





Supplementary File 4. Ligand binding sites extracted from SARS protein targets and mapped on the sequence of wNsp5 protein aligned with the closest homologs found in UniProt. Shown is the first group of ligands.


Ligand BS:


 benzyl (2-oxopropyl)carbamate (3D62-959, SARS)


 N-[(1R)-2-(tert-butylamino)-2-oxo-1-(pyridin-3-yl)ethyl]-N-(4-tert-butylphenyl)furan-2-carboxamide (3V3M-0EN, SARS)


 N-[4-(acetylamino)phenyl]-2-(1H-benzotriazol-1-yl)-N-[(1R)-2-[(2-methylbutan-2-yl)amino]-1-(1-methyl-1H-pyrrol-2-yl)-2-oxoethyl]acetamide (4MDS-23H, SARS)


 (2S)-2-([[(3S,4aR,8aS)-2-(4-bromobenzoyl)decahydroisoquinolin-3-yl]methyl]amino)-3-(1H-imidazol-5-yl)propanal (4TWW-3A7, SARS)


 (2S)-2-([[(3S,4aR,8aS)-2-(biphenyl-4-ylcarbonyl)decahydroisoquinolin-3-yl]methyl]amino)-3-(1H-imidazol-5-yl)propanal (4TWY-3BL, SARS)


 (2S)-2-([[(3R,4aS,8aR)-2-(biphenyl-4-ylcarbonyl)decahydroisoquinolin-3-yl]methyl]amino)-3-(1H-imidazol-5-yl)propanal (4WY3-3X5, SARS)


 N-(3-FUROYL)-D-VALYL-L-VALYL-N~1~-((1R,2Z)-4-ETHOXY-4-OXO-1-[(3S)-2-OXOPYRROLIDIN-3-YL]METHYL)BUT-2-ENYL)-D-LEUCINAMIDE (2AMD-9IN, SARS)


 (5S,8S,14R)-ETHYL 11-(3-AMINO-3-OXOPROPYL)-8-BENZYL-14-HYDROXY-5-ISOBUTYL-3,6,9,12-TETRAOXO-1-PHENYL-2-OXA-4,7,10,11-TETRAAZAPENTADECAN-15-OATE (2A5K-AZP, SARS)

 N-((3S,6R)-6-((S,E)-4-ETHOXYCARBONYL-1-((S)-2-OXOPYRROLIDIN-3-YL)BUT-3-EN-2-YLCARBAMOYL)-2,9-DIMETHYL-4-OXODEC-8-EN-3-YL)-5-METHYLISOXAZOLE-3-CARBOXAMIDE (2ALV-CY6, SARS)

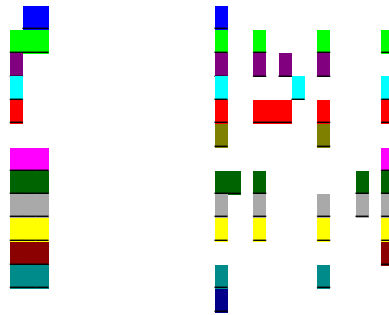
 ETHYL (4R)-4-([[(2R,5S)-5-{N-(TERT-BUTOXYCARBONYL)-L-SERYL}AMINO]-6-METHYL-2-(3-METHYLBUT-2-EN-1-YL)-4-OXOHEPTANOYL]AMINO)-5-[(3R)-2-OXOPYRROLIDIN-3-YL]PENTANOATE (2QIQ-CYV, SARS)

 ETHYL (2E,4S)-4-([[(2R)-2-{N-(TERT-BUTOXYCARBONYL)-L-VALYL}AMINO]-2-PHENYLETHANOYL)AMINO)-5-[(3S)-2-OXOPYRROLIDIN-3-YL]PENT-2-ENOATE (2D2D-ENB, SARS)

 ETHYL (4R)-4-([N-[(BENZYLOXY)CARBONYL]-L-PHENYLALANYL]AMINO)-5-[(3S)-2-OXOPYRROLIDIN-3-YL]PENTANOATE (3SZN-G75, SARS)

 ETHYL (4R)-4-([N-(TERT-BUTOXYCARBONYL)-L-PHENYLALANYL]AMINO)-5-[(3S)-2-OXOPYRROLIDIN-3-YL]PENTANOATE (3TIT-G81, SARS)

