

Supporting information:

Table S1. The 392 crystal structures of the protein-ligand complexes selected for this study.

index	PDB code	Protein/Ligand	resolution
1	1gvu	Endothiapepsin/H189	0.94
2	1bxo	Penicillopepsin/Phosphonate Inhibitor	0.95
3	1gvw	Endothiapepsin/Pd-130,328	1.00
4	1gvx	Endothiapepsin/H256	1.00
5	1lkk	Human P56 Tyrosine Kinase/pYEEI peptide	1.00
6	1kzk	HIV Protease /Je-2147	1.09
7	1jet	Oligo-Peptide Binding Protein (Oppa)/Peptide KAK	1.20
8	1jeu	Oligo-Peptide Binding Protein (Oppa)/Peptide KEK	1.25
9	1qft	Histamine Binding Protein /Histamine	1.25
10	1fcy	Retinoic Acid Receptor -1/Cd564	1.30
11	1flm	Fmn-Binding Protein/Flavin Mononucleotide	1.30
12	1hyo	Fumarylacetoacetate Hydrolase/Phosphorus-Based Inhibitor	1.30
13	1jev	Oligo-Peptide Binding Protein (Oppa)/Peptide KWK	1.30
14	1jr0	Cholera Toxin B Subunit/Bmsc-0011	1.30
15	1gyx	Ydce, A 4-Oxalocrotonate Tautomerase Homologue /Benzoic acid	1.35
		Ydce, A 4-Oxalocrotonate Tautomerase Homologue /	
16	1gyy	(E)-2-Fluoro-P-Hydroxycinnamate	1.35
17	5p21	c-H-Ras p21 Protein /5'-Guanosyl-Imido-Triphosphate	1.35
18	1c5s	Trypsin/Benzo[B]thiophene-2-Carboxamidine	1.36
19	1c1r	Trypsin/BABIM derivative	1.37
20	1c5t	Trypsin/Thieno[2,3-B]Pyridine-2-Carboxamidine	1.37
21	1gi4	Trypsin/APC-1144	1.37

22	1kug	Metalloproteinase /Penw	1.37
23	1fcz	Retinoic Acid Receptor -1/Bms181156	1.38
24	1fd0	Retinoic Acid Receptor -1/Sr11254	1.38
25	1gi2	Trypsin/APC-1144_810sm	1.38
26	1ghz	Trypsin/APC-10273	1.39
27	1f8d	Neuraminidase/9-amino-DANA	1.40
28	1f8e	Neuraminidase/4,9-diamino-DANA	1.40
29	1hmr	Fatty Acid Binding Protein /Elaidate	1.40
30	1hms	Fatty Acid Binding Protein /Oleic acid	1.40
31	1hmt	Fatty Acid Binding Protein/Stearic Acid	1.40
32	2ctc	Carboxypeptidase A/L-Phenyl Lactate	1.40
33	2olb	Oligopeptide Binding Protein (Oppa) /Tri-Lysine	1.40
34	1bxq	Penicillopepsin/Phosphonate Inhibitor	1.41
35	1c5p	Trypsin/Benzamidine	1.43
36	1c5q	Trypsin/4-iodobenzo[b]thiophene 2-carboxamidine	1.43
37	1kuk	Metalloproteinase/Pekw	1.45
38	1vwl	Streptavidin/Cyclo-[5-S-Valeramide-Hpqqgppc]K-Nh2	1.45
39	1fcx	Retinoic Acid Receptor -1/Bms184394	1.47
40	2izl	Streptavidin/Biotin	1.48
41	1gi6	Trypsin/APC-8328	1.49
42	8abp	Arabinose-Binding Protein Mutant (M108L)/D-Galactose	1.49
43	1b8o	Purine Nucleoside Phosphorylase/Immucillin-H	1.50
44	1c5n	Thrombin/4-iodobenzo[b]thiophene 2-carboxamidine	1.50
45	1gj6	Ser190 Trypsin-Like Serine Protease/APC-8696	1.50
46	1gj7	Urokinase-Type Plasminogen Activator/APC-10302	1.50
47	1hn4	Prophospholipase A2/MJ33	1.50
48	1kl	Mitomycin-Binding Protein/Mitomycin C Metabolite	1.50
49	1kui	Metalloproteinase /Peqw	1.50
50	1loq	Orotidine 5'-Monophosphate Decarboxylase/UMP	1.50

