Table S1: List of protein structures of different families selected for docking with identified SARS-CoV-2 enzymes binding molecule to evaluate the specificity

Protein ID	Protein Family ID	Protein ID	Protein Family ID
5U7Z	CBAH (PF02275)	3OHM	G-alpha (PF00503)
5W45	NAD1 (PF18778)	3PUF	RNase_H2-Ydr279 (PF09468)
4E49	Carb_anhydrase (PF00194)	3R4O	HSP90 (PF00183)
1BL1	7tm_2 (PF00002)	3R6I	Aldo_ket_red (PF00248)
1CWF	Pro_isomerase (PF00160)	3UVU	Arm (PF00514)
1HF0	Pou (PF00157)	3WO2	IL1 (PF00340)
1IKN	Ank (PF00023)	3ZR0	NUDIX (PF00293)
1JT3	FGF (PF00167)	4A7U	OSCP (PF00213)
1OE9	14-3-3 (PF00244)	4FAD	PI3_PI4_kinase (PF00454)
1QE6	IL8 (PF00048)	4GWG	6PGD (PF00393)
1W6K	Prenyltrans (PF00432)	4IA0	PDEase_I (PF00233)
1Z3U	Fibrinogen_C (PF00147)	4IP9	SAA (PF00277)
1ZXM	DNA_gyraseB (PF00204)	4IRG	Ets (PF00178)
2CF9	Ycf9 (PF01737)	4JKJ	Peptidase_C12 (PF01088)
2CZK	Inositol_P (PF00459)	4JXJ	RrnaAD (PF00398)
2FM5	PDEase_I (PF00233)	4KTV	S-AdoMet_synt_N (PF00438)
2G6P	Peptidase_M24 (PF00557)	4MWS	Peptidase_S10 (PF00450)
2IYB	LIM (PF00412)	4NY0	FERM_M (PF00373)
2J0S	Helicase_C (PF00271)	4NYH	DSPc (PF00782)
2J8B	UPAR_LY6 (PF00021)	4OJ2	MIP (PF00230)
2Q7N	fn3 (PF00041)	4U7D	DEAD (PF00270)
2QFZ	RabGAP-TBC (PF00566)	4URW	RasGEF_N (PF00618)
2QX4	Flavodoxin_2 (PF02525)	4UV8	Myb_DNA-binding (PF00249)
2UW9	Pkinase_C (PF00433)	4W9O	FKBP_C (PF00254)
2V5Y	MAM (PF00629)	4WB7	DnaJ (PF00226)
2X1X	ig (PF00047)	4X1L	Profilin (PF00235)
2XMS	Ndr (PF03096)	4MXV	TNF (PF00229)
3BYI	RhoGAP (PF00620)	4Y5O	PB1 (PF00564)

3DOF	Arf (PF00025)	4ZMV	Cadherin (PF00028)
3EHI	Thymidylat_synt (PF00303)	4ZWJ	Arrestin_N (PF00339)
3EHT	HRM (PF02793)	5A2E	SRCR (PF00530)
3GR4	PK (PF00224)	5AIU	ubiquitin (PF00240)
3H91	Chromo (PF00385)	5C5X	MIP (PF00230)
3HRZ	A2M (PF00207)	5D1M	UQ_con (PF00179)
3I69	GST_C (PF00043)	5F6D	UQ_con (PF00179)
3I7H	X (PF00739)	5FFG	Integrin_beta (PF00362)
3KLT	Filament (PF00038)	5FN3	Presenilin (PF01080)
3MWE	Ligase_CoA (PF00549)	5FUG	YL1 (PF05764)
3OE9	7tm_1 (PF00001)	5GNT	Dynamin_N (PF00350)
5H0V	Transthyretin (PF00576)	5HZJ	PH_13 (PF16652)
5HEX	Hexokinase_1 (PF00349)	5IOH	Metallophos (PF00149)
5HKJ	C1q (PF00386)	5K10	Iso_dh (PF00180)
5L6D	MT-A70 (PF05063)	5WG5	RGS (PF00615)
5M3D	Tetraspanin (PF00335)	5Z90	Bromodomain (PF00439)
5N7E	RhoGEF (PF00621)	6DK3	SHMT (PF00464)
5OKF	Crystallin (PF00525)	6F39	CUB (PF00431)
5POQ	Bromodomain (PF00439)	6FFI	Phage_lysozyme (PF00959)
5T40	Endonuclease_NS (PF01223)	6PAX	PAX (PF00292)
5UZP	Citrate_synt (PF00285)	4GWN	MAM (PF00629)
5VZ3	TGF_beta (PF00019)	3VJ9	SQS_PSY (PF00494)

