

A Novel *In Silico* Benchmarked Pipeline Capable of Complete Protein Analysis: A Possible Tool for Potential Drug Discovery

Authors

D. D. B. D. Perera ^{1,*,\,†,\‡}, K.Minoli L. Perera ¹ and Dinithi C. Peiris ^{2,*,\,†}

Affiliations

¹ Department of Zoology, Faculty of Applied Sciences, University of Sri Jayewardenepura,

Nugegoda 10250, Sri Lanka; mperera95826@gmail.com

² Genetics & Molecular Biology Unit (Center for Biotechnology), Department of Zoology, Faculty of Applied Sciences, University of Sri Jayewardenepura, Nugegoda 10250, Sri Lanka

* Correspondence: desh.02236@gmail.com (D.D.B.D.P.); dinithi@sci.sjp.ac.lk (D.C.P.); Tel.: +94-714-018-537 (D.C.P.)

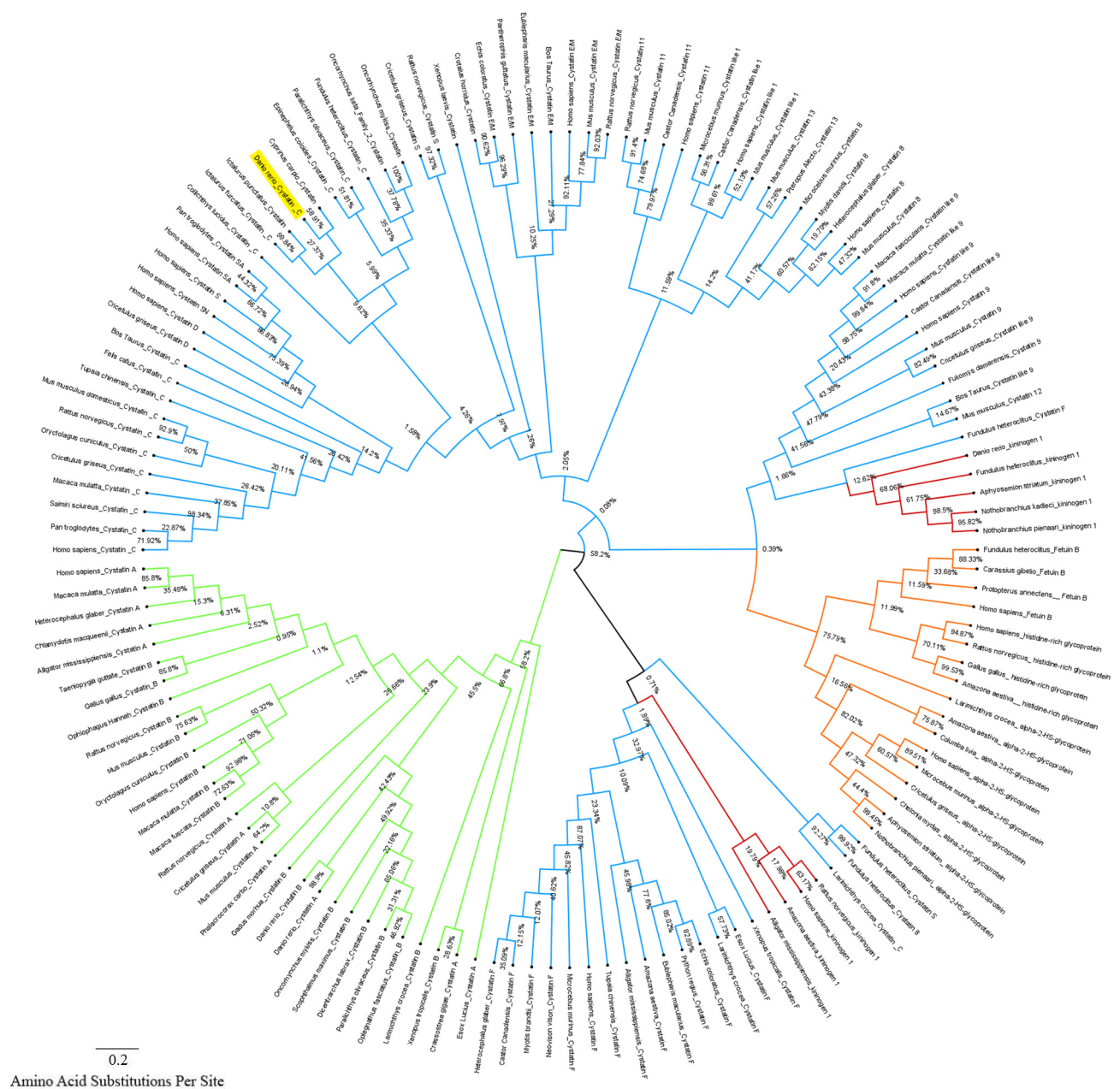
† Current address: Department of Biochemistry & Molecular Biology, Cumming School of Medicine, University of Calgary, Calgary, AB T2N 1N4, Canada.

\‡ Equal corresponding authors.

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1. Analysis of Cystatin C



Supplementary Figure S1: Complete initial phylogenetic tree. Type 1 Cystatins in Green, Type 2 Cystatins in Blue, Type 3 Cystatins in Red and Type 4 Cystatins in Orange. The *Danio rerio* amino sequence highlighted yellow. This was filtered to formulate the final refined tree available in the main text.

Supplementary Table S1: Detailed description of the electrostatic charge and hydrophobic residue distribution on the protein surface of Cystatin C of *D. rerio*.