51	1df8	S45A Mutant Of Streptavidin /Biotin	1.51
52	1qq9	Aminopeptidase/Methionine	1.53
53	1gja	Urokinase-Type Plasminogen Activator/APC-7136	1.56
54	1moq	Glucosamine 6-Phosphate Synthase/Glucosamine 6-Phosphate	1.57
55	1akr	G61A Oxidized Flavodoxin Mutant/Flavin Mononucleotide	1.58
56	1gzc	Erythrina Crista-Galli Lectin/LACTOSE	1.58
57	1nox	Nadh Oxidase/Flavin Mononucleotide	1.59
58	16pk	3-Phosphoglycerate Kinase/Bisubstrate Analog	1.60
59	1adl	Adipocyte Lipid-Binding Protein /Arachidonic Acid	1.60
60	1cil	Carbonic Anhydrase II/inhibitor ETS	1.60
61	1f74	N-Acetyl-Neuraminase Lyase/4-Deoxy-Sialic Acid	1.60
62	1g7q	H-2 Class I Histocompatibility Antigen/peptide from the MUC1	1.60
63	1gi5	Trypsin/APC-6665	1.60
64	1iup	Meta-Cleavage Product Hydrolase/Isobutyric acid	1.60
65	1j16	Trypsin Mutant X99/175/190Rt/Benzamidine	1.60
66	1jlx	Phosphoribosylglycinamide Formyltransferase/ Epoxide-Derived Multisubstrate Adduct Inhibitor Orotidine Monophosphate Decarboxylase/	1.60
67	1lor	6-Hydroxyuridine-5'-Phosphate	1.60
68	2aac	Gene Regulatory Protein Arac /D-Fucose	1.60
69	2dri	D-ribose-binding protein /Ribose	1.60
70	2qwc	R292K Of Tern N9 Influenza Virus Neuraminidase/Neu5Ac2En	1.60
71	2sim	Salmonella typhimurium LT2 neuraminidase /Neu5Ac2en	1.60
72	2tmn	Thermolysin/P-Leu-NH2	1.60
73	5tmn	Thermolysin /Cbz-GlyP-Leu-Leu	1.60
74	6tmn	Thermolysin /Cbz-GlyP-(O)-Leu-Leu	1.60
75	830c	Collagenase-3 (Mmp-13) /Sulphone-Based Hydroxamic Acid	1.60

76	1c5c	Chimeric Decarboxylase Antibody 21D8/hapten	1.61
77	1gny	Xylanase 10C/Xylopentaose	1.63
78	1ciz	Stromelysin-1/nonpeptide inhibitor	1.64
79	1gj8	Urokinase-Type Plasminogen Activator/APC-10950	1.64
80	1c2d	Trypsin/keto-BABIM	1.65
81	1ghx	Thrombin/APC-1144	1.65
82	1lcp	Leucine Aminopeptidase/L-Leucine Phosphonic Acid	1.65
83	1qk3	Hypoxanthine-Guanine Phosphoribosyltransferase/GMP	1.65
84	1snc	Staphylococcal Nuclease /Deoxythymidine-3',5'-Bisphosphate	1.65
85	1sri	Streptavidin/3',5'-Dimethyl-Haba	1.65
86	3std	Scytalone Dehydratase/Cyanocinnoline Inhibitor	1.65
87	1anf	Maltodextrin-Binding Protein/Glucose	1.67
88	6abp	L- Arabinose-binding protein /Arabinose	1.67
89	7abp	L-Arabinose-Binding Protein Mutant M108L /D-Fucose	1.67
90	1abe	L-Arabinose-Binding Protein /L-Arabinose	1.70
91	1afk	Ribonuclease A/5'-Diphosphoadenosine-3'-Phosphate	1.70
92	1afl	Ribonuclease A/5'-diphosphoadenosine 2'-phosphate	1.70
		Transforming Protein P21/H-Ras-1/	
93	1clu	Diaminobenzophenone- β , γ -Imido- GTP	1.70
94	1duv	Ornithine Transcarbamoylase/Psorn	1.70
95	1e2k	Thymidine Kinase/MCT	1.70
96	1f2o	Aminopeptidase/L-Leucine	1.70
97	1f8c	Neuraminidase/4-amino-DANA	1.70
98	1fkb	Fk506 Binding Protein /Rapamycin	1.70
99	1fkf	FK506 Binding Protein /FK506	1.70
100	1fv0	Phospholipase A2/9-Hydroxy Aristolochic Acid	1.70
101	1fzk	Mhc Class I Natural Mutant H-2Kbm1 Heavy Chain /SEV9	1.70
102	1fzq	ADP-Ribosylation Factor-Like Protein 3/GDP	1.70

