Supplementary Data

Figure S1: RMSD values of the sites occurring in the cluster 3C1H-1.

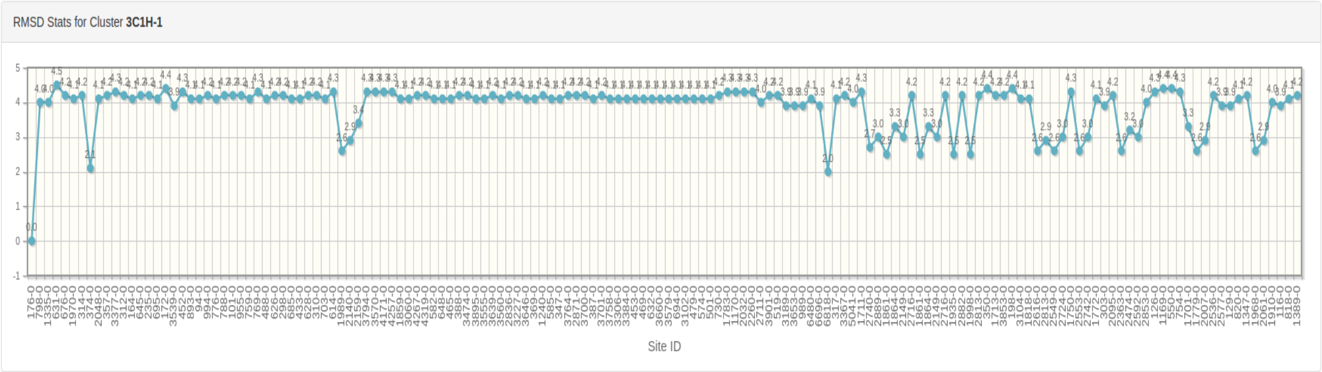


Figure S1: The Y-axis the RMSD values are shown and in the X-axis the ID of the sites that are part of the cluster 3C1H-1 are listed (full results https://appsbio.utalca.cl/3d-pp/results/1556639834.1218/).

Figure S2: Sites detected that correspond to the Cadmium ion binding site of the chain A and B of the PDBid:4c3d.

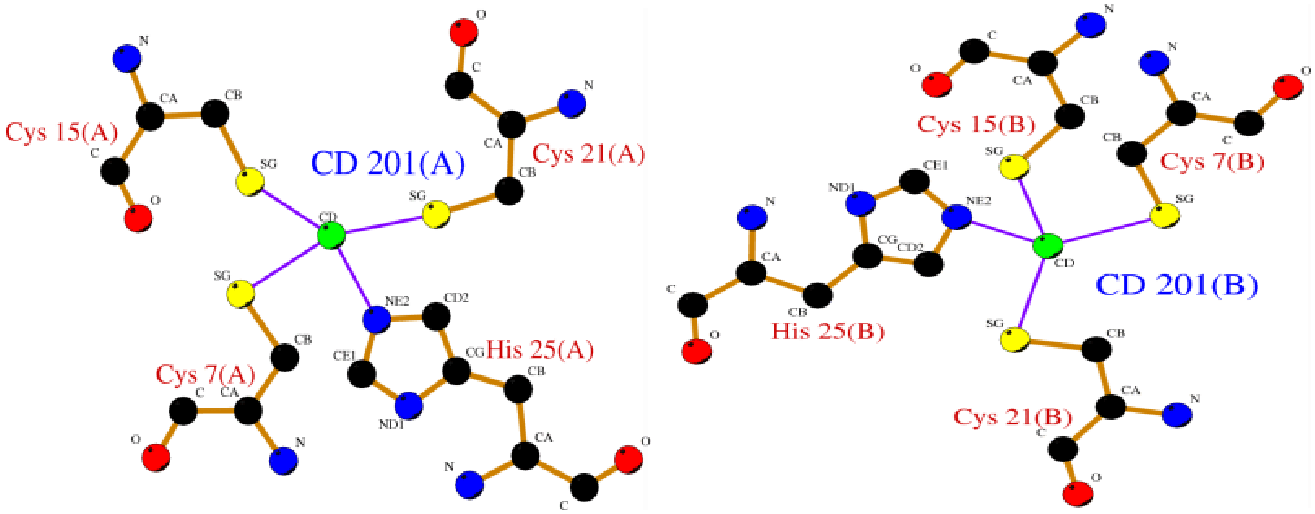
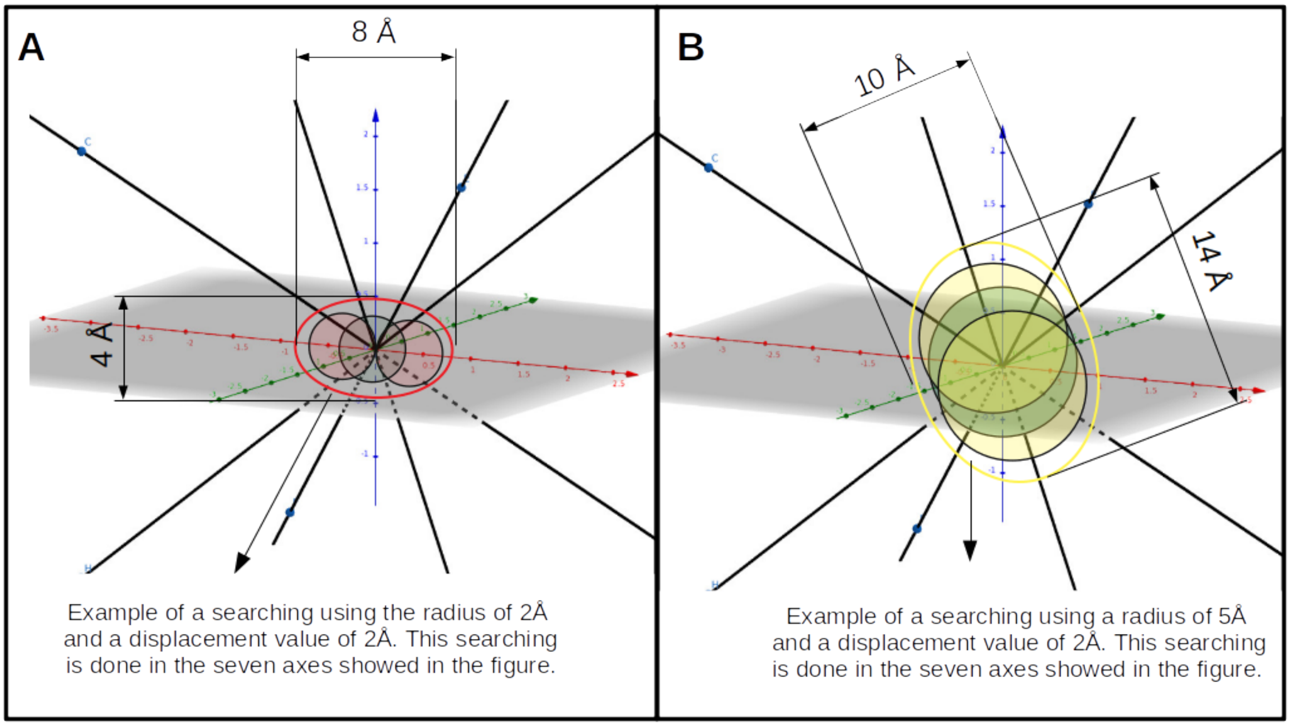


Figure S2: Two green spheres represent the Cadmium ions which are being coordinated by the residues present at the new sites discovered by 3D-PP (images obtained from PDBsum).

Figure S3: Representation of the expanded searching method implemented on 3D-PP to find non-spherical 3D-patterns.