Patch	Type	Size (Å ²)	Score	Intensity (Score / Size)
1	Positive	1024.2	866.788	0.846
2	Positive	43.4	38.615	0.89
3	Positive	15.4	0	0
4	Positive	672.4	597.782	0.889
5	Positive	21.5	17.476	0.811
6	Positive	18.4	7.222	0.393
7	Negative	120.9	115.675	0.957
8	Negative	60.1	77.194	1.284
9	Negative	86.8	105.921	1.221
10	Negative	251.3	281.105	1.119
11	Negative	79.9	80.66	1.01
12	Negative	104.4	154.691	1.482
13	Negative	23.4	24.225	1.035
14	Negative	206.6	253.733	1.228
15	Negative	41.3	34.583	0.837
16	Negative	29.9	21.893	0.732
17	Negative	25.6	12.23	0.477
18	Negative	17.9	13.604	0.76
19	Negative	176.2	251.095	1.425
20	Negative	25	32.309	1.294
21	Hydrophobic	1223.1	858.725	0.702
22	Hydrophobic	104.5	75.331	0.721
23	Hydrophobic	51.1	35.154	0.688
24	Hydrophobic	84.9	43.78	0.516
25	Hydrophobic	143	92.19	0.645
26	Hydrophobic	112.5	62.656	0.557
27	Hydrophobic	107.4	53.777	0.501
28	Hydrophobic	53.9	43.302	0.803

Supplementary Table S2: Protein Surface Analysis of the interacting surfaces between Cystatin C (A) and Papain (B). Details regarding the types of bonding including Hydrogen Bonding (HB), Salt Bridges (SB), Pi Stacking (Pi), Disulfide bonding (DS) and Vander Waal interactions (VW).

Residue	Closest	Distance (Å)	HB	SB	Pi	DS	VW
A:53:Tyr			0	0	0	0	0
A:58:Ser			0	0	0	0	0
A:59:Lys			0	0	0	0	1
A:78:Asp	B:156:Lys	2.7	0	1	0	0	11
A:80:Ala			0	0	0	0	0
A:83:Thr	B:64:Asn	2.1	0	0	0	0	9
A:84:Cyx			0	0	0	0	0
A:85:Arg			0	0	0	0	0
A:90:Glu			0	0	0	0	0
A:92:Leu	B:61:Tyr	2.2	0	0	0	0	1
A:93:Cyx			0	0	0	0	0
A:94:Ala			0	0	0	0	0
A:95:Ile	B:158:Asp	2.4	0	0	0	0	15
A:96:His	B:158:Asp	2.9	0	0	0	0	0
A:97:Glu	B:25:Cys B:159:His B:158:Asp B:66:Gly	2.3 2.3 2.7 3.0	1	0	0	0	9
A:98:Asn	B:19:Gln	2.2	0	0	0	0	2
A:99:Pro	B:177:Trp B:142:Gln	1.8 2.5	0	0	0	0	20
A:100:Glu			0	0	0	0	0
A:101:Ile			0	0	0	0	0
A:102:Ala			0	0	0	0	0
A:103:Gln			0	0	0	0	0

Supplementary Table S3: Protein Surface Analysis of interacting surfaces between Cystatin C (A), Cathepsin B (B). Details regarding the types of bonding including Hydrogen Bonding (HB), Salt Bridges (SB), Pi Stacking (Pi), Disulfide bonding (DS) and Vander Waal interactions (VW).

Residue	Closest	Distance (Å)	HB	SB	Pi	DS	VW
A:2:Phe			0	0	0	0	0
A:3:Leu	B:65:Ser	3.0 A	0	0	0	0	1
A:4:Lys			0	0	0	0	0
A:9:Phe			0	0	0	0	0
A:12:Val			0	0	0	0	0
A:43:Ala			0	0	0	0	0
A:44:Gln	B:196:Met	2.4 A	1	0	0	0	0
A:45:Tyr			0	0	0	0	0
A:47:Arg	B:196:Met	2.2 A	0	0	0	0	5
A:48:Gln			0	0	0	0	0
A:49:Ser			0	0	0	0	0
A:50:Asn			0	0	0	0	0
A:86:Lys			0	0	0	0	0
A:87:Gly			0	0	0	0	0
A:105:Lys			0	0	0	0	0
A:108:Lys			0	0	0	0	0

Supplementary Table S4: Protein Surface Analysis of interacting surfaces between Cystatin C (A), Cathepsin H (B). Details regarding the types of bonding including Hydrogen Bonding (HB), Salt Bridges (SB), Pi Stacking (Pi), Disulfide bonding (DS) and Vander Waal interactions (VW).

Residue	Closest	Distance (Å)	HB	SB	Pi	DS	VW
A:1:Met	B:21:Ser B:63:Cyx	1.3 A 2.6 A	0	0	0	0	21
A:2:Phe			0	0	0	0	0
A:3:Leu			0	0	0	0	4
A:4:Lys	B:142:Leu	1.9 A	0	0	0	0	21
A:7:Val			0	0	0	0	0
A:8:Ala	B:63:Cyx B:23:Gly	2.0 A 2.8 A	0	0	0	0	9
A:9:Phe	B:23:Gly B:158:Asn	2.7 A 2.9 A	0	0	0	0	13
A:10:Leu			0	0	0	0	0
A:12:Val			0	0	0	0	1
A:13:Ile			0	0	0	0	0
A:25:Pro			0	0	0	0	0
A:66:Gln			0	0	0	0	0
A:72:Lys			0	0	0	0	0
A:74:Ile			0	0	0	0	0
A:108:Lys			0	0	0	0	0
A:110:Val			0	0	0	0	0
A:124:Glu			0	0	0	0	0
A:125:Asn			0	0	0	0	0
A:126:Ser			0	0	0	0	0
A:127:Cyx			0	0	0	0	0
A:128:Leu			0	0	0	0	0