103	1gca	Glucose/Galactose-Binding Protein/D-Galactose	1.70
104	1gz9	Erythrina Crista-Galli Lectin/L-Fucosyllactose	1.70
105	1h0a	Epsin Enth /Ins(1,4,5)P3	1.70
106	1h4w	Trypsin Iva/Benzamidine	1.70
107	1h6h	Neutrophil Cytosol Factor 4/Phosphatidylinositol 3-Phosphate	1.70
108	1hfs	Stromelysin-1/L-764,004	1.70
109	1k4g	tRNA-Guanine Transglycosylase/2-aminoquinazolinone derivative	1.70
110	1kdk	Sex Hormone-Binding Globulin/Dihydrotestosterone	1.70
111	1183	Lysozyme/Benzene	1.70
112	1lgt	Biphenyl-2,3-Diol 1,2-Dioxygenase/2'-Cl Dihydroxybiphenyl	1.70
113	1mfa	Fv Fragment (Murine Se155-4) /carbohydrate antigen	1.70
114	1ppl	Penicillopepsin/Iva-Val-Val-Leu(P)-(O)Phe-Ome	1.70
115	1ppm	Penicillopepsin/Cbz-Ala-Ala-Leu(P)-(O)Phe-Ome	1.70
116	1qhc	Ribonuclease A/3',5'-Pyrophosphate-Linked Dinucleotide Inhibitor	1.70
117	1thl	Thermolysin /Glutaramide Derivative	1.70
118	3mbp	Maltodextrin-Binding Protein/Maltotriose	1.70
119	3ptb	Trypsin/Benzylidiamine	1.70
120	3tmn	Thermolysin /Val-Trp	1.70
121	4dfr	Dihydrofolate Reductase /Methotrexate	1.70
122	4mbp	Maltodextrin Binding Protein;/Maltetrose	1.70
123	4tmn	Thermolysin /Cbz-PheP-Leu-Ala	1.70
124	2xis	Xylose Isomerase /D-Xylitol	1.71
125	1fh9	β -1,4-Xylanase/Lactam Oxime Inhibitor	1.72
126	1gj5	Thrombin/APC-7806	1.73
127	1gjc	Urokinase-Type Plasminogen Activator/APC-8696	1.73
128	1akw	G61L Oxidized Flavodoxin Mutant/Flavin Mononucleotide	1.75
129	1b32	Oligo-Peptide Binding Protein/Peptide KMK	1.75

130	1b4z	Oligo-Peptide Binding Protein/Peptide KDK	1.75
131	1b6l	Retropepsin/Macrocytic Peptidomimetic Inhibitor 4	1.75
132	1bap	L-Arabinose-Binding Protein Mutant P254G/L-Arabinose	1.75
133	1c1u	Thrombin/BABIM Analogue	1.75
134	1d4l	HIV-1 Protease/Macrocytic Peptidomimetic Inhibitor 1	1.75
135	1elc	Elastase/Trifluoroacetyl-L-Phenylalanyl-P-Isopropylanilide	1.75
136	1f4g	Thymidylate Synthase/Sp-876	1.75
137	1f57	Carboxypeptidase A/D-Cysteine	1.75
138	1g2o	Purine Nucleoside Phosphorylase/transition-state analogue ImmH	1.75
139	1gi8	Urokinase-Type Plasminogen Activator/APC-1144	1.75
140	1gjd	Urokinase-Type Plasminogen Activator/APC-11421	1.75
141	1hew	Lysozyme /Tri-N-Acetylchitotriose	1.75
142	1ikt	β -Estradiol 17 -Dehydrogenase/Oxtoxynol-10	1.75
143	1mtr	HIV-1 Protease/Cyclic Phe-Ile-Val Peptidomimetic Inhibitor	1.75
144	3cla	Type III Chloramphenicol Acetyltransferase /Chloramphenicol	1.75
145	1apb	L-Arabinose-Binding Protein Mutant P254G/D-Fucose	1.76
146	1slg	Streptavidin/Peptide Fchpqt	1.76
147	1sre	Streptavidin/Haba	1.78
148	1gi7	Urokinase-Type Plasminogen Activator/APC-10273	1.79
149	1a4w	Thrombin/Thiazole-Containing Inhibitors	1.80
150	1ag9	Oxidized Flavodoxin/Flavin Mononucleotide	1.80
151	1akt	G61N Oxidized Flavodoxin Mutant/Flavin Mononucleotide	1.80
152	1apt	Penicillopepsin/Isovaleryl (Iva)-Val-Val-Lysta-O-Et	1.80
153	1apu	Penicillopepsin/A Pepstatin Analogue	1.80
154	1apv	Penicillopepsin/Difluorostatone-Containing Peptides	1.80
155	1b3f	Oligo-Peptide Binding Protein/Peptide KHK	1.80
156	1b46	Oligo-Peptide Binding Protein/Peptide KPK	1.80
157	1apw	Penicillopepsin/Difluorostatine containing peptide	1.80