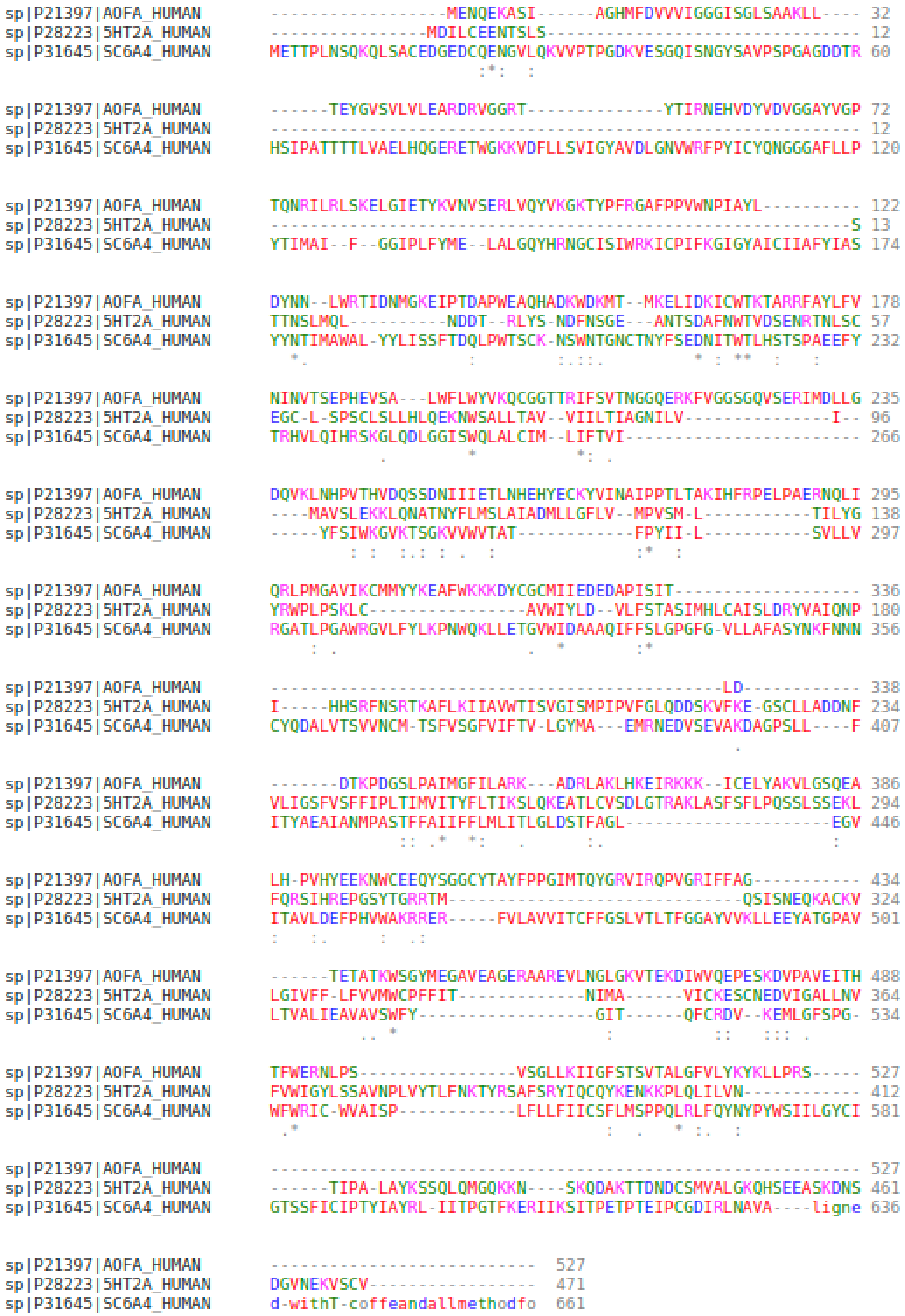


Example of a searching using the radius of 2Å and a displacement value of 2Å. This searching is done in the seven axes showed in the figure.

Example of a searching using a radius of 5Å and a displacement value of 2Å. This searching is done in the seven axes showed in the figure.

Figure S3: For both cases, A and B, the translucent green sphere represents the center of the searching space for each dummy atom of the Virtual Grid of Coordinates. By default, the search only considers spherical 3D-patterns on that space, but if the user changes the “Displacement threshold” parameter, seven different searching spaces are used for the analysis. In the Figure two examples of “Displacement threshold” values are depicted. Example A shows an elliptical shape of searching, whereas example B shows an oval shape of searching.

Figure S4: Multiple sequence alignment among SERT, MAO-A and 5-HTR2a



```
sp|P21397|AOFA_HUMAN       ------------------MENQEKASI------AGHMFDVVVIGGGISGLSAAKLL---- 32
sp|P28223|5HT2A_HUMAN      ----------------MDILCEENTSLS-------------------------------- 12
sp|P31645|SC6A4_HUMAN      METTPLNSQKQLSACEDGEDCQENGVLQKVVPTPGDKVESGQISNGYSAVPSPGAGDDTR 60
                                                :*:  :

sp|P21397|AOFA_HUMAN       ------TEYGVSVLVLEARDRVGGRT--------------YTIRNEHVDYVDVGGAYVGP 72
sp|P28223|5HT2A_HUMAN      ------------------------------------------------------------ 12
sp|P31645|SC6A4_HUMAN      HSIPATTTTLVAELHQGERETWGKKVDFLLSVIGYAVDLGNVWRFPYICYQNGGGAFLLP 120


sp|P21397|AOFA_HUMAN       TQNRILRLSKELGIETYKVNVSERLVQYVKGKTYPFRGAFPPVWNPIAYL---------- 122
sp|P28223|5HT2A_HUMAN      -----------------------------------------------------------S 13
sp|P31645|SC6A4_HUMAN      YTIMAI--F--GGIPLFYME--LALGQYHRNGCISIWRKICPIFKGIGYAICIIAFYIAS 174


sp|P21397|AOFA_HUMAN       DYNN--LWRTIDNMGKEIPTDAPWEAQHADKWDKMT--MKELIDKICWTKTARRFAYLFV 178
sp|P28223|5HT2A_HUMAN      TTNSLMQL----------NDDT--RLYS-NDFNSGE---ANTSDAFNWTVDSENRTNLSC 57
sp|P31645|SC6A4_HUMAN      YYNTIMAWAL-YYLISSFTDQLPWTSCK-NSWNTGNCTNYFSEDNITWTLHSTSPAEEFY 232
                             *.                :        :.::.         * : **  :   :

sp|P21397|AOFA_HUMAN       NINVTSEPHEVSA---LWFLWYVKQCGGTTRIFSVTNGGQERKFVGGSGQVSERIMDLLG 235
sp|P28223|5HT2A_HUMAN      EGC-L-SPSCLSLLHLQEKNWSALLTAV--VIILTIAGNILV---------------I-- 96
sp|P31645|SC6A4_HUMAN      TRHVLQIHRSKGLQDLGGISWQLALCIM--LIFTVI------------------------ 266
                                      .        *          *: .

sp|P21397|AOFA_HUMAN       DQVKLNHPVTHVDQSSDNIIIETLNHEHYECKYVINAIPPTLTAKIHFRPELPAERNQLI 295
sp|P28223|5HT2A_HUMAN      ----MAVSLEKKLQNATNYFLMSLAIADMLLGFLV--MPVSM-L-----------TILYG 138
sp|P31645|SC6A4_HUMAN      -----YFSIWKGVKTSGKVVWVTAT------------FPYII-L-----------SVLLV 297
                                   : :  :.: : .  :              :*  :

sp|P21397|AOFA_HUMAN       QRLPMGAVIKCMMYYKEAFWKKKDYCGCMIIEDEDAPISIT------------------- 336
sp|P28223|5HT2A_HUMAN      YRWPLPSKLC----------------AVWIYLD--VLFSTASIMHLCAISLDRYVAIQNP 180
sp|P31645|SC6A4_HUMAN      RGATLPGAWRGVLFYLKPNWQKLLETGVWIDAAAQIFFSLGPGFG-VLLAFASYNKFNNN 356
                               : .                   .  *       :*

sp|P21397|AOFA_HUMAN       ----------------------------------------------LD------------ 338
sp|P28223|5HT2A_HUMAN      I-----HHSRFNSRTKAFLKIIAVWTISVGISMPIPVFGLQDDSKVFKE-GSCLLADDNF 234
sp|P31645|SC6A4_HUMAN      CYQDALVTSVVNCM-TSFVSGFVIFTV-LGYMA---EMRNEDVSEVAKDAGPSLL----F 407
                                                                          .

sp|P21397|AOFA_HUMAN       -------DTKPDGSLPAIMGFILARK---ADRLAKLHKEIRKKK--ICELYAKVLGSQEA 386
sp|P28223|5HT2A_HUMAN      VLIGSFVSFFIPLTIMVITYFLTIKSLQKEATLCVSDLGTRAKLASFSFLPQSSLSSEKL 294
sp|P31645|SC6A4_HUMAN      ITYAEAIANMPASTFFAIIFFLMLITLGLDSTFAGL---------------------EGV 446
                                        :: .*  *:   .      :.                       :

sp|P21397|AOFA_HUMAN       LH-PVHYEEKNWCEEQYSGGCYTAYFPPGIMTQYGRVIRQPVGRIFFAG----------- 434
sp|P28223|5HT2A_HUMAN      FQRSIHREPGSYTGRRTM------------------------------QSISNEQKACKV 324
sp|P31645|SC6A4_HUMAN      ITAVLDEFPHVWAKRRER-----FVLAVVITCFFGSLVTLTFGGAYVVKLLEEYATGPAV 501
                           :   :.     :  .:

sp|P21397|AOFA_HUMAN       ------TETATKWSGYMEGAVEAGERAAREVLNGLGKVTEKDIWVQEPESKDVPAVEITH 488
sp|P28223|5HT2A_HUMAN      LGIVFF-LFVVMWCPFFIT-------------NIMA------VICKESCNEDVIGALLNV 364
sp|P31645|SC6A4_HUMAN      LTVALIEAVAVSWFY------------------GIT------QFCRDV--KEMLGFSPG- 534
                                    .. *                     :          ::   ::: .

sp|P21397|AOFA_HUMAN       TFWERNLPS----------------VSGLLKIIGFSTSVTALGFVLYKYKLLPRS----- 527
sp|P28223|5HT2A_HUMAN      FVWIGYLSSAVNPLVYTLFNKTYRSAFSRYIQCQYKENKKPLQLILVN------------ 412
sp|P31645|SC6A4_HUMAN      WFWRIC-WVAISP------------LFLLFIICSFLMSPPQLRLFQYNYPYWSIILGYCI 581
                            .*                               :  .   * :.  :

sp|P21397|AOFA_HUMAN       ------------------------------------------------------------ 527
sp|P28223|5HT2A_HUMAN      ------TIPA-LAYKSSQLQMGQKKN----SKQDAKTTDNDCSMVALGKQHSEEASKDNS 461
sp|P31645|SC6A4_HUMAN      GTSSFICIPTYIAYRL-IITPGTFKERIIKSITPETPTEIPCGDIRLNAVA----ligne 636


sp|P21397|AOFA_HUMAN       ---------------------------   527
sp|P28223|5HT2A_HUMAN      DGVNEKVSCV-----------------   471
sp|P31645|SC6A4_HUMAN      d-withT-coffeandallmethodfo   661
```

Figure S4: In the figure S4 are shown the results of the multiple sequence alignment among the serotonin target proteins evaluated. Only 15 residues are conserved (*).