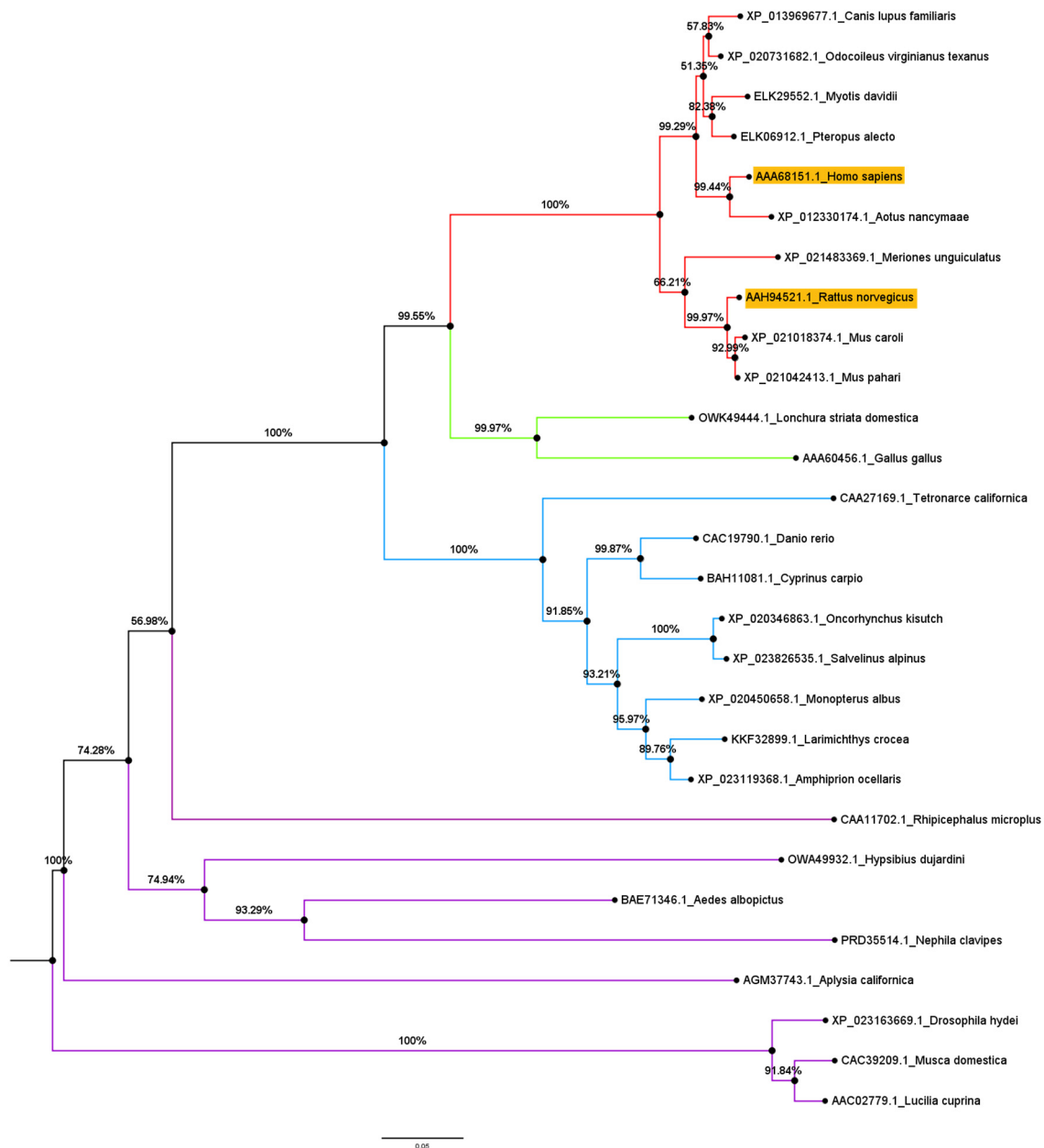
Supplementary Table S5: Protein Surface Analysis of interacting surfaces between Cystatin C (A), Cathepsin L1 (B). Details regarding the types of bonding including Hydrogen Bonding (HB), Salt Bridges (SB), Pi Stacking (Pi), Disulfide bonding (DS) and Vander Waal interactions (VW).

Residue	Closest	Distance (Å)	HB	SB	Pi	DS	VW
A:1:Met			0	0	0	0	0
A:2:Phe	B:66:Asn	2.1 A	0	0	0	0	5
A:3:Leu	B:66:Asn B:65:Cyx B:67:Gly	2.0 A 2.8 A 2.9 A	0	0	0	0	22
A:4:Lys	B:19:Gln	2.7 A	0	0	0	0	6
A:5:Ile			0	0	0	0	0
A:9:Phe	B:162:Asp	2.5 A	0	0	0	0	17
A:10:Leu			0	0	0	0	0
A:11:Ala			0	0	0	0	0
A:12:Val			0	0	0	0	0
A:13:Ile	B:21:Gln	2.0 A	0	0	0	0	6
A:14:Leu			0	0	0	0	0
A:16:Val			0	0	0	0	0
A:17:Ser			0	0	0	0	0
A:44:Gln			0	0	0	0	0
A:45:Tyr			0	0	0	0	0
A:48:Gln			0	0	0	0	0
A:72:Lys			0	0	0	0	0
A:110:Val			0	0	0	0	0
A:121:Lys			0	0	0	0	0
A:122:Val			0	0	0	0	0
A:123:Thr			0	0	0	0	0
A:124:Glu			0	0	0	0	2
A:125:Asn			0	0	0	0	0
A:126:Ser			0	0	0	0	0

Supplementary Table S6: Protein Surface Analysis of interacting surfaces between Cystatin C (A), Cathepsin S (B). Details regarding the types of bonding including Hydrogen Bonding (HB), Salt Bridges (SB), Pi Stacking (Pi), Disulfide bonding (DS) and Vander Waal interactions (VW).

