ± 0.09	224.92 ± 5.18	40.50	−85.43 ± 14.23
UGT2B10-UDPGlcA-DHVCZ	308.33 ± 9.97	1.21 ± 0.83	0.43 ± 0.04	2.29 ± 1.13*10^{-2}	0.20 ± 0.10	227.99 ± 4.71	43.27	−86.34 ± 25.35
UGT2B10-UDPGlcA-4HVCZ	309.36 ± 11.59	0.00 ± 0.00	0.44 ± 0.03	2.26 ± 8.81*10^{-3}	0.18 ± 0.09	223.49 ± 6.05	38.55	−95.43 ± 18.47
UGT2B10-UDPGlcA-VCZ-N-O	303.01 ± 10.28	1.38 ± 0.78	0.43 ± 0.05	2.30 ± 1.28*10^{-2}	0.22 ± 0.11	233.91 ± 5.20	58.16	− 12.41 ± 19.02
UGT2B10-UDPGlcA-VCZ-N-O-intermediate UK-215,364 [35]	305.54 ± 12.28	0.72 ± 0.52	0.38 ± 0.03	2.3 ± 1.19*10^{-2}	0.18 ± 0.1	227.28 ± 4.55	37.75	− 164.44 ± 13.38

Results are indicated as mean ± SD of the MD simulation's analysis results. *4HVCZ* 4-hydroxy voriconazole, *AMT* amitriptyline, *APAP* acetaminophen, *BIL* bilirubin, *DHVCZ* Di-hydroxy voriconazole, *HVCZ* Hydroxy voriconazole, *ITZ* itraconazole, *LOR* lorazepam, *MPA* mycophenolic acid, *NC* Not calculated, *VCZ-N-O* voriconazole N-oxide, *RMSD* root mean square deviation, *RMSF* root mean square fluctuation, *RoG* radius of gyration, *UDPGlcA* UDP-glucuronic acid