

Supplementary material:

Table 1: Top ten compounds against NS2B protein [The amino acids are represented by their one letter code]

Rank	PubChem ID	Molecular formula	M.W. (g/mol)	LogP value	Energy Score (kcal/mol)	No. of H-bonds; hydrophobic contacts	Inhibitor constant K_i (nM) at 298.15 K
1	636530	C ₂₅ H ₂₈ O ₄	392.487	5.6	-9.95	2(G80,D81);10	51.07
2	45280006	C ₂₅ H ₂₈ O ₄	392.487	5.6	-9.94	0; 10	51.36
3	21858822	C ₂₀ H ₁₆ O ₅	336.338	3.5	-9.89	2(G80,T108);10	56.11
4	6476085	C ₂₀ H ₂₀ O ₅	340.369	4.1	-8.78	1(C101);7	363.76
5	57175290	C ₁₉ H ₂₀ O ₃	296.360	3.6	-8.63	1(C101);9	473.63
6	20763922	C ₂₀ H ₂₀ O ₄	324.370	4.6	-8.53	2(C101,L104);9	561.78
7	23069388	C ₁₆ H ₁₆ O ₄	272.295	3.9	-8.45	2(Y119,C101);9	635.33
8	22673586	C ₁₅ H ₁₅ O ₈ P	354.248	1.6	-8.40	2(D81,C101);8	691.03
9	2733750	C ₁₇ H ₁₈ O ₃	270.323	4.8	-8.40	1(C101);8	693.75
10	22673906	C ₁₅ H ₁₅ O ₈ P	354.248	1.6	-8.39	2(C101,L104);9	709.72