Residue	Closest	Distance (Å)	HB	SB	Pi	DS	VW
A:1:Met	B:57C:Lys	2.5 A	0	0	0	0	5
A:2:Phe			0	0	0	0	0
A:3:Leu			0	0	0	0	0
A:8:Ala			0	0	0	0	0
A:9:Phe	B:113:Tyr	2.3 A	0	0	0	0	4
A:25:Pro			0	0	0	0	1
A:45:Tyr			0	0	0	0	0
A:48:Gln			0	0	0	0	0
A:61:Thr			0	0	0	0	0
A:62:Lys			0	0	0	0	0
A:64:Gln			0	0	0	0	0
A:66:Gln			0	0	0	0	0
A:72:Lys			0	0	0	0	0
A:74:Ile	B:61:Lys	2.2 A	0	0	0	0	12
A:75:Phe			0	0	0	0	0
A:76:Thr			0	0	0	0	1
A:105:Lys			0	0	0	0	0
A:106:Glu			0	0	0	0	0
A:108:Lys	B:61:Lys	2.8 A	0	0	0	0	13
A:124:Glu	B:67:Phe	2.4 A	0	0	0	0	3
A:125:Asn			0	0	0	0	0
A:126:Ser			0	0	0	0	0
A:127:Cyx			0	0	0	0	1
A:128:Leu			0	0	0	0	2

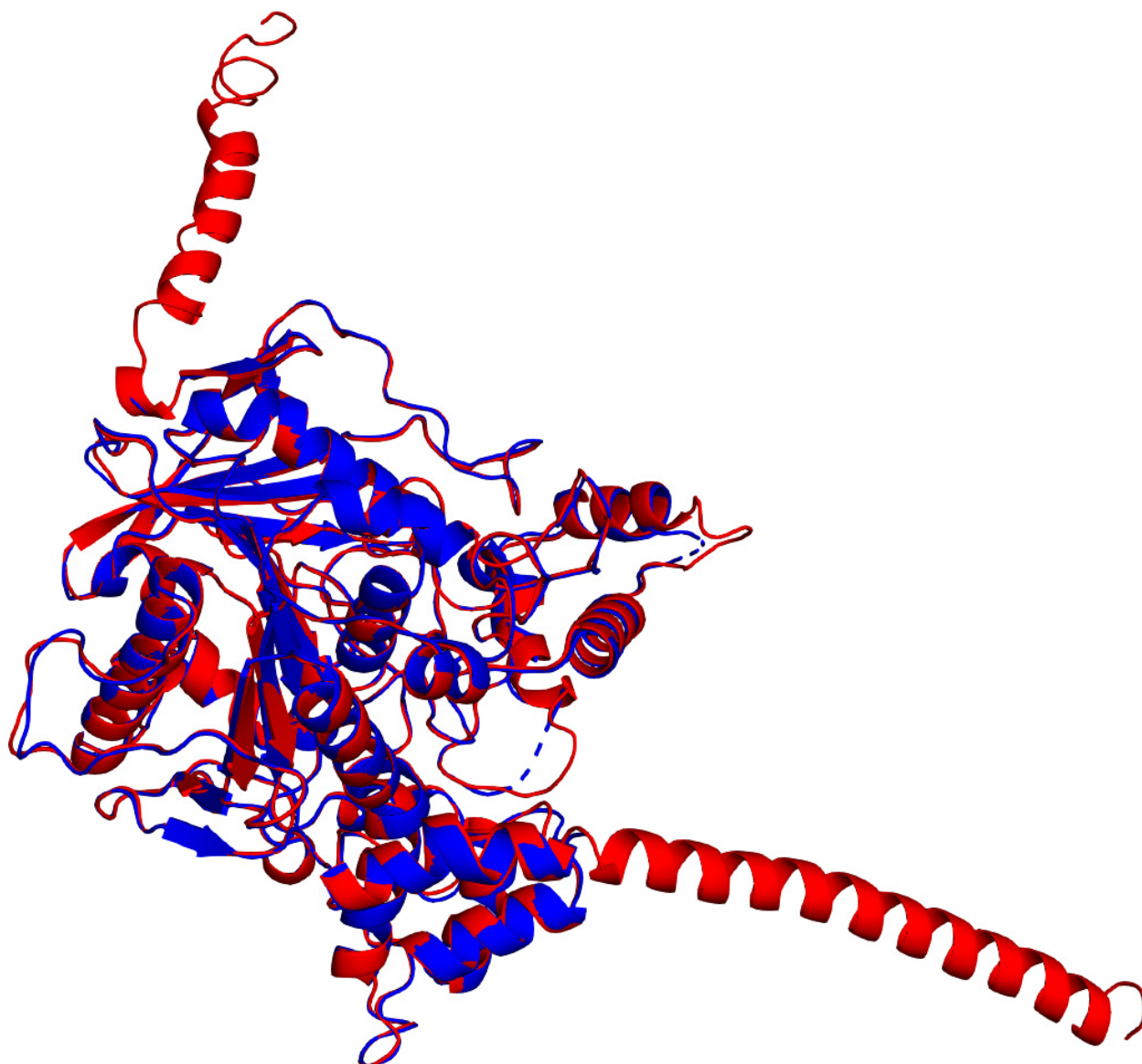
2. Analysis of Human and Rat AChE



Supplementary Figure S5: Phylogenetic Tree Analysis of Acetylcholinesterase. Clear distinct clade separation represented as follows with Mammalian Ache in Red, Aves Ache in Green, Pisces in Blue and Invertebrate Ache in Purple. *Homo sapiens* and *Rattus norvegicus* highlighted in yellow.