Figure S5: Implemented architecture and essential components and services of 3D-PP.

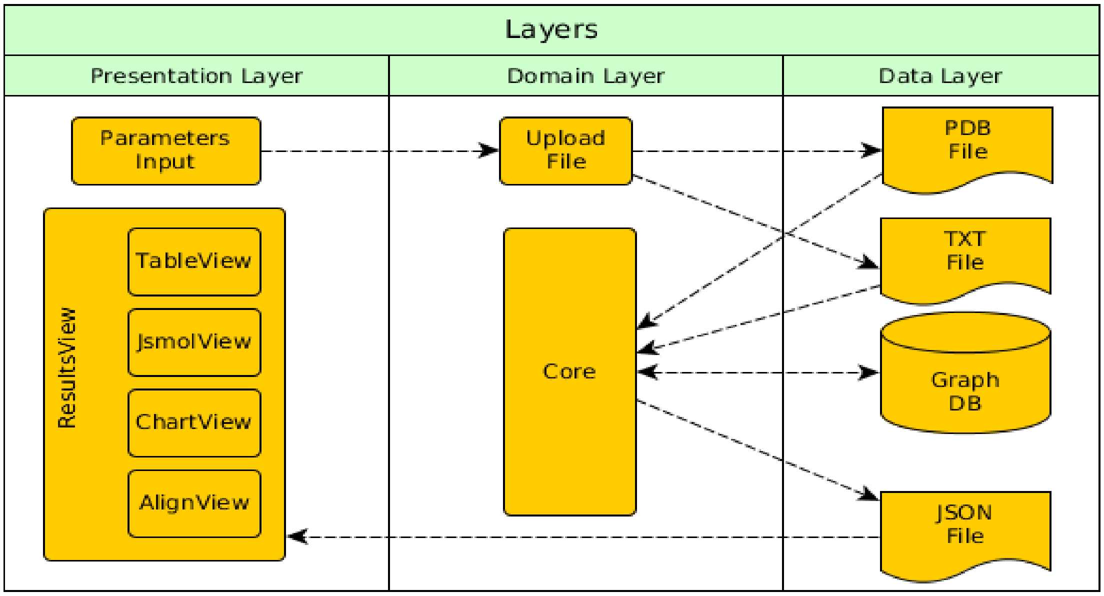


Figure S5: The architecture consists of three main layers: the presentation, domain and data layers, representing the interaction between the essential components of the solution.

This representation is divided into three main layers: the presentation, the domain, and the data layers. I) The presentation layer represents the user's view and the interaction with the domain layer. It consists of two modules: first, ParametersInput which is responsible for obtaining the necessary data to compute the request (Homology model files or PDBids). The second module is the ResultsView, which is composed of the following items: a) a chart showing the frequency of each 3D-pattern discovered (ChartView), b) data tables showing all clusters that belong to each 3D-pattern and all sites that reside into each cluster (TableView), c) a 3D viewer for the structural visualization of the 3D-patterns (JsmolView), d) a picture showing the sequence-based alignment of the sites forming each 3D-pattern (AlignView), e) a graph showing the RMSD of the sites of a cluster. II) The domain layer represents the core of 3D-PP and denotes the communication link between the presentation and data layers. This layer has the following components: a) UploadFile for uploading the file with the PDBids or the homology models delivered by the user, b) Core, for the processing of each protein, the discovering of 3D-patterns and cluster generation, the creation of graph databases, the preparation in JSON format of the results. III) The data layer has three components which are responsible for store the data: a) the PDBFile represents the protein structures under analysis, b) the GraphDB stores all information generated in the Domain Layer, c) the JSONFile contains the processed results of 3D-PP. This component delivers the results to the ResultsView of the Presentation layer.

Figure S6: Graph Database Models.

A

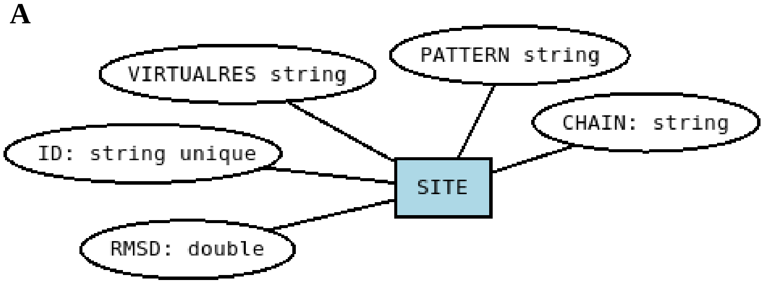


Figure S6A: The model of the graph database implemented for each protein processed.

B

.

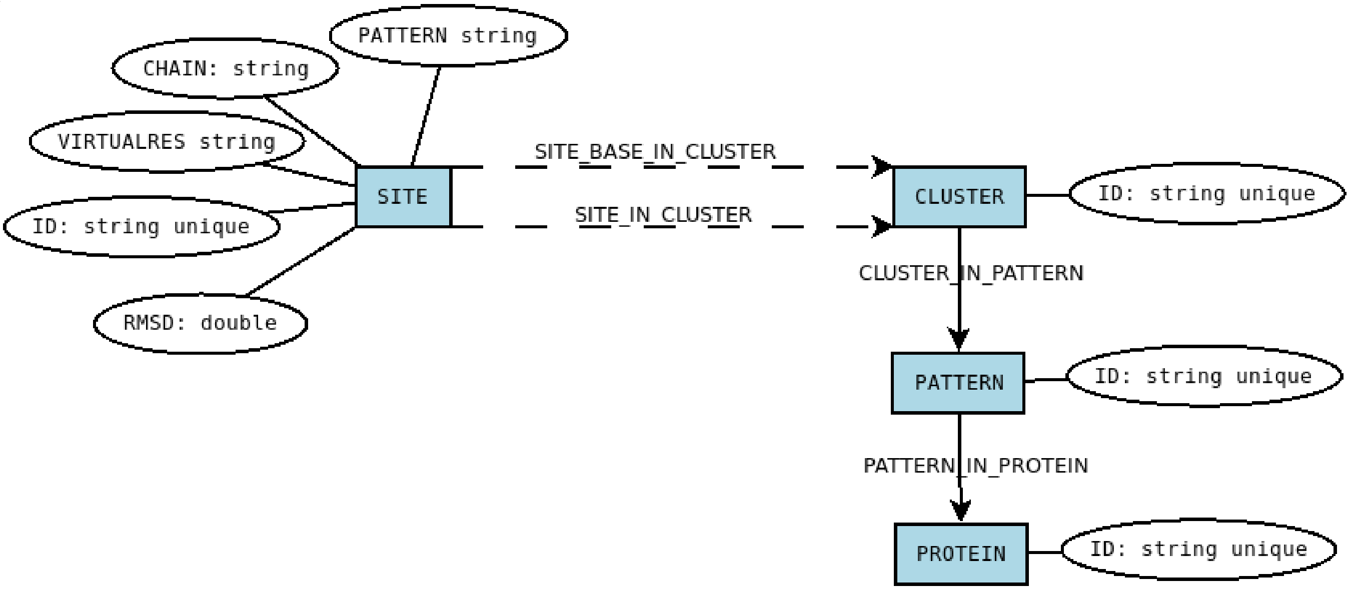


Figure S6B: The graph database model that unifies all the sites found in all proteins.

Table S1: Comparative table showing the occurrence of sites in the original protein structure (pdbSUM), in the primary sequence (C-x(8)-C-x(5)-C-x(3)-H) and in the results obtained with 3D-PP.