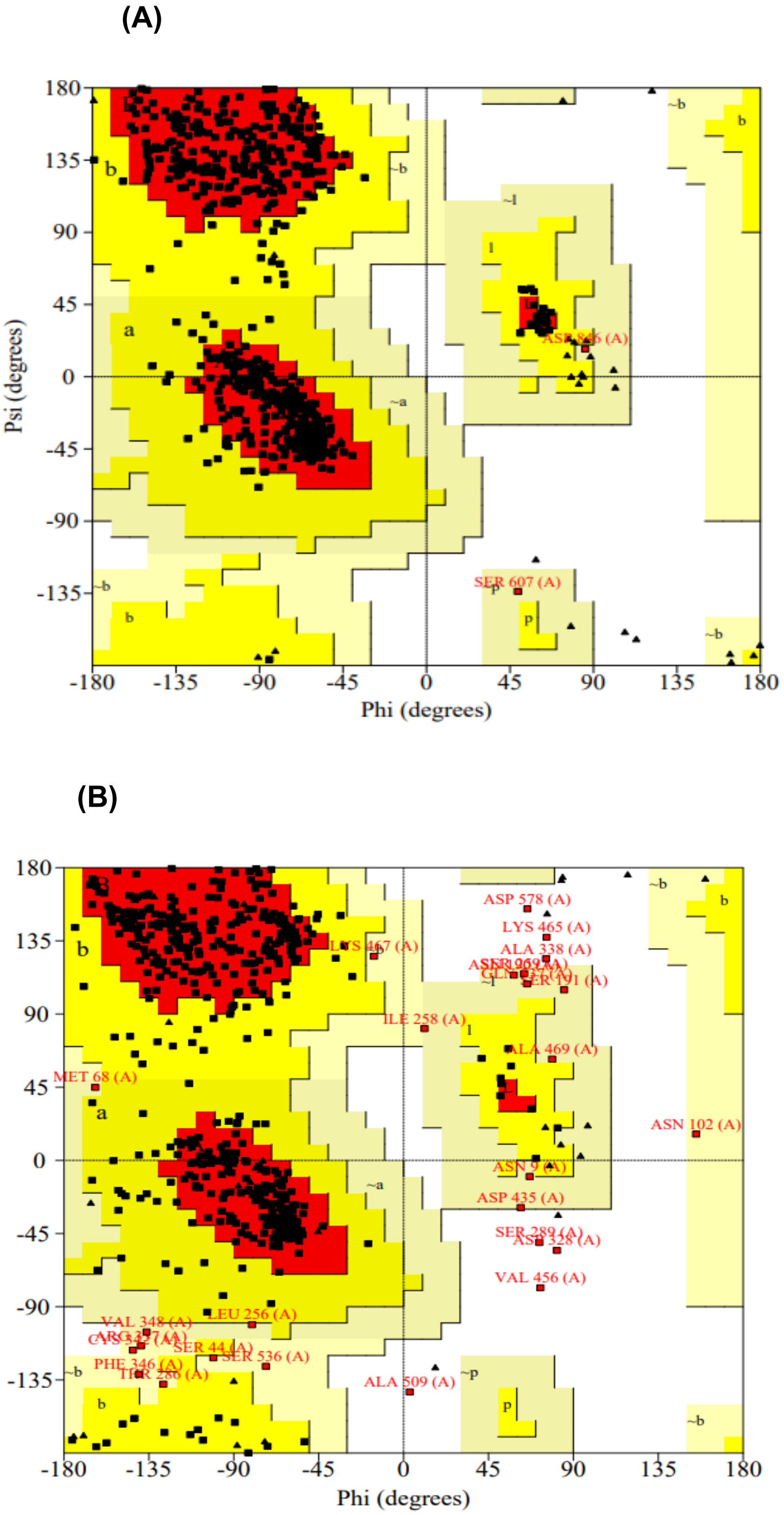

Figure S1: Ramachandran plot analysis of homology models (A) SARS-CoV-2RdRp and (B**)** SARS-CoV-2 helicase. The most favorable regions are marked as A, B and L (red). The additional allowed regions are marked as a, b, l, p (dark yellow). All residues except glycine and proline, are represented as filled black squares, glycine residues are shown as filled triangles. Disallowed residues are filled red.

Table S2: Summary of main-chain parameters of SARS-CoV-2 RdRp homology model

Stereochemical parameter	No of data points	Parameter value	Comparison typical value	Value band width	No. of band width from mean	Interpretation
% residues in A, B, L	735	92.5	88.2	10.0	0.4	INSIDE
Omega angle St. Dev.	801	6.1	6.0	3.0	0.0	INSIDE
Bad Contact/100 Residues	0	0.0	1.0	10.0	-0.1	INSIDE
Zeta angle St. Dev.	763	2.0	3.1	1.6	-0.7	INSIDE
H-bond Energy St. Dev.	501	0.8	0.7	0.2	0.3	INSIDE
Overall G-Fator	805	-0.0	-0.2	0.3	0.5	INSIDE

St. Dev. Represent the standard deviation of observed scores. The structure accuracy can be interpreted in the order BETTER> INSIDE> WORSE for each parameter