XP_013969677.1 1 -----MRPFWCLH--PSIASLILMLILGGGAS--DPLILVVRGRI
 XP_020731682.1 60 GRRRLPALAMRPFWCLH--PSIASLILMLILGGGAS--DPLILVVRGRI
 ELK29552.1_Myot 1 -----MRPFWCLH--PSIASLILMLILGGGAS--DPLILVVRGRI
 ELK06912.1_Pter 1 -----MRPFWCLH--LFFPSLILMLILGG--RAERLEDELLVVRGRI
AA68151.1_Homo 1 -----MRPFWCLH--PSIASLILMLILGGGAS--DPLILVVRGRI
 XP_012330174.1 59 SDFACP--AMRPFWCLH--PSIASLILMLILGGGAS--DPLILVVRGRI
 XP_021483369.1 1 -----MRPFWCLH--PSIASLILMLILGGGAS--DPLILVVRGRI
AN94521.1_Ratt 1 -----MRPFWCLH--PSIASLILMLILGGGAS--DPLILVVRGRI
 XP_021018374.1 1 -----MRPFWCLH--PSIASLILMLILGGGAS--DPLILVVRGRI
 XP_021042413.1 1 -----MRPFWCLH--PSIASLILMLILGGGAS--DPLILVVRGRI
 consensus 61 *****
 XP_013969677.1 46 RGRIRKAGGCVSAFLGIFPAEPVVGPRFLPEPRKFWSGVLDATIRQSVQYQVDTLL
 XP_020731682.1 117 RGRIRKAGGCVSAFLGIFPAEPVVGPRFLPEPRKFWSGVLDATIRQSVQYQVDTLL
 ELK29552.1_Myot 51 RGRIRKAGGCVSAFLGIFPAEPVVGPRFLPEPRKFWSGVLDATIRQSVQYQVDTLL
 ELK06912.1_Pter 47 RGRIRKAGGCVSAFLGIFPAEPVVGPRFLPEPRKFWSGVLDATIRQSVQYQVDTLL
AA68151.1_Homo 47 RGRIRKAGGCVSAFLGIFPAEPVVGPRFLPEPRKFWSGVLDATIRQSVQYQVDTLL
 XP_012330174.1 49 RGRIRKAGGCVSAFLGIFPAEPVVGPRFLPEPRKFWSGVLDATIRQSVQYQVDTLL
 XP_021483369.1 38 RGRIRKAGGCVSAFLGIFPAEPVVGPRFLPEPRKFWSGVLDATIRQSVQYQVDTLL
AN94521.1_Ratt 49 RGRIRKAGGCVSAFLGIFPAEPVVGPRFLPEPRKFWSGVLDATIRQSVQYQVDTLL
 XP_021018374.1 49 RGRIRKAGGCVSAFLGIFPAEPVVGPRFLPEPRKFWSGVLDATIRQSVQYQVDTLL
 XP_021042413.1 49 RGRIRKAGGCVSAFLGIFPAEPVVGPRFLPEPRKFWSGVLDATIRQSVQYQVDTLL
 consensus 121 *****
 XP_013969677.1 106 PGFGETDMNPNIRELSDCLYNVWTPYPRRSPTPVLWIIYGGGFYSGASSLDVYDGR
 XP_020731682.1 177 PGFGETDMNPNIRELSDCLYNVWTPYPRRSPTPVLWIIYGGGFYSGASSLDVYDGR
 ELK29552.1_Myot 111 PGFGETDMNPNIRELSDCLYNVWTPYPRRSPTPVLWIIYGGGFYSGASSLDVYDGR
 ELK06912.1_Pter 107 PGFGETDMNPNIRELSDCLYNVWTPYPRRSPTPVLWIIYGGGFYSGASSLDVYDGR
AA68151.1_Homo 109 PGFGETDMNPNIRELSDCLYNVWTPYPRRSPTPVLWIIYGGGFYSGASSLDVYDGR
 XP_012330174.1 175 PGFGETDMNPNIRELSDCLYNVWTPYPRRSPTPVLWIIYGGGFYSGASSLDVYDGR
 XP_021483369.1 98 PGFGETDMNPNIRELSDCLYNVWTPYPRRSPTPVLWIIYGGGFYSGASSLDVYDGR
AN94521.1_Ratt 109 PGFGETDMNPNIRELSDCLYNVWTPYPRRSPTPVLWIIYGGGFYSGASSLDVYDGR
 XP_021018374.1 109 PGFGETDMNPNIRELSDCLYNVWTPYPRRSPTPVLWIIYGGGFYSGASSLDVYDGR
 XP_021042413.1 109 PGFGETDMNPNIRELSDCLYNVWTPYPRRSPTPVLWIIYGGGFYSGASSLDVYDGR
 consensus 181 *****
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 XP_020731682.1 237 LAQAGGVLVSNVVRGARGFIALPGSREAGNVGLLDORLALQWQENVAAPGDDPMSV
 ELK29552.1_Myot 171 LAQAGGVLVSNVVRGARGFIALPGSREAGNVGLLDORLALQWQENVAAPGDDPMSV
 ELK06912.1_Pter 167 LAQAGGVLVSNVVRGARGFIALPGSREAGNVGLLDORLALQWQENVAAPGDDPMSV
AA68151.1_Homo 169 LAQAGGVLVSNVVRGARGFIALPGSREAGNVGLLDORLALQWQENVAAPGDDPMSV
 XP_012330174.1 235 LAQAGGVLVSNVVRGARGFIALPGSREAGNVGLLDORLALQWQENVAAPGDDPMSV
 XP_021483369.1 158 LAQAGGVLVSNVVRGARGFIALPGSREAGNVGLLDORLALQWQENVAAPGDDPMSV
AN94521.1_Ratt 169 LAQAGGVLVSNVVRGARGFIALPGSREAGNVGLLDORLALQWQENVAAPGDDPMSV
 XP_021018374.1 169 LAQAGGVLVSNVVRGARGFIALPGSREAGNVGLLDORLALQWQENVAAPGDDPMSV
 XP_021042413.1 169 LAQAGGVLVSNVVRGARGFIALPGSREAGNVGLLDORLALQWQENVAAPGDDPMSV
 consensus 241 *****
 XP_013969677.1 226 ILFGSAGAASVGMHLLSPFSRGLFHRVAVLQSGFENGFWATVGEARRRATILARIYGG
