Table S3. Interaction layer, minimal distance and MFCC binding energies between each one of the 72 amino acid residues in the uPA and the compound 172 atoms. The energy values were calculated within the GGA + D/PBE/DNP+ theory with ε = 40. Bold 172 ligand atoms correspond to atoms involved in intermolecular interactions with uPA. We considered as ring1 the benzimidazole closest ring to amine group, and as ring 2 the furthest ring (Fig. 3A).

Interaction layer (°A)	Minimal distance			Energy (kcal mol^{-1})	Interaction layer (°A)	Minimal distance			Energy (kcal mol^{-1})
	uPA	d (°A)	172			uPA	d (°A)	172	
7.5	ILE16	7.04	ii(ring1), ii(ring2)	-0.1	8	ASP185	7.57	i(N14)NH2	0.0
6	ILE17	5.59	i(N14)NH2	-0.2	8	GLN185B	7.57	i(N14)NH2	0.2
9	GLY18	8.77	i(N14)NH2	-0.1	8.5	TRP186	8.44	i(N14)NH2	0.0
9	TYR40	8.87	ii(O17)OH	0.0	9.5	LYS187	9.08	i(N14)NH2	-0.1
9	VAL41	8.52	ii(O17)OH	-0.2	6.5	THR188	6.07	i(N14)NH2	-0.2
8	CYS42-CYS58	7.70;7.97	ii(ring2)	-1.8	2.5	ASP189	2.08	**i(N14)NH2**	-4.9
8.5	GLY43	8.19	ii(ring2)	0.0	2.5	SER190	2.17	**ii(ring1), ii(ring2)**	**-4.0**
9.5	SER54	9.21	ii(ring2)	0.0	3	CYS191-CYS220	2.71;3.20	**ii(ring1), ii(ring2)**	-4.9
8	ALA55	7.71	ii(ring2)	0.1	3	GLN192	2.57	ii(O17)OH	-1.4
4.5	HIS57	4.24	ii(ring2)	-0.8	3.5	GLY193	3.44	ii(O17)OH	-0.1
10	TYR94	9.91	ii(ring2)	0.1	4	ASP194	3.78	ii(ring2)	0.0
8	LEU97B	7.86	ii(ring2)	-0.1	3	SER195	2.51	**ii(C6)CH2**	-2.2
9.5	ALA98	9.29	ii(ring2)	0.5	6	GLY196	5.96	ii(ring2)	-0.1
7	HIS99	6.69	ii(O17)OH	0.4	7	GLY197	6.53	ii(ring2)	-0.1
8	ASP102	7.69	ii(ring2)	-0.3	9.5	PRO198	9.07	ii(ring2)	0.0
6	ILE138	5.71	i(ring1)	-0.4	8.5	LEU199	8.03	i(ring1)	0.0
9	THR139	8.57	ii(ring2)	0.1	10	GLY211	9.91	ii(ring2)	0.0
8.5	GLY140	8.12	ii(ring2)	0.0	7	ILE212	6.97	ii(ring2)	0.0
9.5	PHE141	9.17	ii(ring2)	0.0	2.5	VAL213	2.07	ii(ring2)	-1.4
7.5	GLY142	7.08	ii(O17)OH	0.0	4.5	SER214	4.06	ii(ring2)	-0.9
7	LYS143	6.79	ii(O17)OH	-0.6	4	TRP215	3.60	**ii(ring2)**	-3.1
10	ASN145	9.74	ii(ring2)	0.0	3	GLY216	2.65	**ii(ring1), ii(ring2)**	-3.0
7	SER146	6.90	ii(ring2	-0.1	4	ARG217	3.95	i(ring1)	**-0.8**
7	TYR151	6.80	ii(O17)OH	-0.5	3.5	GLY219	3.03	**ii(ring1), i(N14)NH2**	5.0
8.5	THR158	8.25	i(N14)NH2	0.2	3.5	ALA221	3.34	i(N14)NH2	0.0
6.5	VAL160	6.42	i(N14)NH2	-0.1	5.5	LEU222	5.23	i(N14)NH2	-0.1
10	LYS161	10.00	i(N14)NH2	-0.1	9	LYS223	8.80	i(N14)NH2	0.1
10	ILE163	9.82	i(N14)NH2	**0.0**	8	ASP223A	7.99	i(N14)NH2	-0.4
8	CYS168-CYS182	9.39;7.67	i(N14)NH2	-2.0	4	LYS224	3.68	i(N14)NH2	-0.8
10	TYR171	9.70	i(N14)NH2	-0.5	3.5	PRO225	3.34	i(N14)NH2	-0.9
4	TYR172	3.81	i(N14)NH2	0.1	3	GLY226	2.69	**i(N14)NH2**	-2.5
10	VAL176	9.63	i(N14)NH2	-0.3	4.5	VAL227	4.16	ii(ring1)	-0.7
8.5	LEU181	8.23	ii(ring1)	**0.1**	4	TYR228	3.76	ii(ring1)	-0.6
6.5	ALA183	6.14	i(N14)NH2	0.1	8.5	THR229	8.24	ii(ring1)	-0.8
5.5	ALA184	5.45	i(N14)NH2	-0.1					