PDBid	Resolution	Pos.	Sequence C-x(8)-C-x(5)-C-x(3)-H	Fasta from PDB	Site PDB (3D-PP)	pdbSUM	Seq.	3d-pp	Pdb SUM (LigPlot	Comments
1M9O	N/A	95 – 123	RYKTELCRTYSESGRCRYGAKCQFAHGLG	A:GSHMTTSSRYKTELCRTYSESGRCRYGAKCQFAHGLGELRQANRHPKYKTELCHKFKLQGRCPYGSRCHFIHNPTED	A:CYS15:CYS24:CYS30:HIS34	A:CYS15:CYS24:CYS30:HIS34	Yes	Yes	Yes	
1RGO	N/A	153 – 181	RYKTELCRPFEESGTCKYGEKCQFAHGFH	A:STRYKTELCRPFEESGTCKYGEKCQFAHGFHELRSLTRHPKYKTELCRTFHTIGFCPYGPRCHFIHNADE	A:CYS159:CYS168:CYS174:HIS178	A:CYS159:CYS168:CYS174:HIS178	Yes	Yes	Yes	
		191 – 219	KYKTELCRTFHTIGFCPYGPRCHFIHNAD		A:CYS197:CYS206:CYS212:HIS216	A:CYS197:CYS206:CYS212:HIS216	Yes	Yes	Yes	
2CQE	N/A	419 – 446	PKKRELCKFYITGFCARAENCPYMHGDF	A:GSSGSSGELPKKRELCKFYITGFCARAENCPYMHGDFPCKLYHTTGNCINGDDCMFSHDPLTEETRELLDKMLADDAEAGAEDEKEVEELKKSGPSSG	A:CYS437:CYS445:CYS451:HIS455	A:CYS437:CYS445:CYS451:HIS455	Yes	Yes	Yes	
		447 – 470	PCKLYHTTGNCINGDDCMFSHDPL		A:CYS460:CYS469:CYS475:HIS479	A:CYS460:CYS469:CYS475:HIS479	Yes	Yes	Yes	
2D9M	N/A	906 – 928	ICDRYMNGTCPEGNSCKFAHGNA	A:GSSGSSGQYCWQHRFPTGYFSICDRYMNGTCPEGNSCKFAHGNAELHEWEERRDALKMKLNKASGPSSG	A:CYS907:CYS915:CYS921:HIS925	A:CYS907:CYS915:CYS921:HIS925	Yes	Yes	Yes	
2D9N	N/A	62 – 89	GEKTVVCKHWLRGLCKKGDQCEFLHEYD	A:GSSGSSGEKTVVCKHWLRGLCKKGDQCEFLHEYDMTKMPECYFYSKFGECSNKECPFLHIDPESKIKDCPWSGPSSG	A:CYS68:CYS76:CYS82:HIS70	X	No	Yes	No	New site.
		90 – 117	MTKMPECYFYSKFGECSNKECPFLHIDP		A:CYS68:CYS76:CYS82:HIS86	A:CYS68:CYS76:CYS82:HIS86	Yes	Yes	Yes	
					A:CYS105:CYS110:CYS96:HIS114	A:CYS96:CYS105:CYS110:HIS114	Yes	Yes	Yes	
2E5S	N/A	176 – 204	TDKLEVCREFQRGNCARGETDCRFAHPAD	A:GSSGSSGSTATQKLLRTDKLEVCREFQRGNCARGETDCRFAHPADSTMIDTSDNTVTVCMDYIKGRCMREKCKYFHPPAHLQAKIKAAQHQANQAAVA	A:CYS23:CYS31:CYS38:HIS42	A:CYS23:CYS31:CYS38:HIS42	Yes	Yes	Yes	
		212 – 238	DNTVTVCMDYIKGRCMREKCKYFHPPA		A:CYS59:CYS67:CYS72:HIS76	A:CYS59:CYS67:CYS72:HIS76	Yes	Yes	Yes	
2FC6	N/A	294 – 322	PHPTSICDNFSAYGWCPLGPQCPQSHDID	A:GSSGSSGCCLPPATHRPHPTSICDNFSAYGWCPLGPQCPQSHDISGPSSG	A:CYS23:CYS32:CYS38:HIS42	A:CYS23:CYS32:CYS38:HIS42	Yes	Yes	Yes	

2RHK	1.95 A	62 – 89	GEKTVVCKHWLRGLCKKGDQCEFLHEYD	C:MGHHHHHHSHMSGEKTVVCKHWLRGLCKKGDQCEFLHEYDMTKMSECYFYSKFGECSNKECPFLHIDPESKI D:MGHHHHHHSHMSGEKTVVCKHWLRGLCKKGDQCEFLHEYDMTKMSECYFYSKFGECSNKECPFLHIDPESKI	C:CYS105:CYS110:CYS96:HIS114	C:CYS96:CYS105:CYS110:HIS114	Yes	Yes	Yes	
		90 – 117	MTKMPECYFYSKFGECSNKECPFLHIDP		C:CYS68:CYS76:CYS82:HIS86	C:CYS68:CYS76:CYS82:HIS86	Yes	Yes	Yes	
					D:CYS105:CYS110:CYS96:HIS114	D:CYS96:CYS105:CYS110:HIS114	Yes	Yes	Yes	
					D:CYS68:CYS76:CYS82:HIS86	D:CYS68:CYS76:CYS82:HIS86	Yes	Yes	Yes	
2RPP	N/A	13 – 41	WLTLEVCRQFQRGTCSRSDEECKFAHPPK	A:GSSGSSGPVRDTKWLTLEVCRQFQRGTCSRSDEECKFAHPPKSCQVENGRVIACFDSLKGRCSRENCKYLHPPTHLKTQLEINSGPSSG	A:CYS26:CYS34:CYS41:HIS45	A:CYS26:CYS34:CYS41:HIS45	Yes	Yes	Yes	
		47 – 73	NGRVIACFDSLKGRCSRENCKYLHPPT		A:CYS60:CYS68:CYS73:HIS77	A:CYS60:CYS68:CYS73:HIS77	Yes	Yes	Yes	
3D2N	2.7A	13 – 41	WLTLEVCREFQRGTCSRPDTECKFAHPSK	A:SRDTKWLTLEVCREFQRGTCSRPDTECKFAHPSKSCQVENGRVIACFDSLKGRCSRENCKYLHPPPHLKTQLEINGRNNLIQQ	A:CYS19:CYS27:CYS34:HIS38	A:CYS19:CYS27:CYS34:HIS38	Yes	Yes	Yes	
		47 – 73	NGRVIACFDSLKGRCSRENCKYLHPPP		A:CYS53:CYS61:CYS66:HIS70	A:CYS53:CYS61:CYS66:HIS70	Yes	Yes	Yes	
3D2Q	1.5A	179 – 207	TDRLEVCREYQRGNCNRGENDCRFAHPAD	A:SRTDRLEVCREYQRGNCNRGENDCRFAHPADSTMIDTNDNTVTVCMDYIKGRCSREKCKYFHPPAHLQAK B:SRTDRLEVCREYQRGNCNRGENDCRFAHPADSTMIDTNDNTVTVCMDYIKGRCSREKCKYFHPPAHLQAK C:SRTDRLEVCREYQRGNCNRGENDCRFAHPADSTMIDTNDNTVTVCMDYIKGRCSREKCKYFHPPAHLQAK D:SRTDRLEVCREYQRGNCNRGENDCRFAHPADSTMIDTNDNTVTVCMDYIKGRCSREKCKYFHPPAHLQAK	A:CYS185:CYS193:CYS200:HIS204 A:CYS221:CYS229:CYS234:HIS238	A:CYS185:CYS193:CYS200:HIS204 A:CYS221:CYS229:CYS234:HIS238	Yes	Yes	Yes	
		215 – 241	DNTVTVCMDYIKGRCSREKCKYFHPPA		B:CYS185:CYS193:CYS200:HIS204 B:CYS221:CYS229:CYS234:HIS238	B:CYS185:CYS193:CYS200:HIS204 B:CYS221:CYS229:CYS234:HIS238	Yes	Yes	Yes	
					C:CYS185:CYS193:CYS200:HIS204 C:CYS221:CYS229:CYS234:HIS238	C:CYS185:CYS193:CYS200:HIS204 C:CYS221:CYS229:CYS234:HIS238	Yes	Yes	Yes	
					D:CYS185:CYS193:CYS200:HIS204 D:CYS221:CYS229:CYS234:HIS238	D:CYS185:CYS193:CYS200:HIS204 D:CYS221:CYS229:CYS234:HIS238	Yes	Yes	Yes	
3D2S	1.7A	179 – 207	TDRLEVCREYQRGNCNRGENDCRFAHPAD	A:SRTDRLEVCREYQRGNCNRGENDCRFAHPADSTMIDTNDNTVTVCMDYIKGRCSREKCKYFHPPAHLQAK	A:CYS185:CYS193:CYS200:HIS204 A:CYS221:CYS229:CYS234:HIS238	A:CYS185:CYS193:CYS200:HIS204 A:CYS221:CYS229:CYS234:HIS238	Yes	Yes	Yes	
		215 –	DNTVTVCMDYIKGRCSREKCKYFHPPA		B:CYS185:CYS193:CYS200:HIS204 B:CYS221:CYS229:CYS234:HIS238	B:CYS185:CYS193:CYS200:HIS204 B:CYS221:CYS229:CYS234:HIS238	Yes	Yes	Yes	