 XP_020731682.1 297 ILFGSAGAASVGMHLLSPFSRGLFHRVAVLQSGFENGFWATVGEARRRATILARIYGG
 ELK29552.1_Myot 231 ILFGSAGAASVGMHLLSPFSRGLFHRVAVLQSGFENGFWATVGEARRRATILARIYGG
 ELK06912.1_Pter 227 ILFGSAGAASVGMHLLSPFSRGLFHRVAVLQSGFENGFWATVGEARRRATILARIYGG
AA68151.1_Homo 229 ILFGSAGAASVGMHLLSPFSRGLFHRVAVLQSGFENGFWATVGEARRRATILARIYGG
 XP_012330174.1 295 ILFGSAGAASVGMHLLSPFSRGLFHRVAVLQSGFENGFWATVGEARRRATILARIYGG
 XP_021483369.1 218 ILFGSAGAASVGMHLLSPFSRGLFHRVAVLQSGFENGFWATVGEARRRATILARIYGG
AN94521.1_Ratt 229 ILFGSAGAASVGMHLLSPFSRGLFHRVAVLQSGFENGFWATVGEARRRATILARIYGG
 XP_021018374.1 229 ILFGSAGAASVGMHLLSPFSRGLFHRVAVLQSGFENGFWATVGEARRRATILARIYGG
 XP_021042413.1 229 ILFGSAGAASVGMHLLSPFSRGLFHRVAVLQSGFENGFWATVGEARRRATILARIYGG
 consensus 301 *****
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 XP_020731682.1 357 PGGGAGNDTELVACLRTPAQDLVDEHNVLPQESVFRFSFVFWVDGDFLSDTPEALIN
 ELK29552.1_Myot 291 PGGGAGNDTELVACLRTPAQDLVDEHNVLPQESVFRFSFVFWVDGDFLSDTPEALIN
 ELK06912.1_Pter 287 PGGGAGNDTELVACLRTPAQDLVDEHNVLPQESVFRFSFVFWVDGDFLSDTPEALIN
AA68151.1_Homo 289 PGGGAGNDTELVACLRTPAQDLVDEHNVLPQESVFRFSFVFWVDGDFLSDTPEALIN
 XP_012330174.1 355 PGGGAGNDTELVACLRTPAQDLVDEHNVLPQESVFRFSFVFWVDGDFLSDTPEALIN
 XP_021483369.1 278 PGGGAGNDTELVACLRTPAQDLVDEHNVLPQESVFRFSFVFWVDGDFLSDTPEALIN
AN94521.1_Ratt 289 PGGGAGNDTELVACLRTPAQDLVDEHNVLPQESVFRFSFVFWVDGDFLSDTPEALIN
 XP_021018374.1 289 PGGGAGNDTELVACLRTPAQDLVDEHNVLPQESVFRFSFVFWVDGDFLSDTPEALIN
 XP_021042413.1 289 PGGGAGNDTELVACLRTPAQDLVDEHNVLPQESVFRFSFVFWVDGDFLSDTPEALIN
 consensus 361 *****
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 XP_020731682.1 417 AGDFHGLQVLGVWVKDEGSYFLVYGAGFSGSDNESLISRAQFLAGVGVQASDLAAEA
 ELK29552.1_Myot 351 AGDFHGLQVLGVWVKDEGSYFLVYGAGFSGSDNESLISRAQFLAGVGVQASDLAAEA
 ELK06912.1_Pter 347 AGDFHGLQVLGVWVKDEGSYFLVYGAGFSGSDNESLISRAQFLAGVGVQASDLAAEA
AA68151.1_Homo 349 AGDFHGLQVLGVWVKDEGSYFLVYGAGFSGSDNESLISRAQFLAGVGVQASDLAAEA
 XP_012330174.1 415 AGDFHGLQVLGVWVKDEGSYFLVYGAGFSGSDNESLISRAQFLAGVGVQASDLAAEA
 XP_021483369.1 335 AGDFHGLQVLGVWVKDEGSYFLVYGAGFSGSDNESLISRAQFLAGVGVQASDLAAEA
AN94521.1_Ratt 349 AGDFHGLQVLGVWVKDEGSYFLVYGAGFSGSDNESLISRAQFLAGVGVQASDLAAEA
 XP_021018374.1 349 AGDFHGLQVLGVWVKDEGSYFLVYGAGFSGSDNESLISRAQFLAGVGVQASDLAAEA
 XP_021042413.1 349 AGDFHGLQVLGVWVKDEGSYFLVYGAGFSGSDNESLISRAQFLAGVGVQASDLAAEA
 consensus 421 *****
 XP_013969677.1 406 VVLYHTDNLHPEDEPARLEANSVVGSDNVVCPVAQLAGRLAAQGARVYATIFERRASTI
 XP_020731682.1 477 VVLYHTDNLHPEDEPARLEANSVVGSDNVVCPVAQLAGRLAAQGARVYATIFERRASTI
 ELK29552.1_Myot 411 VVLYHTDNLHPEDEPARLEANSVVGSDNVVCPVAQLAGRLAAQGARVYATIFERRASTI
 ELK06912.1_Pter 407 VVLYHTDNLHPEDEPARLEANSVVGSDNVVCPVAQLAGRLAAQGARVYATIFERRASTI
AA68151.1_Homo 409 VVLYHTDNLHPEDEPARLEANSVVGSDNVVCPVAQLAGRLAAQGARVYATIFERRASTI
 XP_012330174.1 475 VVLYHTDNLHPEDEPARLEANSVVGSDNVVCPVAQLAGRLAAQGARVYATIFERRASTI
 XP_021483369.1 395 VVLYHTDNLHPEDEPARLEANSVVGSDNVVCPVAQLAGRLAAQGARVYATIFERRASTI
AN94521.1_Ratt 409 VVLYHTDNLHPEDEPARLEANSVVGSDNVVCPVAQLAGRLAAQGARVYATIFERRASTI
 XP_021018374.1 409 VVLYHTDNLHPEDEPARLEANSVVGSDNVVCPVAQLAGRLAAQGARVYATIFERRASTI
 XP_021042413.1 409 VVLYHTDNLHPEDEPARLEANSVVGSDNVVCPVAQLAGRLAAQGARVYATIFERRASTI
 consensus 481 *****

