

Electronic Supplementary Information

Binding energies of the drugs Capreomycin and Streptomycin in complex with tuberculosis bacterial ribosome subunits

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Capreomycin - 30S				Capreomycin - 50S			
Residue	Atomic group	r	Energy	Residue	Atomic group	r	Energy
C26	i(C)O	2	-11.71	A1913	ii(NH)OH	2	-25.26
A1408	iii(NH ₄ ⁺)NH ₃	2.5	-12.83	C1914	v(NH ₂)C	2.5	-9.01
G1491	iii(NH ₄ ⁺)NH ₃	2.5	-19.27	A1912	ii(C)OH	6	-3.80
A1492	iv(C)C	2.5	-14.75	U1915	v(NH ₂)C	6.5	-4.58
A1493	ii(OH)H; iv (NH)O	2.5	-29.69	A1916	iii(O)NH ₂	9	-3.24
G1494	ii(NH ₄ ⁺)N	2.5	-26.94	U1917	iii(O)NH ₂	12	-2.47
A36	ii(NH ₄ ⁺)N	3	-9.66	U1911	ii(C)OH; i(NH ₄ ⁺)O	12.5	-2.56
C1409	iii(NH)O	3.5	-5.96	A1918	ii(C)C	12.5	-2.98
A25	i(C)O	3.5	-5.95	A1919	iii(NH ₂)C	13	-2.98
G1410	v(O) C	5	-4.84	C1920	ii(C)C; iii(C)C	16	-2.76
C27	v(O) C	5.5	-3.89	G1910	i(NH ₂) OH	17.5	-3.63
G35	i(C)OH	5.5	-4.08	G1921	ii(C)C	20	-3.92
U38	i(NH ₄ ⁺)C	5.5	-5.90	C1962	iii(NH ₂)P	23	-2.95
C1407	iii(NH ₄ ⁺)NH ₂	6	-1.94	C1909	i(NH ₄ ⁺)O	23.5	-2.48
U1495	iii(NH ₄ ⁺)C	6	-4.10	G1922	ii(C)C	24	-3.33
C24	i(C)O	6	-4.05	C1961	iii(C)O	24.5	-2.17
C1490	iii(C)NH ₂	7	-2.34	U1963	iii(NH ₂)O	24.5	-3.64
C39	i(NH ₄ ⁺)NH ₂	7	-2.43	U1946	iii(O)OH	26	-1.70
A30	i(NH ₄ ⁺)NH ₂	8	-2.15	C1947	iii(O)C	26	-2.32
C519	iv(C)O	8.5	-4.34	C1908	iii(O)NH ₂	27	-2.12
C1411	v(O)O	8.5	-2.14	G1948	iii(O)C	27.5	-3.48
G530	iv(NH ₄ ⁺)NH ₂	9	-3.09	G1945	v(O)NH ₂	28	-1.30
U1406	iii(NH ₄ ⁺)O	9	-1.72	A1932	v(NH ₂)O	28.5	-1.83
C1496	iii(NH ₄ ⁺)NH ₂	9	-2.20	G1933	iii(NH ₂)O	28.5	-3.32
G28	i(NH ₄ ⁺)O	9	-3.84	G1935	iii(NH ₂)O	28.5	-2.93
C40	i(NH ₄ ⁺)NH ₂	9	-2.50	U1923	iii(O)O	28.5	-1.87
C518	iv(NH ₄ ⁺)OH	9.5	-3.08	U1931	iii(O)C	29	-1.97
G1489	iii(C)O	10	-2.36	C1934	iii(NH ₂)NH ₂	29	-2.38
G10	i(NH ₄ ⁺)C	10	-2.29	G1964	iii(NH ₂)O; v(O)O	30	-4.46
G529	iv(C)NH	10.5	-2.14	G1907	iii(O)O	30	-1.26
G1405	iii(NH ₄ ⁺)O	10.5	-1.87				
U31	i(NH ₄ ⁺)NH	10.5	-2.61				
G42	i(C)NH	10.5	-2.41				
A520	iv(C)O	11	-2.50				
C1404	iii(NH ₄ ⁺)NH ₂	11	-1.72				
C11	v(NH ₂)H	11	-2.20				
U34	i(C)OH	11	-2.59				
G23	i(NH ₄ ⁺)OH	11.5	-2.65				
G1497	iii(NH ₄ ⁺)O	12	-3.26				
C1412	v(O)C	12.5	-3.87				
G29	i(NH ₄ ⁺)O	12.5	-3.47				
U32	i(NH ₄ ⁺)O	12.5	-2.63				
G521	iv(C)N	13	-2.87				
C1403	iii(NH ₄ ⁺)NH ₂	14	-2.54				

TABLE S1. Residue Atomic group, radius (in Å) and the interaction energies (in kcal/mol) of the anti-tuberculosis drug capreomycin in complex with the 30S and 50S tuberculosis bacterial ribosome subunits.