		241		B:SRTDRLEVCREYQRGNCNRGENDCRFAHPADSTMIDTNDNTVTVCMDYIKGRCSREKCKYFHPPAHLQAK C:SRTDRLEVCREYQRGNCNRGENDCRFAHPADSTMIDTNDNTVTVCMDYIKGRCSREKCKYFHPPAHLQAK D:SRTDRLEVCREYQRGNCNRGENDCRFAHPADSTMIDTNDNTVTVCMDYIKGRCSREKCKYFHPPAHLQAK	C:CYS185:CYS193:CYS200:HIS204 C:CYS221:CYS229:CYS234:HIS238	C:CYS185:CYS193:CYS200:HIS204 C:CYS221:CYS229:CYS234:HIS238	Yes	Yes	Yes	
					D:CYS185:CYS193:CYS200:HIS204 D:CYS221:CYS229:CYS234:HIS238	D:CYS185:CYS193:CYS200:HIS204 D:CYS221:CYS229:CYS234:HIS238	Yes	Yes	Yes	
3JB9	3.6A	111 – 138	NPGSFFCLYFARGMCSEGSKCEYLHRLP	Y:MSENGLEQEVTVEEKNNDVTEKILVEGEKSKEYEETPRKVKIVKRKKQPARKQIETRPEYEMEPEQPGQVYNLWYNKWSGGMRQDPLKSQVKSETRCVISRDSGYTKADKNPGSFFCLYFARGMCSEGSKCEYLHRLPKDTDFFNANVDCFGREKHADYRDDMGGVGSFLRQNYTLYVGGITPTDDIEEIVSRHFAEWGDIERIRVLNSRGIAFITYLNEANAQFAKEAMAHQSLDHDECLNVRWATTDPNPASQARNQRRLEERAANAVKKLLPKQFLLDLEETKNGKXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX	e:CYS102:CYS105:CYS137:HIS136	X	No	Yes	No	New site.
					e:CYS105:CYS117:CYS134:HIS136	X	No	Yes	No	New site.
					e:CYS105:CYS134:CYS137:HIS136	X	No	Yes	No	New site.
					Y:CYS117:CYS125:CYS131:HIS135	Y:CYS117:CYS125:CYS131:HIS135	Yes	Yes	Yes	
3TP2	2.4A	67 – 94	DGQLFFCLFFAKGMCCLGPKCEYLHHIP	A:GAMTSWRDKSAKVQVKESELPSSIPAQTGLTFNIWYNKWSQGFAGNTRFVSPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEVLDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFS	A:CYS73:CYS81:CYS87:HIS91	A:CYS73:CYS81:CYS87:HIS91	Yes	Yes	Yes	
					B:CYS73:CYS81:CYS87:HIS91	B:CYS73:CYS81:CYS87:HIS91	Yes	Yes	Yes	

				RLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQTLLLPSDKEWDDRREGTGLLVKWAN B:GAMTSWRDKSAKVQVKESELPSSIPAQTGLTFNIWYNKWSQGFAGNTRFVSPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEVLDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFSRLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQTLLLPSDKEWDDRREGTGLLVKWAN						
3U1L	1.64 A	67 – 94	DGQLFFCLFFAKGMCCLGPKCEYLHHIP	A:MTSWRDKSAKVQVKESELPSSIPAQTGLTFNIWYNKWSQGFAGNTRFVSPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEVLDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFSRLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQTLLLPSDKEWDDRREGTGLLVKWANEDPDPAAQKRLQE	A:CYS73:CYS81:CYS87:HIS91	A:CYS73:CYS81:CYS87:HIS91	Yes	Yes	Yes	
3U1M	1.95 A	67 – 94	DGQLFFCLFFAKGMCCLGPKCEYLHHIP	A:MTSWRDKSAKVQVKESELPSSIPAQTGLTFNIWYNKWSQGFAGNTRFVSPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEVLDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFSRLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQTLLLPSDKEWDDRREGTGLLVKWANEDPDPAAQKRLQE	A:CYS73:CYS81:CYS87:HIS91	A:CYS73:CYS81:CYS87:HIS91	Yes	Yes	Yes	
3U	1.8A	73 – 86	CRRKYCQRPCDSLH	A:GPLGMADPGVCCFITKILCAHGGRMTLEELLG	A:CYS106:CYS88:CYS96:HIS110	A:CYS106:CYS88:CYS96:HIS110	Yes	Yes	Yes	

9G		88 – 110	CKLNLLGRCHYAQSQRNLCKYSH	EIRLPEAQLYELLETAGPDRFVLLETGGQAGITRSVVATTRARVCRRKYCQRPCDSLHLCKLNLLGRCHYAQSQRNLCKYSHDVLSEQNFQILKNHELSGLNQEELACLLVQSDPFFLPEICKSYKGEGRKQTCGQPQPCERLHICEHFTRGNCSYLNCLRSHNLMDRKVLTIMREHGLSPDVVQNIQDICNNKHAR	A:CYS73:CYS78:CYS82:HIS86	A:CYS73:CYS78:CYS82:HIS86	Yes	Yes	Yes	
		150 – 172	CKSYKGEGRKQTCGQPQPCERLH		A:CYS174:CYS182:CYS187:HIS191	A:CYS174:CYS182:CYS187:HIS191	Yes	Yes	Yes	
		169 – 193	ERLHICEHFTRGNCSYLNCLRSHNL		A:CYS150:CYS162:CYS168:HIS172	A:CYS150:CYS162:CYS168:HIS172	Yes	Yes	Yes	
4C3B	2.95 A	1 – 28	MSRRNPCKFEIRGHCLNGKRCHFSHNYF	A:B:C:D:E:F:G:H:I:J:K:L:M:N:O:P GPLGSMSRRNPCKFEIRGHCLNGKRCHFSHNYFEWPPHALLVRQNFMLNRILKSMDKSIDTLSEISGAAELDRTEEYALGVVGVLESYIGSINNITKQSACVAMSKLLTELNSDDIKKLRDNEELNSPKIRVYNTVISYIESNRKNNKQTIHLLKRLPADVLKKTIKNTLDIHKSITINNPKESTVSDTNDHAKNNDTT	A:CYS15:CYS21:CYS7:HIS25	A:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					B:CYS15:CYS21:CYS7:HIS25	B:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					C:CYS15:CYS21:CYS7:HIS25	C:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					D:CYS15:CYS21:CYS7:HIS25	D:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					E:CYS15:CYS21:CYS7:HIS25	E:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					F:CYS15:CYS21:CYS7:HIS25	F:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					G:CYS15:CYS21:CYS7:HIS25	G:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					H:CYS15:CYS21:CYS7:HIS25	H:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					I:CYS15:CYS21:CYS7:HIS25	I:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					J:CYS15:CYS21:CYS7:HIS25	J:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					K:CYS15:CYS21:CYS7:HIS25	K:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					L:CYS15:CYS21:CYS7:HIS25	L:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					M:CYS15:CYS21:CYS7:HIS25	M:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					N:CYS15:CYS21:CYS7:HIS25	N:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					O:CYS15:CYS21:CYS7:HIS25	O:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					P:CYS15:CYS21:CYS7:HIS25	P:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
4C3D	2.52 A	1 – 28	MSRRNPCKFEIRGHCLNGKRCHFSHNYF	A:GPLGSMSRRNPCKFEIRGHCLNGKRCHFSHNYFEWPPHALLVRQNFMLNRILKSMDKSIDTLSEISGAAELDRTEEYALGVVGVLESYIGSINNITKQSACVAMSKLLTELNSDDIKKLRDNEELNSPKIRVYNTVISYIESNRKNNKQTIHLLKRLPADVLKKTIKNTLDIHKSITINNPKESTVSDTNDHAKNNDTT B:GPLGSMSRRNPCKFEIRGHCLNGKRCHFSHNY	A:CYS15:CYS21:CYS7:HIS25	A:CYS15:CYS21:CYS7:HIS25 (not ZN → CD)	Yes	Yes	Yes	CD binding site.
					B:CYS15:CYS21:CYS7:HIS25	B:CYS15:CYS21:CYS7:HIS25 (not ZN → CD)	Yes	Yes	Yes	CD binding site.

				FEWPPHALLVRQNFMLNRILKSMDKSIDTLSEISGAAELDRTEEYALGVVGVLESYIGSINNITKQSACVAMSKLLTELNSDDIKKLRDNEELNSPKIRVYNTVISYIESNRKNNKQTIHLLKRLPADVLKKTIKNTLDIHKSITINNPKESTVSDTNDHAKNNDTT						
4C3E	2.4A	1 – 28	MSRRNPCKFEIRGHCLNGKRCHFSHNYF	A:B:C:D:E:F:G:H:I:J:K:L:M:NO:P GPLGSMSRRNPCKFEIRGHCLNGKRCHFSHNYFEWPPHALLVRQNFMLNRILKSMDKSIDTLDEIDGAAELDRTEEYALGVVGVLESYIGSINNITKQSACVAMSKLLTELNSDDIKKLRDNEELNSPKIRVYNTVISYIESNRKNNKQTIHLLKRLPADVLKKTIKNTLDIHKSITINNPKESTVSDTNDHAKNNDTT	A:CYS15:CYS21:CYS7:HIS25	A:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					B:CYS15:CYS21:CYS7:HIS25	B:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					C:CYS15:CYS21:CYS7:HIS25	C:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					D:CYS15:CYS21:CYS7:HIS25	D:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					E:CYS15:CYS21:CYS7:HIS25	E:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					F:CYS15:CYS21:CYS7:HIS25	F:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					G:CYS15:CYS21:CYS7:HIS25	G:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					H:CYS15:CYS21:CYS7:HIS25	H:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					I:CYS15:CYS21:CYS7:HIS25	I:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					J:CYS15:CYS21:CYS7:HIS25	J:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					K:CYS15:CYS21:CYS7:HIS25	K:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					L:CYS15:CYS21:CYS7:HIS25	L:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					M:CYS15:CYS21:CYS7:HIS25	M:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					N:CYS15:CYS21:CYS7:HIS25	N:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					O:CYS15:CYS21:CYS7:HIS25	O:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
					P:CYS15:CYS21:CYS7:HIS25	P:CYS15:CYS21:CYS7:HIS25	Yes	Yes	Yes	
4CYK	N/A	8 – 37	WAKDIPCRNITIYGYCKKEKEGCPFKHSDN	A:MDKINPDWAKDIPCRNITIYGYCKKEKEGCPFKHSDNTTAT	A:CYS14:CYS23:CYS30:HIS34	A:CYS14:CYS23:CYS30:HIS34	Yes	Yes	Yes	
4II1	2.65A	175 – 201	KSLKPCPFFLEGKCRFKENCRFSHGQV	A:B:C:D MHHHHHHSSGRENLYFQGEEEGEDEEELSGTKVSAPYYSSWGTLEYHNAMVVGTEEAEDGSAGVRVLYLYPTHKSLKPCPFF	A:CYS180:CYS188:CYS194:HIS198	A:CYS180:CYS188:CYS194:HIS198	Yes	Yes	Yes	
					B:CYS180:CYS188:CYS194:HIS198	B:CYS180:CYS188:CYS194:HIS198	Yes	Yes	Yes	
					C:CYS180:CYS188:CYS194:HIS198	C:CYS180:CYS188:CYS194:HIS198	Yes	Yes	Yes	
					D:CYS180:CYS188:CYS194:HIS198	D:CYS180:CYS188:CYS194:HIS198	Yes	Yes	Yes	