Supplementary Figure S6: Multiple Sequence Alignment by ClustalW of mammalian Ache. Symbol * depicts highly conserved sequence motifs. *Homo sapiens* sequence highlighted in yellow and *Rattus norvegicus* highlighted in green.



Supplementary Figure S7: The three-dimensional alignment of the AChE crystal structure of *Rattus norvegicus* (red) against the AChE crystal structure of *Homo sapiens* (blue).

Supplementary Table S7: AutoDock Vina results for protein ligand docking between hAChE and Echothiophate.

Mode	Affinity	Distance from best mode	
	(kcal/mol)	rmsd l.b.	rmsd u.b.
1	-5.6	0	0
2	-5.5	1.91	3.012
3	-5.5	3.554	5.917
4	-5.4	1.434	3.414
5	-5.3	3.056	5.733
6	-5.2	3.6	5.82
7	-4.9	2.177	3.504
8	-4.8	3.555	5.875
9	-4.7	2.272	3.646

Supplementary Table S8: AutoDock Vina results for protein ligand docking between rAChE and Echothiophate.

Mode	Affinity	Distance from best mode	
	(kcal/mol)	rmsd l.b.	rmsd u.b.
1	-4.7	0	0
2	-4.5	1.906	2.462
3	-4.5	3.9	4.962
4	-4.5	3.912	4.817
5	-4.4	1.957	2.752
6	-4.4	1.951	2.9
7	-4.4	1.099	3.189
8	-4.3	3.788	4.826
9	-4.1	1.58	3.36

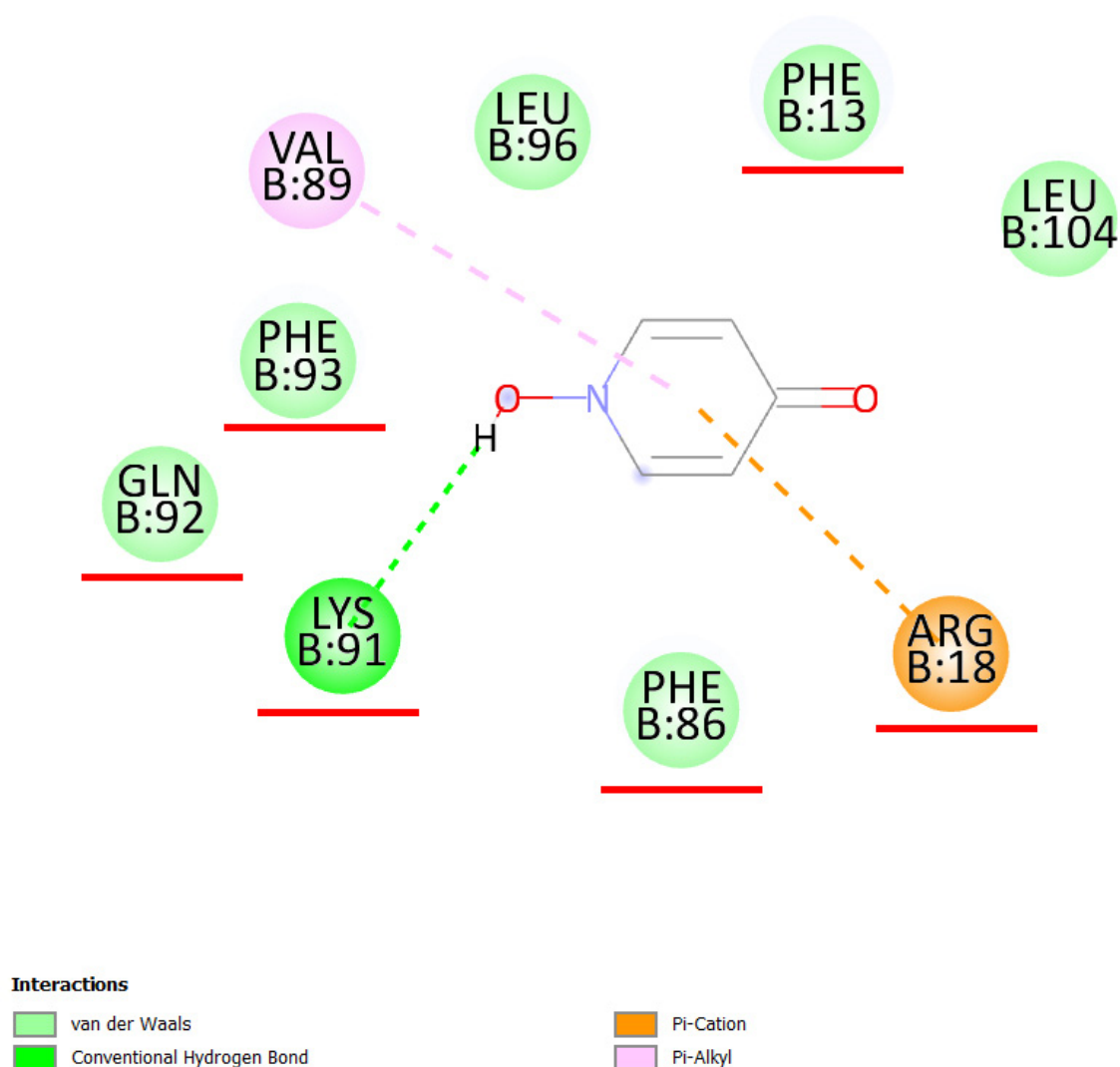
Supplementary Table S9: AutoDock Vina results for protein ligand docking between hAChE and the negative control Imidazole.

