

Supplementary File 3. Ligand binding sites extracted from non-SARS protein targets and mapped on the sequence of wNsp5 protein aligned with the closest homologs found in UniProt.

Ligand BS:

 N-{4-[(1H-benzotriazol-1-ylacetyl)(thiophen-3-ylmethyl)amino]phenyl}thiophene-2-carboxamide (4YOI-4F4, HKU4)

 N-[4-(acetylamino)phenyl]-2-(1H-benzotriazol-1-yl)-N-[(1R)-2-(tert-butylamino)-2-oxo-1-(thiophen-3-yl)ethyl]acetamide (4YOG-4F5, HKU4)

 ADENOSINE-5-DIPHOSPHORIBOSE (4MEA-APR, HKU4)

 N-{4-[(1H-benzotriazol-1-ylacetyl)(thiophen-3-ylmethyl)amino]phenyl}benzamide (4YOJ-RFM, HKU4)

 (1R,2S)-2-{{N-([4-benzyl-1-(tert-butoxycarbonyl)piperidin-4-yl]oxy)carbonyl}-L-leucyl}amino}-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (5WKL-AVY, MERS)

 (1S,2S)-2-{{N-([2-(3-chlorophenyl)ethoxy]carbonyl)-L-leucyl}amino}-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (5WKK-AW4, MERS)

 (1R,2S)-2-{{N-([benzyloxy]carbonyl)-L-leucyl}amino}-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (5WKJ-B1S, MERS)

 (1R,2S)-2-{{N-([2-(3-chlorophenyl)ethoxy]carbonyl)-L-leucyl}amino}-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (5WKK-B3G, MERS)

 (1S,2S)-2-{{N-([4-benzyl-1-(tert-butoxycarbonyl)piperidin-4-yl]oxy)carbonyl}-L-leucyl}amino}-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (5WKL-B3J, MERS)

 (1R,2S)-2-{{N-([1-(tert-butoxycarbonyl)-4-ethylpiperidin-4-yl]oxy)carbonyl}-L-leucyl}amino}-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (5WKM-B6Y, MERS)

 (1S,2S)-2-{{N-([benzyloxy]carbonyl)-L-leucyl}amino}-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (5WKJ-K36, MERS)

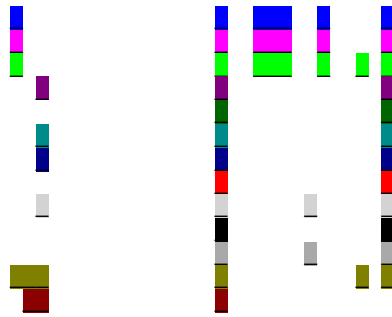
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 (S)-N-benzyl-3-((S)-2-cinnamamido-3-phenylpropanamido)-2-oxo-4-((S)-2-oxopyrrolidin-3-yl)butanamide (6FV2-D03, NL63)

 (2-{S})-4-methyl-{N}-[(2-{S}),3-{R}]-3-oxidanyl-4-oxidanylidene-1-[(3-{S})-2-oxidanylidene-3-yl]-4-[(phenylmethyl)amino]butan-2-yl]-2-[(~{E})-3-phenylprop-2-enoyl]amino]pentanamide (6FV1-E8E, NL63)

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TR Q6JH48 Q6JH48_CVHSA	EAACCHLAKALNDFSNSGADVLYQPPQTSITSAVLQSGFRKMAFP	SGKVEGCMVQVTCGT	3264
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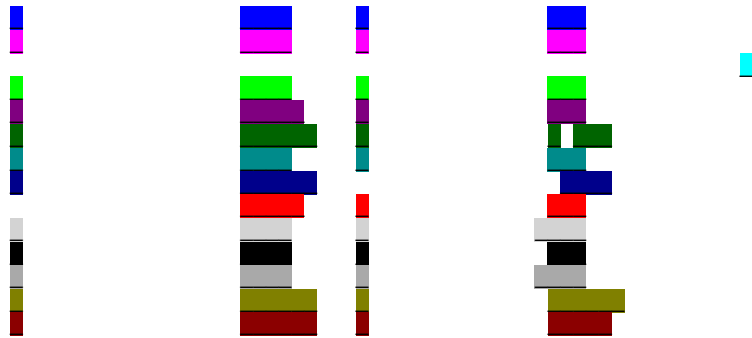
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TR	Q6UZF5	Q6UZF5_CVHSA	TTLNGLWLDDTVYCPRHVICTAEDMLNPNYEDLLIRKSNHSLVQAGNVQLRVIGHSMQN	3324
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SP	P0C6V9 R1AB_BC279	CAALKELLQNGMNGRTILGSTILEDEFTPFDDVVRQCSGVTFQGKFKKIVKGTHHWMLLTF	3570
TR	A0A0U1WHI4 A0A0U1WHI4_CVHSA	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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