

Supplementary material

Drug-likeness of linear pentamidine analogues and their impact on hERG K⁺ channel – correlation with structural features

Teresa Żółek^{a*}, Muge Qile^b, Paweł Kaźmierczak^a, Meye Bloothoof^b, Marcel A. G. van der Heyden^b and Dorota Maciejewska^{a*}

Table S1 Probability of metabolism by human uridine 5'-diphosphate-glucuronosyltransferases (UGT) for **1 – 9**.

Table S2 Values of CDOCKER interaction energy for pentamidine derivatives (**4**, **5** and **6**).

Figure S1. Predicted intermolecular interactions by CDOCKER for compounds **4**, **5** and **6**.

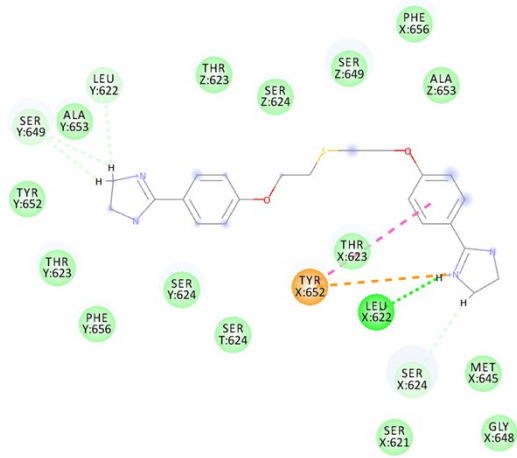
Table S1

Compound	UGT								
	1A1	1A3	1A4	1A6	1A8	1A9	1A10	2B7	2B15
1	Yes	No	Yes	No	No	Yes	No	Yes	No
2	Yes	Yes	Yes	No	No	Yes	No	Yes	No
3	Yes	Yes	Yes	No	No	No	No	Yes	No
4	Yes	Yes	Yes	No	No	Yes	No	Yes	No
5	Yes	Yes	Yes	No	No	No	No	Yes	No
6	Yes	Yes	Yes	No	No	No	No	No	No
7	No	No	No	No	No	Yes	No	Yes	No
8	No	No	No	No	Yes	No	No	No	No
9	No	No	No	No	No	Yes	No	No	No

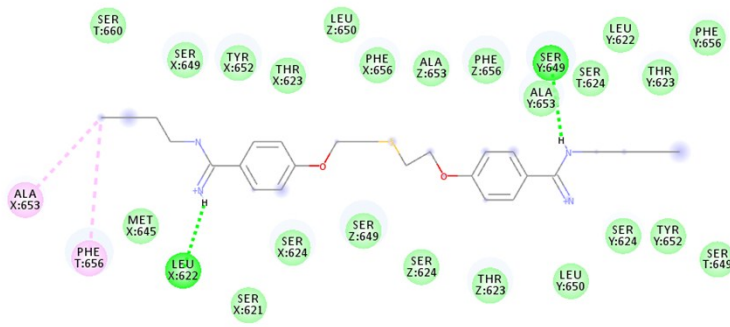
Table S2

Pose number	CDOCKER interaction energy (kcal/mol)		
	4	5	6
1	-48,9474	-59,0164	-55,1398
2	-49,6748	-52,6177	-56,6219
3	-43,7155	-55,7457	-53,9279
4	-46,4077	-57,0773	-54,1317
5	-41,6959	-52,8375	-49,0274
6	-44,5029	-52,7724	-55,2444
7	-42,2372	-47,7179	-49,6112
8	-42,2035	-52,9497	-48,2851
9	-41,7638	-48,8009	-50,2068
10	-42,6056	-52,007	-45,8554

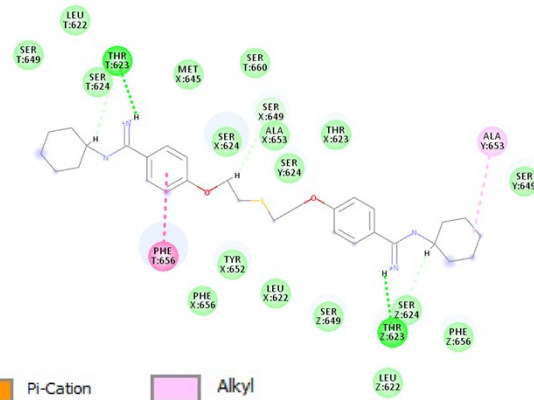
4



5



6



Interactions

 van der Waals	 Pi-Cation	 Alkyl
 Conventional Hydrogen Bond	 Pi-Pi Stacked	 Pi-Alkyl
 Carbon Hydrogen Bond		

Fig. S1.