Mode	Affinity	Distance from best mode	
	(kcal/mol)	rmsd l.b.	rmsd u.b.
1	-3.3	0	0
2	-3.3	16.04	16.42
3	-3.2	16.927	17.148
4	-3.2	11.862	12.551
5	-3	16.012	16.246
6	-3	11.788	12.15
7	-3	16.386	16.685
8	-3	17.025	17.716
9	-2.9	16.189	16.412

Supplementary Table S10: AutoDock Vina results for protein ligand docking between rAChE and the negative control Imidazole.

Mode	Affinity	Distance from best mode	
	(kcal/mol)	rmsd l.b.	rmsd u.b.
1	-3.2	0	0
2	-3.2	12.014	12.21
3	-3.1	13.551	13.739
4	-3.1	16.373	16.682
5	-3.1	15.291	15.815
6	-3	17.291	17.651
7	-3	12.631	13.237
8	-3	5.996	6.58
9	-2.8	16.366	16.565

3. Docking analysis between Survivin protein and 4-hydroxypyridine 1-oxide pyridin-4-ol 1-oxide

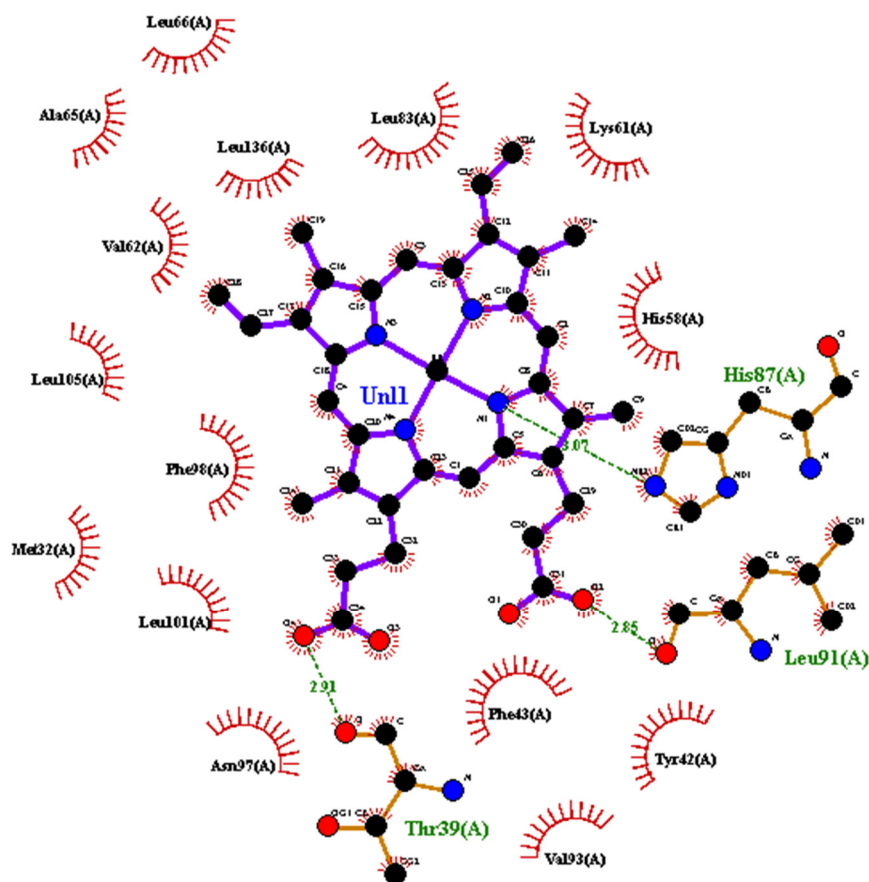


Supplementary Figure S8: The 2D representation of the protein-ligand complex formed in the Survivin protein and 4-hydroxypyridine 1-oxide pyridin-4-ol 1-oxide. The amino acid residues that were present in the original study have been marked by a red underline.

Supplementary Table S11: AutoDock Vina results for protein ligand docking between Survivin protein and 4-hydroxypyridine 1-oxide pyridin-4-ol 1-oxide.

Mode	Affinity	Distance from best mode	
	(kcal/mol)	rmsd l.b.	rmsd u.b.
1	-4.6	0	0
2	-4.5	1.799	2.119
3	-4.5	3.621	4.458
4	-4.4	1.973	3.053
5	-4.3	1.095	3.186
6	-4.3	3.834	4.07
7	-4.2	3.581	4.581
8	-4.1	3.174	4.023
9	-4.1	3.626	4.078

4. Docking analysis between Haemoglobin and Heam.



Supplementary Figure S9: The 2D representation of the protein-ligand complex formed in the Hemoglobin and the heam ligand. The characteristic “heme coordinated to the histidine residue” protein-ligand interaction can be seen between the heam ligand’s central iron atom and the Haemoglobin's Histidine amino acid.

Supplementary Table S12: AutoDock Vina results for protein ligand docking between Haemoglobin and Heam.

Mode	Affinity	Distance from best mode	
	(kcal/mol)	rmsd l.b.	rmsd u.b.
1	-11.4	0	0
2	-11.3	2.448	6.798
3	-11.1	2.469	6.164
4	-11.1	0.357	6.347
5	-10.8	4.346	9.924
6	-9.7	2.932	6.106
7	-9.7	4.683	10.216
8	-8.8	4.031	8.964
1	-11.4	0	0