				LEGKCRFKENCRFSHGQVVSLDELRPFQDPDLSSLQAGSACLAKHQDGLWHAARITDVDNGYYTVKFDSLLLREAVVEGDGILPP						
4YH8	1.7A	12 – 40	EQDKVNCSFYYKIGACRHGERCSRKHVKP	A:MASHLASIYGTEQDKVNCSFYYKIGACRHGERCSRKHVKPNFSQTILCPNMYKNPIHEPNGKKFTQRELAEQFDAFYEDMFCEFSKYGEVEQLVVCDNVGDHLVGNVYVRFKYEESAQNAIDDLNSRWYSQRPVYAELSPVTDFREACCRQHETSECQRGGLCNFMHAKKPSPQLLRDLVLAQRKYLALNAAEEMKKEPNSDSTNRWVSVTAERKN	A:CYS149:CYS157:CYS163:HIS167	A:CYS149:CYS157:CYS163:HIS167	Yes	Yes	Yes	
		143 – 170	DFREACCRQHETSECQRGGLCNFMHAKK		A:CYS18:CYS27:CYS33:HIS37	A:CYS18:CYS27:CYS33:HIS37	Yes	Yes	Yes	
5ELH	1.8A	84 – 113	YSPDVYCTKYDEATGLCPEGDECPFLHRTT	A:SPQHYTYLKEFRTEQCPLFVQHKCTQHRPYTCFHWHFVNQRRRRSIRRDGTFNYSPDVYCTKYDEATGLCPEGDECPFLHRTTGDTERRYHLRYYKTGICIHETDSKGNCTKNGLHCAFAHGPHDLRSPVYDIRELQAMEALQN B:SPQHYTYLKEFRTEQCPLFVQHKCTQHRPYTCFHWHFVNQRRRRSIRRDGTFNYSPDVYCTKYDEATGLCPEGDECPFLHRTTGDTERRYHLRYYKTGICIHETDSKGNCTKNGLHCAFAHGPHDLRSPVYDIRELQAMEALQN	A:CYS130:CYS140:CYS147:HIS151	A:CYS130:CYS140:CYS147:HIS151	Yes	Yes	Yes	
		124 – 154	YYKTGICIHETDSKGNCTKNGLHCAFAHGPH		A:CYS100:CYS106:CYS90:HIS110	A:CYS100:CYS106:CYS90:HIS110	Yes	Yes	Yes	
					A:CYS45:CYS53:CYS61:HIS65	A:CYS45:CYS53:CYS61:HIS65	Yes	Yes	Yes	
					B:CYS130:CYS140:CYS147:HIS132	X	No	Yes	No	New site.
					B:CYS100:CYS106:CYS90:HIS110	B:CYS100:CYS106:CYS90:HIS110	Yes	Yes	Yes	
					B:CYS130:CYS140:CYS147:HIS151	B:CYS130:CYS140:CYS147:HIS151	Yes	Yes	Yes	
					B:CYS45:CYS53:CYS61:HIS65	B:CYS45:CYS53:CYS61:HIS65	Yes	Yes	Yes	
5ELK	2.3A	215 – 241	NYKTEPCKKPPRLCRQGYACPYYHNSK	A:SPRWQETAYVLGNYKTEPCKKPPRLCRQGYACPYYHNSKDRRRSPRKHKYRSSPCPNVKHGDEWGDPGKCENGDACQYCHTRTEQQFHPEIYKSTKCNDMQQAGSCPRGPFCAFAHIEPPPLSDDVQPSSAVS	A:CYS299:CYS308:CYS314:HIS318	A:CYS299:CYS308:CYS314:HIS318	Yes	Yes	Yes	
		251 – 285	KYRSSPCPNVKHGDEWGDPGKCENGDACQYCHTRT		A:CYS257:CYS272:CYS278:HIS282	A:CYS257:CYS272:CYS278:HIS282	Yes	Yes	Yes	
		293 – 321	IYKSTKCNDMQQAGSCPRGPFCAFAHIEP		A:CYS221:CYS228:CYS234:HIS238	A:CYS221:CYS228:CYS234:HIS238	Yes	Yes	Yes	
5G	3.4A	67 – 94	DGQLFFCLFFAKGMCCLGPKCEYLHHIP	R:MTSWRDKSAKVQVKESELPSSIPAQTGLTFNI	R:CYS73:CYS81:CYS87:HIS91	R:CYS73:CYS81:CYS87:HIS91	Yes	Yes	Yes	

MK				WYNKWSQGFAGNTRFVSPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEVLDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFSRLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQTLLLPSDKEWDDRREGTGLLVKWANEDPDPAAQKRLQEELKLESLNMMVHLINNNTNSAGTEVNNKNNERLDRTFPEASVDNVKKRLLPLDNGMESDDFIEKLKKVKKNISRENISSKPSVGKLGGPLLDYLSSDED						
					T:CYS108:CYS145:CYS148:HIS147	X	No	Yes	No	New site.
					T:CYS108:CYS120:CYS145:HIS147	X	No	Yes	No	New site.
5LJ3	3.8A	67 – 94	DGQLFFCLFFAKGMCCLGPKCEYLHHIP	M:MTSWRDKSAKVQVKESELPSSIPAQTGLTFNIWYNKWSQGFAGNTRFVSPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEALDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFSRLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQTLLLPSDKEWDDRREGTGLLVKWANEDPDPAAQKRLQEELKLESLNMMVHLINNNTNSAGTEVNNKNNERLDRTFPEASVDNVKKRLLPLDNGMESDDFIEKLKKVKKNISRENISSKPSVGKLGGPLLDYLSSDED	L:CYS108:CYS145:CYS148:HIS147	X	No	Yes	No	New site.
					L:CYS108:CYS120:CYS145:HIS147	X	No	Yes	No	New site.
					L:CYS105:CYS108:CYS148:HIS147	X	No	Yes	No	New site.
					M:CYS73:CYS81:CYS87:HIS91	M:CYS73:CYS81:CYS87:HIS91	Yes	Yes	Yes	
5LJ5	3.8A	67 – 94	DGQLFFCLFFAKGMCCLGPKCEYLHHIP	M:MTSWRDKSAKVQVKESELPSSIPAQTGLTFNIWYNKWSQGFAGNTRFVSPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEVLDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFSRLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQ	L:CYS108:CYS145:CYS148:HIS147	X	No	Yes	No	New site.
					L:CYS108:CYS120:CYS145:HIS147	X	No	Yes	No	New site.
					L:CYS105:CYS108:CYS148:HIS147	X	No	Yes	No	New site.
					M:CYS73:CYS81:CYS87:HIS91	M:CYS73:CYS81:CYS87:HIS91	Yes	Yes	Yes	

				TLLLPSDKEWDDRREGTGLLVKWANEDPDPAAQKRLQEELKLESLNMMVHLINNNTNSAGTEVNNKNNERLDRTFPEASVDNVKKRLLPLDNGMESDDFIEKLKKVKKNISRENISSKPSVGKLGGPLLDYLSSDED						
5LQW	5.8A	67 – 94	DGQLFFCLFFAKGMCCLGPKCEYLHHIP	F:MTSWRDKSAKVQVKESELPSSIPAQTGLTFNIWYNKWSQGFAGNTRFVSPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEVLDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFSRLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQTLLLPSDKEWDDRREGTGLLVKWANEDPDPAAQKRLQEELKLESLNMMVHLINNNTNSAGTEVNNKNNERLDRTFPEASVDNVKKRLLPLDNGMESDDFIEKLKKVKKNISRENISSKPSVGKLGGPLLDYLSSDED						
5MPS	3.8A	67 – 94	DGQLFFCLFFAKGMCCLGPKCEYLHHIP	M:MTSWRDKSAKVQVKESELPSSIPAQTGLTFNIWYNKWSQGFAGNTRFVSPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEVLDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFSRLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQTLLLPSDKEWDDRREGTGLLVKWANEDPDPAAQKRLQEELKLESLNMMVHLINNNTNSAGTEVNNKNNERLDRTFPEASVDNVKKRLLPLDNGMESDDFIEKLKKVKKNISRENISSKPSVGKLGGPLLDYLSSDED	L:CYS108:CYS145:CYS148:HIS147	X	No	Yes	No	New site.
					M:CYS73:CYS81:CYS87:HIS91	M:CYS73:CYS81:CYS87:HIS91	Yes	Yes	Yes	