158	1at6	Lysozyme with A Isoaspartate Residue/Tri-N-Acetylchitotriose	1.80
159	1atl	Atrolysin C/Sc 44463	1.80
160	1azl	G61V Flavodoxin Mutant /Flavin Mononucleotide	1.80
161	1b1h	Oligo-Peptide Binding Protein/Tripeptide Lys-Hpe-Lys	1.80
162	1b51	Oligo-Peptide Binding Protein/Peptide KSK T-Lymphocyte-Specific Protein Tyrosine Kinase P56Lck/	1.80
163	1bhf	Inhibitor Ace-Ipa-Glu-Glu-Ile	1.80
164	1bkj	Nadph-Flavin Oxidoreductase/Flavin Mononucleotide	1.80
165	1bma	Elastase/Benzyl Methyl Aminimide Inhibitor	1.80
166	1b58	Oligo-Peptide Binding Protein/Peptide KYK	1.80
167	1b5j	Oligo-Peptide Binding Protein/Peptide KQK HIV-1 Protease (V82F/I84V) Double Mutant /	1.80
168	1bwb	Sd146 Of Dupont Pharmaceuticals	1.80
169	1c83	Protein-Tyrosine Phosphatase 1B/OBA derivative	1.80
170	1c88	Protein-Tyrosine Phosphatase 1B/OBA-1 derivative	1.80
171	1caq	Stromelysin-1/nonpeptide inhibitor	1.80
172	1dhj	Dihydrofolate Reductase Mutant D27S F137S/Methotrexate	1.80
173	1e4h	Transthyretin/Pentaboromophenol	1.80
174	1b6h	Periplasmic Oligo-Peptide Binding Protein/Lysyl-Norvalyl-Lysine	1.80
175	1b9j	Oligo-Peptide Binding Protein (Oppa)/Peptide KLK	1.80
176	1e5a	Transthyretin/2,4,6-Tribromophenol Urokinase-Type Plasminogen Activator/	1.80
177	1ejn	(4-Aminomethyl)Phenylguanidine Derivative	1.80
178	1ela	Elastase/Trifluoroacetyl-L-Lysyl-L-Prolyl-P-Isopropylanilide	1.80
179	1eld	Elastase /Tfa-Phe-Ala-Tfm	1.80
180	1ele	Elastase /Tfa-Val-Ala-Tfm	1.80
181	1evh	Mena Evh1 Domain/Acta Peptide	1.80

182	1f0t	Trypsin/Rpr131247	1.80
183	1f2p	Aminopeptidase/L-Phenylalanine	1.80
184	1f5k	Urokinase-Type Plasminogen Activator/Benzamidine	1.80
185	1f7b	N-Acetyl-Neuraminate Lyase/4-Oxo-Sialic Acid	1.80
186	1f8b	Neuraminidase/DANA Pleckstrin Homology Domain From Dapp1/Phish /	1.80
187	1fao	Inositol 1,3,4,5- Tetrakisphosphate	1.80
188	1fzo	Mhc Class I Natural Mutant H-2Kbm8 Heavy Chain/SEV9	1.80
189	1g35	HIV-1 Protease/Inhibitor Aha024	1.80
190	1g3b	Trypsin/Meta-Amidino Schiff Base Copper (II) Chelate	1.80
191	1g3d	Trypsin/Meta-Amidino Schiff Base Copper (II) Chelate	1.80
192	1g3e	Trypsin/Meta-Amidino Schiff Base Copper (II) Chelate	1.80
193	1g52	Carbonic Anhydrase II/2,3-difluoro-SBB	1.80
194	1g7f	Protein-Tyrosine Phosphatase Catalytic Domain /Pnu177496	1.80
195	1gdo	Glucosamine 6-Phosphate Synthase/Glutamate	1.80
196	1gi9	Urokinase-Type Plasminogen Activator/APC-6669	1.80
197	1gj9	Urokinase-Type Plasminogen Activator/APC-11092	1.80
198	1hi3	Eosinophil-Derived Neurotoxin/Adenosine-2'-5'- Diphosphate	1.80
199	1hi4	Eosinophil-Derived Neurotoxin/Adenosine-3'-5'- Diphosphate	1.80
200	1hi5	Eosinophil-Derived Neurotoxin/Adenosine-5'-Diphosphate	1.80
201	1hn2	Odorant-Binding Protein/Aminoanthracene	1.80
202	1hvh	HIV-1 Protease/Nonpeptide Cyclic Cyanoguanidines	1.80
203	1hvi	HIV-1 Protease /A-77003	1.80
204	1hvk	HIV-1 Protease /A-76928	1.80
205	1hvl	HIV-1 Protease /A-76889	1.80
206	1hwx	HIV-1 Protease/A-84538	1.80
207	1hyx	Immunoglobulin 6D9/Cloramphenicol phosphonate derivate	1.80
208	1j4r	Fk506-Binding Protein/Fkb-001	1.80