Streptomycin - 30S				S12 protein			
Residue	Atomic group	r	Energy	Residue	Atomic group	r	Energy
U14	iii(O)O	2	-4.25	LYS47	i(OH)C	2	1.80
G527	iii(N)O	2	-10.67	LYS46	i(OH)NH ₄ ⁺	2.5	4.13
C912	i(O)O	2	-16.07	PRO48	ii(C)C	2.5	-12.58
A913	i(NH ₂)O	2	-19.84	LYS91	ii(O)C	2.5	8.62
A914	i(NH ₂)O; iii(N)O	2	-38.71	ASP92	ii(C)OH	5.5	-19.08
C1490	i(NH ₂)O	2	-19.68	PRO94	i(NH ₂)C	5.5	-69.20
A915	i(NH ₂)P	2.5	-9.01	ASN49	ii(C)NH ₃	6	-24.36
G1491	i(NH ₂)O	2.5	-10.01	ARG89	i(C)NH ₃ ; ii(O)NH ₄ ⁺	7	-38.63
U12	iii(N)O	3	-2.76	PRO45	ii(C)C	8	-15.54
U13	iii(O)O	3	-7.54	LEU93	ii(C)NH ₃	8.5	-54.92
C526	iii(N)O	3	-2.96	ARG53	ii(C)NH ₃	9	1.78
U911	i(NH)O	4	-2.82	VAL90	ii(C)O	9.5	-0.01
G886	i(NH ₂)H	4.5	-2.52	GLY95	i(OH)NH ₃	9.5	0.01
G1489	i(NH ₂)H	4.5	-2.67	SER50	ii(C)NH ₃	10	-0.07
G15	iii(O)O	5	-3.29	THR44	ii(C)O	11	-0.03
C525	ii(O)H	5.5	-2.44	VAL96	i(OH)NH ₃	11	-0.06
A523	ii(O)N	6	-1.71	ALA51	ii(C)NH ₃	12.5	-0.07
G885	i(NH ₂)H	6.5	-1.83	ARG97	i(OH)C	13	1.71
G887	i(NH ₂)H	6.5	-3.00	VAL43	i(OH)C; ii(C)C	13	0.02
G916	i(NH ₂)P	6.5	-3.96	LYS23	i(C)NH ₄ ⁺ ; ii(O)NH ₄ ⁺	13.5	1.82
A1492	i(H)O	6.5	-3.95	HIS99	ii(C)C	14	-0.06
A16	iii(O)O	7	-2.61	TYR69	ii(C)C	14.5	-0.04
G22	ii(H)N	7	-1.86	LEU52	ii(C)NH ₃	15	0.08
C528	ii(O)O	7	-2.47	THR67	i(OH)C	15	-0.03
G11	iii(C)H	8	-1.92	GLY88	ii(O)C	15	0.05
A1396	iii(O)O	8	-2.67				
C1403	iii(O)P	8	-3.13				
G21	iii(C)N	8.5	-1.52				
C522	ii(C)N	8.5	-1.57				
C1397	iii(O)C	8.5	-2.51				
C1395	i(NH ₂)O	9	-2.61				
G1410	i(C)N	9	-1.36				
C23	ii(C)O	10	-2.39				
G505	iii(C)NH ₂	10	-1.53				
G524	ii(C)O	10	-1.86				
G529	ii(C)O	10	-2.14				
G888	i(NH ₂)C	10	-2.44				
C910	i(C)H	10	-1.98				
C1402	iii(OH)C	10	-2.42				
C1404	i(N)P	10	-2.91				
G1488	iii(N)P	10	-1.62				
U24	ii(O)C	10.5	-2.06				
G506	ii(O)NH ₂	10.5	-1.53				
C518	ii(O)NH ₂	10.5	-1.89				
A535	ii(O)C	10.5	-2.04				
U17	iii(OH)O	11	-2.16				
G521	ii(C)O	11	-1.49				
A1394	i(NH ₂)O	11	-2.08				
C18	iii(OH)O	11.5	-1.68				
C19	iii(OH)NH ₂	11.5	-1.63				
G1401	iii(OH)O	11.5	-1.75				
G1405	iii(OH)P	11.5	-2.60				

TABLE S2. Residue Atomic group, radius (in Å) and the interaction energies (in kcal/mol) of the anti-tuberculosis drug streptomycin in complex with the 30S tuberculosis bacterial ribosome subunit and the and S12 protein.