5MQ0	4.17A	67 – 94	DGQLFFCLFFAKGMCCLGPKCEYLHHIP	M:MTSWRDKSAKVQVKESELPSSIPAQTGLTFNIWYNKWSQGFAGNTRFVSPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEVLDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFSRLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQTLLLPSDKEWDDRREGTGLLVKWANEDPDPAAQKRLQEELKLESLNMMVHLINNNTNSAGTEVNNKNNERLDRTFPEASVDNVKKRLLPLDNGMESDDFIEKLKKVKKNISRENISSKPSVGKLGGPLLDYLSSDED	L:CYS108:CYS145:CYS148:HIS147	X	No	Yes	No	New site.
					M:CYS73:CYS81:CYS87:HIS91	M:CYS73:CYS81:CYS87:HIS91	Yes	Yes	Yes	
5MQF	5.9A	159 – 186	RNRPHICSFWVKGECKRGEECPYRHEKP	P:MATSLGSNTYNRQNWEDADFPILCQTCLGENPYIRMTKEKYGKECKICARPFTVFRWCPGVRMRFKKTEVCQTCSKLKNVCQTCLLDLEYGLPIQVRDAGLSFKDDMPKSDVNKEYYTQNMEREISNSDGTRPVGMLGKATSTSDMLLKLARTTPYYKRNRPHICSFWVKGECKRGEECPYRHEKPTDPDDPLADQNIKDRYYGINDPVADKLLKRASTMPRLDPPEDKTITTLYVGGLGDTITETDLRNHFYQFGEIRTITVVQRQQCAFIQFATRQAAEVAAEKSFNKLIVNGRRLNVKWGRSQAARGKEKEKDGTTDSGIKLEPVPGLPGALPPPPAAEEEASANYFNLPPSGPPAVVNIALPPPPGIAPPPPPGFGPHMFHPMGPPPPFMRAPGPIHYPSQDPQRMGAHAGKHSSP						
5U6H	N/A	13 – 41	WLTLEVCREFQRGTCSRPDTECKFAHPSK	A:MAVSVTPIRDTKWLTLEVCREFQRGTCSRPDTECKFAHPSKSCQVENGRVIACFDSLKGRCSRENCKYLHPPPHLKTQLEIN	A:CYS19:CYS27:CYS34:HIS38	A:CYS19:CYS27:CYS34:HIS38	Yes	Yes	Yes	
		47 – 73	NGRVIACFDSLKGRCSRENCKYLHPPP			A:CYS53:CYS61:CYS66:HIS70	Yes	No	Yes	

				GRNNLIQQKN						
5U6L	N/A	179 – 207	TDRLEVCREYQRGNCNRGENDCRFAHPAD	A:AQKLMRTDRLEVCREYQRGNCNRGENDCRFAHPADSTMIDTNDNTVTVCMDYIKGRCSREKCKYFHPPAHLQAKIKAAQYQVN	A:CYS221:CYS229:CYS234:HIS238	A:CYS221:CYS229:CYS234:HIS238	Yes	Yes	Yes	
		215 – 241	DNTVTVCMDYIKGRCSREKCKYFHPPA		A:CYS185:CYS193:CYS200:HIS204	A:CYS185:CYS193:CYS200:HIS204	Yes	Yes	Yes	
5U9B	N/A	13 – 41	WLTLEVCREFQRGTCSRPDTECKFAHPSK	A:MAVSVTPIRDTKWLTLEVCREFQRGTCSRPDTECKFAHPSKSCQVENGRVIACFDSLKGRCSRENCKYLHPPPHLKTQLEINGRNNLIQQKN	A:CYS53:CYS61:CYS66:HIS70	A:CYS53:CYS61:CYS66:HIS70	Yes	Yes	Yes	
		47 – 73	NGRVIACFDSLKGRCSRENCKYLHPPP		A:CYS19:CYS27:CYS34:HIS38	A:CYS19:CYS27:CYS34:HIS38	Yes	Yes	Yes	
5WSG	4.0A	67 – 94	DGQLFFCLFFAKGMCCLGPKCEYLHHIP	R:MTSWRDKSAKVQVKESELPSSIPAQTGLTFNIWYNKWSQGFAGNTRFVSPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEVLDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFSRLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQTLLLPSDKEWDDRREGTGLLVKWANEDPDPAAQKRLQEELKLESLNMMVHLINNNTNSAGTEVNNKNNERLDRTFPEASVDNVKKRLLPLDNGMESDDFIEKLKKVKKNISRENISSKPSVGKLGGPLLDYLSSDED	R:CYS73:CYS81:CYS87:HIS91	R:CYS73:CYS81:CYS87:HIS91	Yes	Yes	Yes	
					T:CYS108:CYS145:CYS148:HIS147	X	No	Yes	No	New site.
					T:CYS108:CYS120:CYS145:HIS147	X	No	Yes	No	New site.
5Y88	3.7A	67 – 94	DGQLFFCLFFAKGMCCLGPKCEYLHHIP	N:MTSWRDKSAKVQVKESELPSSIPAQTGLTFNIWYNKWSQGFAGNTRFVSPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEVLDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFSRLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQTLLLPSDKEWDDRREGTGLLVKWANEDPDPAAQKRLQEELKLESLNMMVHLINNNTNSAGTEVNNKN	L:CYS108:CYS145:CYS148:HIS147	X	No	Yes	No	New site.
					L:CYS108:CYS120:CYS145:HIS147	X	No	Yes	No	New site.
					N:CYS73:CYS81:CYS87:HIS91	N:CYS73:CYS81:CYS87:HIS91	Yes	Yes	Yes	

				NERLDRTFPEASVDNVKKRLLPLDNGMESDDFIEKLKKVKKNISRENISSKPSVGKLGGPLLDYLSSDED						
5YLZ	3.6A	67 – 94	DGQLFFCLFFAKGMCCLGPKCEYLHHIP	N:MTSWRDKSAKVQVKESELPSSIPAQTGLTFNIWYNKWSQGFAGNTRFVSPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEVLDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFSRLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQTLLLPSDKEWDDRREGTGLLVKWANEDPDPAAQKRLQEELKLESLNMMVHLINNNTNSAGTEVNNKNNERLDRTFPEASVDNVKKRLLPLDNGMESDDFIEKLKKVKKNISRENISSKPSVGKLGGPLLDYLSSDED	L:CYS108:CYS145:CYS148:HIS147	X	No	Yes	No	New site.
					L:CYS108:CYS120:CYS145:HIS147	X	No	Yes	No	New site.
					N:CYS73:CYS81:CYS87:HIS91	N:CYS73:CYS81:CYS87:HIS91	Yes	Yes	Yes	
5Z58	4.9A	196 – 224	DYQPDICKDYKETGFCGFGDSCKFLHDRS	M:MAEQLSPGKAVDQVCTFLFKKPGRKGAAGRRKRPACDPEPGESGSSSDEGCTVVRPEKKRVTHNPMIQKTRDSGKQKAAYGDLSSEEEEENEPESLGVVYKSTRSAKPVGPEDMGATAVYELDTEKERDAQAIFERSQKIQEELRGKEDDKIYRGINNYQKYMKPKDTSMGNASSGMVRKGPIRAPEHLRATVRWDYQPDICKDYKETGFCGFGDSCKFLHDRSDYKHGWQIERELDEGRYGVYEDENYEVGSDDEEIPFKCFICRQSFQNPVVTKCRHYFCESCALQHFRTTPRCYVCDQQTNGVFNPAKELIAKLEKHRATGEGGASDLPEDPDEDAIPIT	M:CYS202:CYS211:CYS217:HIS221	M:CYS202:CYS211:CYS217:HIS221	Yes	Yes	Yes	
6BK	3.3A	67 – 94	DGQLFFCLFFAKGMCCLGPKCEYLHHIP	G:MTSWRDKSAKVQVKESELPSSIPAQTGLTFNIWYNKWSQGFAGNTRFV	G:CYS73:CYS81:CYS87:HIS91	G:CYS73:CYS81:CYS87:HIS91	Yes	Yes	Yes	
					I:CYS108:CYS145:CYS148:HIS147	X	No	Yes	No	New Site