209	1jcx	2-Dehydro-3-Deoxyphosphooctonate Aldolase/Api	1.80
210	1jq9	Phospholipase A2/Phe-Leu-Ser-Tyr-Lys	1.80
211	1k4h	tRNA-Guanine-Transglycoylase/2-aminoquinazolinone derivative	1.80
212	1kpm	Phospholipase A2/Vitamin E Messenger RNA 5' Cap-Binding Protein (Eif4E) /	1.80
213	1l8b	7-Methyl-Guanosine-5'-Triphosphate	1.80
214	1lf2	Plasmepsin /Inhibitor Rs370	1.80
215	1lkl	Human P56 Tyrosine Kinase/pYEEG peptide	1.80
216	1m21	Peptide Amidase/Chymostatin Cation-Dependent Mannose-6-Phosphate Receptor/	1.80
217	1m6p	α -D-Mannose-6-Phosphate	1.80
218	1mem	Cathepsin K/Vinyl Sulfone Inhibitor Macrophage Migration Inhibitory Factor/	1.80
219	1mfi	(E)-2-Fluoro-P-Hydroxycinnamate	1.80
220	1pot	Spermidine/Putrescine-Binding Protein/Spermidine	1.80
221	1ppc	Trypsin/NAPAP	1.80
222	1ppk	Penicillopepsin/Phosphinic Acid Analogue Of Statine	1.80
223	1pro	HIV-1 Protease/A-98881	1.80
224	1qb1	Trypsin/Zk- 806974	1.80
225	1qb6	Trypsin/Zk-805623	1.80
226	1qb9	Trypsin/Zk- 806450	1.80
227	1qbn	Trypsin/Zk-806688	1.80
228	1qbo	Trypsin/Zk-806711 Inhibitor	1.80
229	1qbv	Thrombin /Guanidine-Mimetic Inhibitor	1.80
230	1qka	Oligo-Peptide Binding Protein (Oppa) /Peptide KRK	1.80
231	1qkb	Oligo-Peptide Binding Protein (Oppa) /Peptide KVK	1.80
232	1rdi	Mannose-Binding Protein-C/ α -Methyl-L-Fucopyranoside	1.80
233	1rdj	Mannose-Binding Protein-C/ β -L-Methyl-Fucose	1.80

234	1rdn	Mannose-Binding Protein-C/ α -Methyl-D-N-Acetylglucosaminide	1.80
235	1rpj	D-Allose Binding Protein /D-Allopyranose	1.80
236	1srg	Streptavidin/3'-Methyl-Haba	1.80
237	1str	Streptavidin/Peptide Ac-Chpqnt-Nh2	1.80
238	1swg	Streptavidin E51/A46 /biotin	1.80
239	1tng	Trypsin /Inhibitor Aminomethylcyclohexane	1.80
240	1tnh	Trypsin /Inhibitor 4-Fluorobenzylamine	1.80
241	1tnj	Trypsin /Inhibitor 2-Phenylethylamine	1.80
242	1tnk	Trypsin /Inhibitor 3-Phenylpropylamine	1.80
243	1tom	Thrombin/Hirugen	1.80
244	1usn	Stromelysin-1/Thiadiazole Inhibitor Pnu-142372	1.80
245	2gst	Glutathione S-Transferase /(9S,10S)-addition product	1.80
246	2qwg	Neuraminidase/Neu5Ac2en analogue inhibitor	1.80
247	2rkm	Oligo-Peptide Binding Protein/Peptide Lys-Lys	1.80
248	2rnt	Lys 25-Ribonuclease T1 /Guanylyl-2',5'-Guanosine	1.80
249	3kiv	Apolipoprotein/6-Aminohexanoic Acid	1.80
250	3mag	Vaccinia Methyltransferase Vp39/6-Amino-3-Methylpurine	1.80
251	4sga	Proteinase A /Tetrapeptide Ace-Pro-Ala-Pro-Phe	1.80
252	5abp	L-Arabinose-Binding Protein /D-Galactose	1.80
253	5er2	Endothia Aspartic Proteinase/Cp-69,799	1.80
254	5sga	Proteinase A /Tetrapeptide Ace-Pro-Ala-Pro-Tyr	1.80
255	6rnt	Ribonuclease T1 /2'-Adenylic Acid	1.80
256	6std	Scytalone Dehydratase/SD Inhibitor 3	1.80
257	7est	Elastase/TFAP	1.80
258	7std	Scytalone Dehydratase/Inhibitor Carpropamide	1.80
259	1fzm	Mhc Class I Natural Mutant H-2Kbm8 Heavy Chain /VSV8	1.80
260	1gj4	Thrombin/APC-10302	1.81
261	1fh7	β -1,4-Xylanase/Deoxynojirimycin Inhibitor	1.82