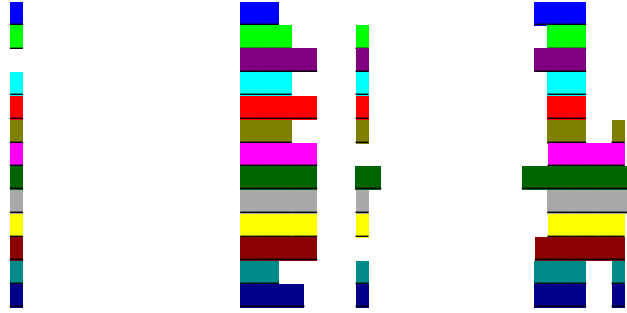
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SP P0C6X7 R1AB_CVHSA	EAACCHLAKALNDFSNSGADVLYQPPQTSITSAVLQSGFRKMAFPSPGKVEGCMVQVTCGT	3264
TR Q6UZF5 Q6UZF5_CVHSA	EAACCHLAKALNDFSNSGADVLYQPPQTSITSAVLQSGFRKMAFPSPGKVEGCMVQVTCGT	3264
TR Q6UZF1 Q6UZF1_CVHSA	EAACCHLAKALNDFSNSGADVLYQPPQTSITSAVLQSGFRKMAFPSPGKVEGCMVQVTCGT	3264
TR Q6JH48 Q6JH48_CVHSA	EAACCHLAKALNDFSNSGADVLYQPPQTSITSAVLQSGFRKMAFPSPGKVEGCMVQVTCGT	3264
TR Q692E6 Q692E6_CVHSA	EAACCHLAKALNDFSNSGADVLYQPPQTSITSAVLQSGFRKMAFPSPGKVEGCMVQVTCGT	3264
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SP P0C6W6 R1AB_BCRP3	EAACCHLAKALNDFSNSGADVLYQPPQTSITSAVLQSGFRKMAFPSPGKVEGCMVQVTCGT	3262
SP P0C6V9 R1AB_BC279	EAACCHLAKALNDFSNSGADVLYQPPQTSITSAVLQSGFRKMAFPSPGKVEGCMVQVTCGT	3270
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TR A0A0U1WHG0 A0A0U1WHG0_CVHSA	EAACCHLAKALNDFSNSGADVLYQPPQTSITSAVLQSGFRKMAFPSPGKVEGCMVQVTCGT	3259
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SP P0C6T7 R1A_BCRP3	EAACCHLAKALNDFSNSGADVLYQPPQTSITSAVLQSGFRKMAFPSPGKVEGCMVQVTCGT	3262
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TR	Q6JH48 Q6JH48_CVHSA	TTLNGLWLDDTVYCPRHVICTAEDMLNPNYEDLLIRKANHSLVQAGNVQLRVIGHSMQN	3324
TR	Q692E6 Q692E6_CVHSA	TTLNGLWLDDTVYCPRHVICTAEDMLNPNYEDLLIRKSNHSLVQAGNVQLRVIGHSMQN	3324
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SP	P0C6W6 R1AB_BCRP3	TTLNGLWLDDTVYCPRHVICTAEDMLNPNYEDLLIRKSNHSLVQAGNVQLRVIGHSMQN	3322
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SP	P0C6U8 R1A_CVHSA	CLLRLKVDTSNPKTPKYKFVRIQPGQTFSSLVACYNGSPSGVYQCAMRPNHTIKGSFLNGS	3384
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SP	P0C6T7 R1A_BCRP3	CLLRLKVDTSNPKTPKYKFVRIQPGQTFSSLVACYNGSPSGVYQCAMRPNHTIKGSFLNGS	3382
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TR |A0A166ZL34| A0A166ZL34_9NIDO CGSVGFNIDYDCVSFCYMHHMELPTGVHAGTDLEGKFYGPFFVDRQTAQAAGDTTITLVN 3246
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TR |A0A0K1Z0N1| A0A0K1Z0N1_CVHSA CGSVGFNIDYDCVSFCYMHHMELPTGVHAGTDLEGKFYGPFFVDRQTAQAAGDTTITLVN 3444
SP |P0C6F5| R1A_BC279 CGSVGFNIDYDCVSFCYMHHMELPTGVHAGTDLEGKFYGPFFVDRQTAQAAGDTTITLVN 3450
SP |P0C6T7| R1A_BCRP3 CGSVGFNIDYDCVSFCYMHHMELPTEVHAGTDLEGKFYGPFFVDRQTAQAAGDTTITLVN 3442
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TR |Q6UZF5| Q6UZF5_CVHSA LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3504
TR |Q6UZF1| Q6UZF1_CVHSA LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3504
TR |Q6JH48| Q6JH48_CVHSA LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3504
TR |Q692E6| Q692E6_CVHSA LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3504
TR |A0A0K1YZY7| A0A0K1YZY7_CVHSA LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3504
SP |P0C6W2| R1AB_BCHK3 LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3498
SP |P0C6W6| R1AB_BCRP3 LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3502
SP |P0C6V9| R1AB_BC279 LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3510
TR |A0A0U1WHI4| A0A0U1WHI4_CVHSA LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3499
TR |A0A0U1WHG0| A0A0U1WHG0_CVHSA LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3499
TR |A0A166ZL34| A0A166ZL34_9NIDO LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3306
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SP |P0C6U8| R1A_CVHSA LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3504
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SP |P0C6F8| R1A_BCHK3 LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3498
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SP |P0C6F5| R1A_BC279 LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3510
SP |P0C6T7| R1A_BCRP3 LAWLYAAVINGDRWFLNRFTTTTLNDFNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDM 3502
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TR	Q6JH48 Q6JH48_CVHSA	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3564
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SP	P0C6W2 R1AB_BCHK3	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3558
SP	P0C6W6 R1AB_BCRP3	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3562
SP	P0C6V9 R1AB_BC279	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3570
TR	A0A0U1WHI4 A0A0U1WHI4_CVHSA	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3559
TR	A0A0U1WHG0 A0A0U1WHG0_CVHSA	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3559
TR	A0A166ZL34 A0A166ZL34_9NIDO	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3366
TR	R9QTB2 R9QTB2_CVHSA	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3556
TR	R9QTH2 R9QTH2_CVHSA	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3565
SP	P0C6U8 R1A_CVHSA	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3564
TR	Q6JH47 Q6JH47_CVHSA	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3564
TR	Q692E5 Q692E5_CVHSA	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3564
SP	P0C6F8 R1A_BCHK3	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3558
TR	A0A0K1Z0N1 A0A0K1Z0N1_CVHSA	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3564
SP	P0C6F5 R1A_BC279	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3570
SP	P0C6T7 R1A_BCRP3	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3562

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