8				SPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEVLDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFSRLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQTLLLPSDKEWDDRREGTGLLVKWANEDPDPAAQKRLQEELKLESLNMMVHLINNNTNSAGTEVNNKNNERLDRTFPEASVDNVKKRLLPLDNGMESDDFIEKLKKVKKNISRENISSKPSVGKLGGPLLDYLSSDED O:MNNNSRNNENRSTINRNKRQLQQAKEKNENIHIPRYIRNQPWYYKDTPKEQEGKKPGNDDTSTAEGGEKSDYLVHHRQKAKGGALDIDNNSEPKIGMGIKDEFKLIRPQKMSVRDSHSLSFCRNCGEAGHKEKDCMEKPRKMQKLVPDLNSQKNNGTVLVRATDDDWDSRKDRWYGYSGKEYNELISKWERDKRNKIKGKDKSQTDETLWDTDEEIELMKLELYKDSVGSLKKDDADNSQLYRTSTRLREDKAAYLNDINSTESNYDPKSRLYKTETLGAVDEKSKMFRRHLTGEGLKLNELNQFARSHAKEMGIRDEIEDKEKVQHVLVANPTKYEYLKKKREQEETKQPKIVSIGDLEARKVDGTKQSEEQRNHLKDLYG						
		120 - 137	SFCRNCGEAGHKEKDCME		I:CYS108:CYS120:CYS145:HIS147	X	No	Yes	No	New Site
					I:CYS105:CYS108:CYS148:HIS147	X	No	Yes	No	New Site
					O:CYS122:CYS125:CYS135:HIS130	O:CYS122:CYS125:CYS135:HIS130	Yes	Yes	Yes	
6DNH	3.4A	35 – 61	KSGAAVCEFFLKAACGKGGMCPFRHIS	C:GMQEIIASVDHIKFDLEIAVEQQLGAQPLPFPGMDKSGAAVCEFFLKAACGKGGMCPFRHISGEKTVVCKHWLRGLCKKGDQCEFLHEYDMTKMPECYFYSKFGECSNKECPFLHIDPESKIKDCPWYDRGFCKHGPLCRHRHTRRVICVNYLVGFCPEGPSCKFMH	C:CYS105:CYS110:CYS96:HIS114	X (2C1H)	Yes	Yes	No	New site.
		62 – 89	GEKTVVCKHWLRGLCKKGDQCEFLHEYD		X	C:CYS68:CYS76:CYS82:HIS86	Yes	No	Yes	
		90 – 117	MTKMPECYFYSKFGECSNKECPFLHIDP		C:CYS41:CYS49:CYS55:HIS:59	C:CYS41:CYS49:CYS55:HIS:59	Yes	Yes	Yes	

				PRFELPMGTTEQPPLPQQTQPPAKQRTPQVIGVMQSQNSSAGNRGPRPLEQVTCYKCGEKGHYANRCTKGHLAFLSGQ						
6EOJ	3.55 A	28 – 59	DPDRPICEFYNSREGPKSCPRGPLCPKKHVLP	B:PSLIHPDTAKYPFKFEPFLRQEYSFSLDPDRPICEFYNSREGPKSCPRGPLCPKKHVLPIFQNKIVCRHWLRGLCKKNDQCEYLHEYNLRKMPECVFFSKNGYCTQSPDCQYLHIDPASKIPKCENYEMGFCPLGSSCPRRHIKKVFCQRYMTGFCPLGKDECDMEHPQFIIPDEGSKLRIKRDDEINTRKMDEEKERRLNAIINGEV	B:CYS67:CYS75:CYS81:HIS85	B:CYS67:CYS75:CYS81:HIS85	Yes	Yes	Yes	
		61 – 88	FQNKIVCRHWLRGLCKKNDQCEYLHEYN		B:CYS34:CYS46:CYS52:HIS56	B:CYS34:CYS46:CYS52:HIS56	Yes	Yes	Yes	
6EXN	3.7A	67 – 94	DGQLFFCLFFAKGMCCLGPKCEYLHHIP	M:MTSWRDKSAKVQVKESELPSSIPAQTGLTFNIWYNKWSQGFAGNTRFVSPFALQPQLHSGKTRGDNDGQLFFCLFFAKGMCCLGPKCEYLHHIPDEEDIGKLALRTEVLDCFGREKFADYREDMGGIGSFRKKNKTLYVGGIDGALNSKHLKPAQIESRIRFVFSRLGDIDRIRYVESKNCGFVKFKYQANAEFAKEAMSNQTLLLPSDKEWDDRREGTGLLVKWANEDPDPAAQKRLQEELKLESLNMMVHLINNNTNSAGTEVNNKNNERLDRTFPEASVDNVKKRLLPLDNGMESDDFIEKLKKVKKNISRENISSKPSVGKLGGPLLDYLSSDED c:MNNNSRNNENRSTINRNKRQLQQAKEKNENIHIPRYIRNQPWYYKDTPKEQEGKKPGNDDTSTAEGGEKSDYLVHHRQKAKGGALDIDNNSEPKIGMGIKDEFKLIRPQKMSVRDSHSLSFCRNCGEAGHKEKDCMEKPRKMQKLVPDLNSQKNNGTVLVRATDDDWDSRKDRWYGYSGKEYNELISKWERDKRNKI	c:CYS122:CYS125:CYS135:HIS130	c:CYS122:CYS125:CYS135:HIS130	Yes	Yes	Yes	
					L:CYS108:CYS145:CYS148:HIS147	X	No	Yes	No	New site.
		120-137	SFCRNCGEAGHKEKDCME		L:CYS108:CYS120:CYS145:HIS147	X	No	Yes	No	New site.
					L:CYS105:CYS108:CYS148:HIS147	X	No	Yes	No	New site.
					M:CYS73:CYS81:CYS87:HIS91	M:CYS73:CYS81:CYS87:HIS91	Yes	Yes	Yes	

				KGKDKSQTDETLWDTDEEIELMKLELYKDSVGSLKKDDADNSQLYRTSTRLREDKAAYLNDINSTESNYDPKSRLYKTETLGAVDEKSKMFRRHLTGEGLKLNELNQFARSHAKEMGIRDEIEDKEKVQHVLVANPTKYEYLKKKREQEETKQPKIVSIGDLEARKVDGTKQSEEQRNHLKDLYG						
6FBS	3.07 A	35 – 61	KSGAAVCEFFLKAACGKGGMCPFRHIS	C:MQEIIASVDHIKFDLEIAVEQQLGAQPLPFPGMDKSGAAVCEFFLKAACGKGGMCPFRHISGEKTVVCKHWLRGLCKKGDQCEFLHEYDMTKMPECYFYSKFGECSNKECPFLHIDPESKIKDCPWYDRGFCKHGPLCRHRHTRRVICVNYLVGFCPEGPSCKFMHPRFELPMGTTEQ	C:CYS105:CYS110:CYS96:HIS114	C:CYS105:CYS110:CYS96:HIS114	Yes	Yes	Yes	
		62 – 89	GEKTVVCKHWLRGLCKKGDQCEFLHEYD		C:CYS68:CYS76:CYS82:HIS86	C:CYS68:CYS76:CYS82:HIS86	Yes	Yes	Yes	
		90 – 117	MTKMPECYFYSKFGECSNKECPFLHIDP		C:CYS41:CYS49:CYS55:HIS59	C:CYS41:CYS49:CYS55:HIS59	Yes	Yes	Yes	
6FF4	3.4A	196 – 224	DYQPDICKDYKETGFCGFGDSCKFLHDRS	t:MAEQLSPGKAVDQVCTFLFKKPGRKGAAGRRKRPACDPEPGESGSSSDEGCTVVRPEKKRVTHNPMIQKTRDSGKQKAAYGDLSSEEEEENEPESLGVVYKSTRSAKPVGPEDMGATAVYELDTEKERDAQAIFERSQKIQEELRGKEDDKIYRGINNYQKYMKPKDTSMGNASSGMVRKGPIRAPEHLRATVRWDYQPDICKDYKETGFCGFGDSCKFLHDRSDYKHGWQIERELDEGRYGVYEDENYEVGSDDEEIPFKCFICRQSFQNPVVTKCRHYFCESCALQHFRTTPRCYVCDQQTNGVFNPAKELIAKLEKHRATGEGGASDLPEDPDEDAIPIT	Q:CYS105:CYS134:CYS137:HIS136	X	No	Yes	No	New site.
					Q:CYS105:CYS117:CYS134:HIS136	X	No	Yes	No	New site.
					t:CYS202:CYS211:CYS217:HIS221	t:CYS202:CYS211:CYS217:HIS221	Yes	Yes	Yes	
6FUW	3.07 A	35 – 61	KSGAAVCEFFLKAACGKGGMCPFRHIS	C:MQEIIASVDHIKFDLEIAVEQQLGAQPLPFPGMDKSGAAVCEFFLKAACGKGGMCPFRHISGEKTVVCKHWLRGLCKKGDQCEFLHEYDMTKMPECYFYSKFGECSNKECPFLHIDPESKIKDCPWYDRGFCK	C:CYS105:CYS110:CYS96:HIS114	C:CYS105:CYS110:CYS96:HIS114	Yes	Yes	Yes	
		62 – 89	GEKTVVCKHWLRGLCKKGDQCEFLHEYD		C:CYS68:CYS76:CYS82:HIS86	C:CYS68:CYS76:CYS82:HIS86	Yes	Yes	Yes	
		90 – 117	MTKMPECYFYSKFGECSNKECPFLHIDP		C:CYS41:CYS49:CYS55:HIS59	C:CYS41:CYS49:CYS55:HIS59	Yes	Yes	Yes	

				HGPLCRHRHTRRVICVNYLVGFCPEGPSCKFMHPRFELPMGTTEQ						

Table S2: Matrix of amino acids sequence identity among the Serotonin Transporter (SERT), the Monoamine Oxidase A (MAO-A) and the Serotonin receptor 2A type (5HT2A).

	MAO-A	5HT2A	SERT
MAO-A	100%	15%	18%
5HT2A	15%	100%	22%
SERT	18%	22%	100%

Table S2: In the table are shown the amino acids sequence identity between MAO-A vs SERT, MAO-A vs 5HT2A, and SERT vs 5HT2A.