262	5a3h	Endoglucanase/2-Deoxy-2-Flouro-B-D-Cellobioside	1.82
263	1g45	Carbonic Anhydrase II Mutant F131V/2-fluro-SBB	1.83
		Peptidyl-Prolyl Cis-Trans Isomerase Nima- Interacting 1/	
264	1f8a	Y(Sep)Pt(Sep)S Peptide	1.84
265	1g46	Carbonic Anhydrase II Mutant F131V/2,3-difluro-SBB	1.84
266	1g4j	Carbonic Anhydrase II Mutant F131V/2,3,4,5,6-Pentafluoro-SBB	1.84
267	1a7t	Metallo--Lactamase/MES	1.85
268	1b6j	HIV-1 Protease /Macrocyclic Peptidomimetic Inhibitor 1	1.85
269	1b6k	HIV-1 Protease /Macrocyclic Peptidomimetic Inhibitor 5	1.85
270	1b6m	HIV-1 Protease /Macrocyclic Peptidomimetic Inhibitor 6	1.85
271	1b6n	HIV-1 Protease /Macrocyclic Peptidomimetic Inhibitor 3	1.85
272	1b6o	HIV-1 Protease /Macrocyclic Peptidomimetic Inhibitor 2	1.85
273	1d4k	HIV-1 Protease/Macrocylic Peptidomimetic Inhibitor 2	1.85
274	1d7j	Fk506-Binding Protein/4-Hydroxy-2-Butanone	1.85
275	1e1x	Cyclin-Dependent Protein Kinase 2/Inhibitor v6027	1.85
276	1ex8	6-Hydroxymethyl-7,8-Dihydropterin Pyrophosphokinase/Hp4A	1.85
277	1f3e	Queuine tRNA-Ribosyltransferase/3,5-Diaminophthalhydrazide	1.85
278	1f3f	Nucleoside Diphosphate Kinase/D4T Triphosphate	1.85
279	1flr	κ -4-4-20 (IgG2A) Fab Fragment/Fluorescein	1.85
280	1ghv	Thrombin/APC-10273	1.85
281	1ghy	Thrombin/APC-1801	1.85
282	1lgw	Lysozyme/2-Fluoroaniline	1.85
283	1li3	Lysozyme/3-Chlorophenol	1.85
284	1vwn	Streptavidin/cyclo-Ac-[Chpqfc]-Nh2 Ig Antibody D2.3 (Light Chain)/	1.85
285	1yej	nitrophenyl phosphonate transition state analog	1.85
286	1g48	Carbonic Anhydrase II Mutant F131V/2,6-difluro-SBB	1.86

