Table S1. Interaction layer, minimal distance and MFCC binding energies between each one of the 84 amino acid residues in the uPA and UI1 ligand atoms. The energy values were calculated within the GGA + D/PBE/DNP+ theory with ε = 40. Bold UI1 ligand atoms correspond to atoms involved in intermolecular interactions with uPA.

Interaction layer (Å)	Minimal distance			Energy (kcal mol^{-1})	Interaction layer (Å)	Minimal distance			Energy (kcal mol^{-1})
	uPA	d (Å)	UI1			uPA	d (Å)	UI1	
7.0	ILE16	6.76	i(N12)NH_3(+); i(N13)NH_3(+)	2	6.0	VAL160	5.69	i(N12)NH_2	0.1
6.0	ILE17	5.89	i(N12)NH_3(+); i(N13)NH_3(+)	-0.5	10.0	LYS161	9.58	i(N12)NH_2	1.4
8.5	ARG35	8.14	iv(C30)CH_2	1.9	9.0	ILE163	8.58	i(N12)NH_2	0.3
9.5	TYR40	9.22	iii(ring)	0.9	8.0	CYS168-CYS182	10.56;7.99	i(N12)NH_2;i(N13)NH_2^+	-1
7.0	VAL41	6.71	iv(ring)	0	6.0	TYR172	5.57	i(N13)NH_2^+	-0.6
5.0	CYS42-CYS58	6.16;4.94	iv(ring)	-2.2	9.0	LEU181	8.54	i(N12)NH_2	0.6
9.0	GLY43	8.76	iv(N23)NH	-0.7	5.5	ALA183	5.46	i(N12)NH_2	-0.8
7.5	ALA55	7.37	iv(N23)NH	-0.2	6.0	ALA184	5.87	i(N12)NH_2	0.1
7.0	THR56	6.94	iv(ring)	0	7.5	ASP185	7.14	i(N12)NH_2	-1.6
2.5	HIS57	2.46	**iv(ring)**	-3.4	7.0	TRP186	6.84	i(N13)NH_2+	-0.3
7.0	PHE59	6.85	iv(C30)CH_2	0.2	9.5	LYS187	9.43	i(N13)NH_2+	1.2
4.5	ILE60	4.29	iv(C30)CH_2	-0.1	6.5	THR188	6.42	i(N12)NH_2	-0.1
3.5	ASP60A	3.14	**iv(N31)NH_3(+)**	-4.6	2.0	ASP189	1.78	**i(N12)NH_3(+); i(N13)NH_3(+)**	-16
6.0	TYR60B	5.86	iv(ring)	-0.2	2.5	SER190	2.15	**i(N12)NH_3(+)**	-6.9
10.0	PRO60C	9.72	iv(C30)CH_2	0.2	2.5	CYS191-CYS220	2.98;2.25	**ii(ring); iii(ring)**	-15.7
9.5	TYR64	9.47	iv(C30)CH_2	-0.7	2.5	GLN192	2.31	**iii(N16)N; ii(ring); iii(C17)CH_3**	-13.4
10.0	LEU90	9.51	iv(C30)CH_2	-0.3	5.0	GLY193	4.90	iv(O9)C=O	-0.5
5.0	TYR94	4.81	iv(ring)	0.4	5.0	ASP194	5.00	ii(ring)	-2.2
8.5	SER95	8.03	iv(ring)	0.8	3.0	SER195	2.66	**ii(ring)**	-3.7
5.5	ALA96	5.03	iv(ring)	0.8	6.0	GLY196	5.67	ii(ring)	0.4
7.0	ASP97	6.97	iv(ring)	-1.9	7.5	GLY197	7.10	ii(ring)	0.3
7.5	THR97A	7.31	iv(ring)	-0.1	9.5	PRO198	9.37	i(N12)NH_2	0.2
6.5	LEU97B	6.09	iii(N13)NH	-0.2	7.5	LEU199	7.44	i(N12)NH_2	0
8.0	ALA98	7.68	ii(ring)	0.1	7.5	ILE212	7.23	ii(ring)	0.2
2.5	HIS99	2.09	iv(ring)	-2.6	3.0	VAL213	2.58	**ii(ring)**	-2.2
9.0	HIS100	8.89	iv(ring)	1.2	3.5	SER214	3.43	**iv(N23)NH**	-3.5
7.0	ASP102	6.61	iv(N23)NH	-2	3.0	TRP215	2.88	**ii(ring)**	-4.3
5.5	ILE138	5.15	i(N12)NH_2	0	3.5	GLY216	3.04	**iii(N14)NH**	-6.4
10.0	THR139	9.55	i(N12)NH_2	0.3	4.0	ARG217	3.87	iii(ring)	-0.7
10.0	GLY140	9.52	i(N12)NH_2	-0.4	2.5	GLY219	2.02	**i(N13)NH_3(+); iii(N14)NH; iii(N20);**	-13.4
8.5	GLY142	8.09	ii(ring)	0.1	3.0	ALA221	2.77	i(N13)NH_2^+	0.4
3.0	LYS143	2.81	iii(ring)	1.3	5.0	LEU222	4.55	i(N13)NH_2^+	-0.3
9.0	GLU144	8.54	iii(ring)	-0.9	9.0	LYS223	8.52	i(N13)NH_2^+	0
6.0	ASN145	5.52	iii(ring)	0.5	9.0	ASP223A	8.95	i(N13)NH_2^+	-1
2.5	SER146	2.40	**iii(ring)**	-3.2	5.0	LYS224	4.53	i(N13)NH_2^+	0.4

5.0	THR147	4.97	iii(ring)	-0.6	4.5	PRO225	4.50	i(N12)NH_2	0.1
6.0	ASP148	5.92	iii(ring)	-1.3	3.0	GLY226	2.83	i(N12)NH_2	-1
7.0	TYR149	6.97	iii(ring)	-1.2	4.5	VAL227	4.19	ii(ring)	-0.5
9.0	LEU150	8.99	iii(ring)	0.2	4.5	TYR228	4.06	i(N12)NH_2	0
6.0	TYR151	5.96	iii(ring)	-0.1	8.5	THR229	8.41	ii(ring)	-0.5
8.0	THR158	7.72	i(N12)NH_2	0.1					