Table S3: Summary of side-chain parameters of SARS-CoV-2 RdRp homology model

Stereochemical parameter	No of data points	Parameter value	Comparison typical value	Value band width	No. of band width from mean	Interpretation
Chi-1 gauche minus St.Dev	99	8.7	13.6	6.5	-0.7	INSIDE
Chi-1 trans St. Dev.	236	8.4	15.3	5.3	-1.3	BETTER
Chi-1 gauche plus St.Dev	348	8.2	13.8	4.9	-1.1	BETTER
Chi-1 pooled St. Dev.	683	8.4	14.3	4.8	-1.2	BETTER
Chi-2 trans St. Dev.	180	9.6	17.7	5.0	-1.6	BETTER

St. Dev. Represent the standard deviation of observed scores. The structure accuracy can be interpreted in the order BETTER> INSIDE> WORSE for each parameter

Table S4: Summary of main-chain parameters of SARS-CoV-2 helicase homology model

Stereochemical parameter	No of data points	Parameter value	Comparison typical value	Value band width	No. of band width from mean	Interpretation
% residues in A, B, L	512	80.5	88.2	10.0	-0.8	INSIDE
Omega angle St. Dev.	591	8.5	6.0	3.0	0.8	INSIDE
Bad Contact/100 Residues	2	0.3	1.0	10.0	-0.1	INSIDE
Zeta angle St. Dev.	564	2.4	3.1	1.6	-0.5	INSIDE
H-bond Energy St. Dev.	300	0.8	0.7	0.2	0.7	INSIDE
Overall G-Fator	599	-0.4	-0.2	0.3	-0.7	INSIDE

Table S5: Summary of side-chain parameters of SARS-CoV-2 Helicase Homology model

Stereochemical parameter	No of data points	Parameter value	Comparison typical value	Value band width	No. of band width from mean	Interpretation
Chi-1 gauche minus St.Dev	96	15.8	13.6	6.5	0.3	INSIDE
Chi-1 trans St. Dev.	155	16.9	15.3	5.3	0.3	INSIDE
Chi-1 gauche plus St.Dev	238	15.3	13.8	4.9	0.3	INSIDE
Chi-1 pooled St. Dev.	489	16.3	14.3	4.8	0.4	INSIDE
Chi-2 trans St. Dev.	115	20.3	17.7	5.0	0.5	INSIDE

St. Dev. Represent the standard deviation of observed scores. The structure accuracy can be interpreted in the order BETTER> INSIDE> WORSE for each parameter

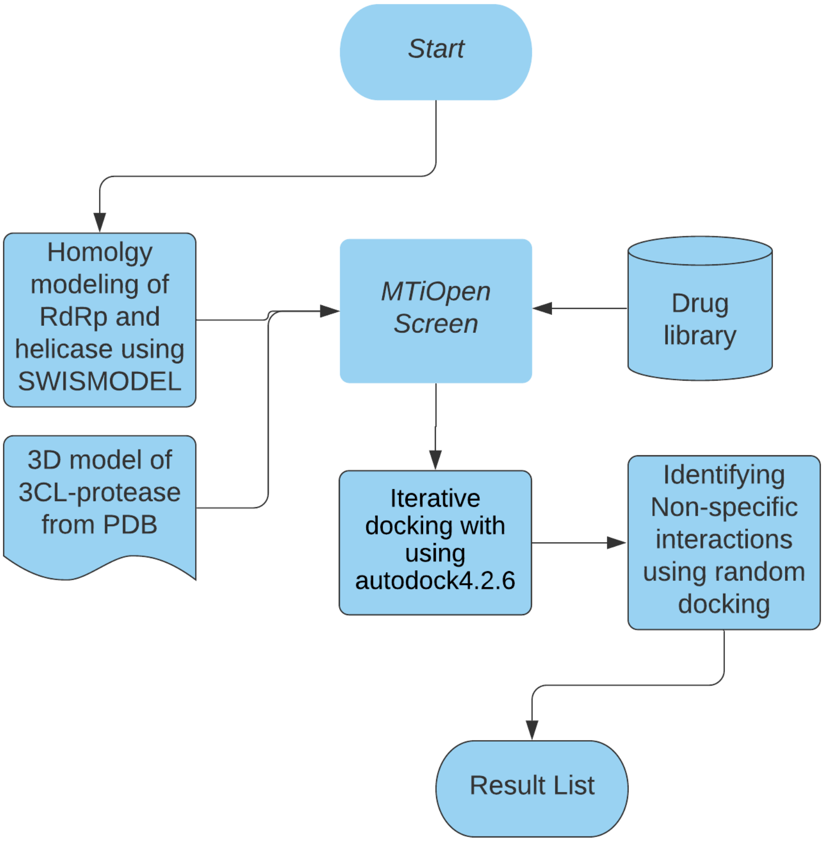

Figure S2: Framework of the computational method to identify potential inhibitors of three viral proteins.