287	1g54	Carbonic Anhydrase II/2,3,4,5,6-Pentafluoro-SBB	1.86
288	1i9n	Carbonic Anhydrase II Mutant F131V/2,5-difluoro-SBB	1.86
289	1k21	Prothrombin/Thrombin-Inhibitor	1.86
290	1rgk	Ribonuclease T1 Mutant E46Q/2'AMP	1.87
291	1hsl	Histidine-Binding Protein/L-Histidine	1.89
292	1abf	L-Arabinose-Binding Protein/D-Fucose	1.90
293	1ax0	Lectin /N-acetylgalactosamine	1.90
294	1b2h	Periplasmic Oligopeptide-Binding Protein/Lysyl-Ornithyl-Lysine	1.90
295	1b4h	Periplasmic Oligo-Peptide Binding Protein/ Lysyl- Diaminobutyric Acid-Lysine	1.90
296	1b5h	Oligo-Peptide Binding Protein/ Lysyl-Diaminopropanoic Acid-Lysine	1.90
297	1b5i	Oligo-Peptide Binding Protein/Peptide KNK	1.90
298	1bcd	Carbonic Anhydrase II /trifluoromethane sulphonamide	1.90
299	1bwa	HIV-1 Protease/Xv638	1.90
300	1c5o	Thrombin/Benzamidine	1.90
301	1ce5	Trypsin /Benzamidine	1.90
302	1cnx	Carbonic Anhydrase II/EG3NH3+	1.90
303	1czk	Flavodoxin mutant/Flavin Mononucleotide	1.90
304	1czt	Flavodoxin/Flavin Mononucleotide	1.90
305	1d7i	Fk506-Binding Protein/Methyl Methylsulfinylmethyl Sulfide	1.90
306	1dhi	Dihydrofolate Reductase Mutant D27S/Methotrexate	1.90
307	1ent	Endothiapepsin/Pd130328	1.90
308	1epp	Endothia Aspartic Proteinase /Pd-130,693	1.90
309	1epq	Endothia Aspartic Proteinase /Pd-133,450	1.90
310	1erb	Retinol Binding Protein /N-ethyl retinamide	1.90
311	1ez9	Maltose-Binding Periplasmic Protein/Maltotetraitol	1.90
312	1f0u	Trypsin/Rpr128515	1.90

313	1f4e	Thymidylate Synthase/Tosyl-D-Proline	1.90
314	1fhd	β -1,4-Xylanase/Imidazole Inhibitor	1.90
315	1fkn	Memapsin 2/Inhibitor Om99-2	1.90
316	1fwu	Cysteine-Rich Domain Of Mannose Receptor/3-So4-Lewis(X)	1.90
317	1fzj	Mhc Class I Natural Mutant H-2Kbm1 Heavy Chain/VSV8	1.90
318	1g98	Phosphoglucose Isomerase/5-Phosphoarabinonate	1.90
319	1gcz	Macrophage Migration Inhibitory Factor/Coumarin Analogue	1.90
320	1gjb	Urokinase-Type Plasminogen Activator/APC-7806	1.90
321	1gui	Laminarinase 16A/Oligosaccharide	1.90
322	1hpv	HIV-1 Protease /C(2) Symmetry-Based Diol Inhibitor	1.90
323	1hsh	HIV-1 Protease/L-735,524	1.90
324	1is0	Tyrosine-Protein Kinase Transforming Protein Src/ 1,2,3-Trisubstituted Cyclopropane	1.90
325	1izh	HIV Proteinase/Inhibitor QF34 Glucose-6-Phosphate Isomerase/	1.90
326	1koj	5-Phospho-D-Arabinonohydroxamic Acid	1.90
327	1lan	Leucine Aminopeptidase /2-Methyl-2,4-Pentanediol	1.90
328	1lee	Plasmepsin /Inhibitor Rs367	1.90
329	1los	Orotidine Monophosphate Decarboxylase/6-Azaump	1.90
330	1lrh	Auxin-Binding Protein 1/1-Naphthalene Acetic Acid Pleckstrin Homology Domain From Phospholipase C /	1.90
331	1mai	Inositol Trisphosphate	1.90
332	1mdq	Maltodextrin-Binding Protein (A301Gs)/Maltose	1.90
333	1mmq	Matrilysin/Hydroxamate Inhibitor	1.90
334	1pph	Trypsin/3-Tapap	1.90
335	1qk4	Hypoxanthine-Guanine Phosphoribosyltransferase/Inosinic Acid	1.90
336	1rdm	Mannose-Binding Protein, Subtilisin Digest Fragment /	1.90

		O1-Methyl-Mannose	
337	1rnb	Barnase (G Specific Endonuclease) /Deoxy-Dinucleotide Inhibitor	1.90
338	1rnt	Ribonuclease T1/2'-Guanylic Acid	1.90
339	1sle	Streptavidin/Cyclic Peptide Ac-Chpqgppc-Nh2	1.90
340	1swr	Core-Streptavidin Mutant W120A /Biotin	1.90
341	1tmn	Thermolysin/N-carboxymethyl dipeptide inhibitor	1.90
342	1tni	Trypsin/4-Phenylbutylamine	1.90
343	1tnl	Trypsin /Tranlycypromine	1.90
		Carbonic Anhydrase II Mutant /	
344	1ydb	Transition State Analogue Acetazolamide	1.90
345	1yei	Ig Antibody D2.3/TSA	1.90
346	2ak3	Adenylate Kinase Isoenzyme-3/AMP	1.90
347	2bpv	HIV-1 Protease/L-738,317	1.90
348	2bpy	HIV-1 Protease/L-739,622	1.90
349	2bza	Trypsin/Benzylamine	1.90
350	2drc	Dihydrofolate Reductase Mutant W22F/Methotrexate	1.90
351	2gbp	D-GalactoseD-glucose binding protein (GGBP)/Glucose	1.90
352	2h4n	Carbonic Anhydrase II/Acetazolamide	1.90
353	2qwf	Neuraminidase/Neu5Ac2en analogue	1.90
354	3gst	Glutathione S-Transferase /(9R,10R)-addition product	1.90
355	3tpi	Trypsinogen/Pancreatic Trypsin Inhibitor	1.90
356	7tim	Triosephosphate Isomerase /Phosphoglycolohydroxamate	1.90
357	8xia	D-Xylose Isomerase /D-Xylose	1.90
358	966c	Mmp-1/Diphenyl-Ether Sulphone Based Hydroxamic Acid	1.90
359	1fjs	Coagulation Factor Xa/Zk-807834	1.92
360	1i9p	Carbonic Anhydrase II Mutant F131V/2,4,6-trifluoro-SBB	1.92
361	1vwf	Streptavidin/Cyclo-Ac-[Chpqgppc]-Nh2 Monomer	1.92
362	1k22	Thrombin/Melagatran	1.93

363	1g53	Carbonic Anhydrase II/2,6-difluoro-SBB	1.94
		Carbonic Anhydrase II/ (S)-N-(3-Indol-1-yl-2- Methyl-Propyl)-4-Sulfamoyl- Benzamide	1.94
364	1if8		
365	1inc	Porcine Pancreatic Elastase /Benzoxazinone Inhibitor	1.94
366	1l2s	β -Lactamase/A Dock-Predicted Non-Covalent Inhibitor	1.94
367	1wdn	Glutamine Binding Protein/glutamine	1.94
368	1ax1	Lectin/Lactose	1.95
369	1ax2	Lectin/N-acetyllactosamine	1.95
370	1axz	Lectin/D-Galactose	1.95
371	1e1v	Cyclin-Dependent Protein Kinase 2/6-O-Cyclohexylmethyl Guanine Protein-Tyrosine Phosphatase 1B/	1.95
372	1ecv	5-Iodo-2-(Oxalyl-Amino)-Benzoic Acid	1.95
373	1f73	N-Acetyl Neuraminase Lyase/Sialic Acid Alditol	1.95
374	1fh8	β -1,4-Xylanase/Isosfagomine Inhibitor	1.95
375	1fkh	Fk506 Binding Protein /Rotamase Inhibitor	1.95
376	1g2k	Protease Retropepsin/Cyclic Sulfamide Inhibitor Aha047	1.95
377	1gaf	Chimeric 48G7 Fab/transition State Analogue	1.95
378	1m48	Interleukin-2/nonpeptidyl small molecule IL-2 ligand	1.95
379	1sm3	Sm3 Antibody/sm3 Peptide Epitope	1.95
380	1sts	Streptavidin/Disulfide-Bonded Peptide Fchpqt-Nh2 Dimer	1.95
381	5std	Scytalone Dehydratase/SD Inhibitor 2	1.95
382	1g4o	Carbonic Anhydrase II Mutant F131V/SBB	1.96
383	1gar	Glycinamide Ribonucleotide Transformylase /1476U89	1.96
384	3pcg	Protocatechuate 3,4-Dioxygenase/Inhibitor Hydroxyphenylacetate	4- 1.96
385	1d4y	HIV-1 Protease/Tipranavir	1.97
386	9abp	L-Arabinose-Binding Protein Mutant P254G/D-Galactose	1.97
387	1c1v	Thrombin/Bis(5-Amidino-2- Benzimidazolyl)Methane	1.98

388	1if7	Carbonic Anhydrase II/Benzamide Derivative	1.98
389	3pcc	Protocatechuate 3,4-Dioxygenase/4-Hydroxybenzoate	1.98
390	4tmk	Thymidylate Kinase/Inhibitor Tp5A	1.98
391	5tmp	Thymidylate Kinase/Inhibitor Aztp5A	1.98
392	1hpx	HIV-1 Protease/KNI-272	2.00