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Appendix A

Supplementary data for chapter 2

CLUSTALX protein colouring:

Green	Thr, Ser, Gln, Asn
Cyan	Ala, Val, Ile, Leu, Met, Phe, Trp
Blue	Tyr, His
Magenta	Asp, Glu
Yellow	Pro
Orange	Gly
Pink	Cys, Lys, Arg

Swissprot accession numbers for multiple sequence alignment

Bos taurus	P50243
Homo sapiens	P17707, Q9BWK4
Mesocricetus auratus	P28918
Mus musculus	P31154
Rattus norvegicus	P17708
Xenopus laevis	P79888
Drosophila melanogaster	P91931, P91925, Q9VKY9
Caenorhabditis elegans	O02655
Onchocerca volvulus	Q27883
Leishmania donovani	Q25264
Trypanosoma brucei brucei	P50244
Trypanosoma cruzi	O76240, Q9UAD2
Arabidopsis thaliana	Q96286, Q96531, Q9M893
Brassica juncea	Q42613
Catharanthus roseus	Q42679

Datura stramonium	Q96555
Dianthus caryophyllus	Q39676
Helianthus annuus	O65354
Hordeum chilense	Q42829
Zea mays	O24575
Nicotiana sylvestris	O80402
Oryza sativa	O24215, O81269
Pisum sativum	Q43820
Pharbitis nil	Q96471
Solanum tuberosum	Q04694
Spinacia oleracea	P46255
Nicotiana tabacum	O04009, O49005
Saccharomyces cerevisiae	P21182

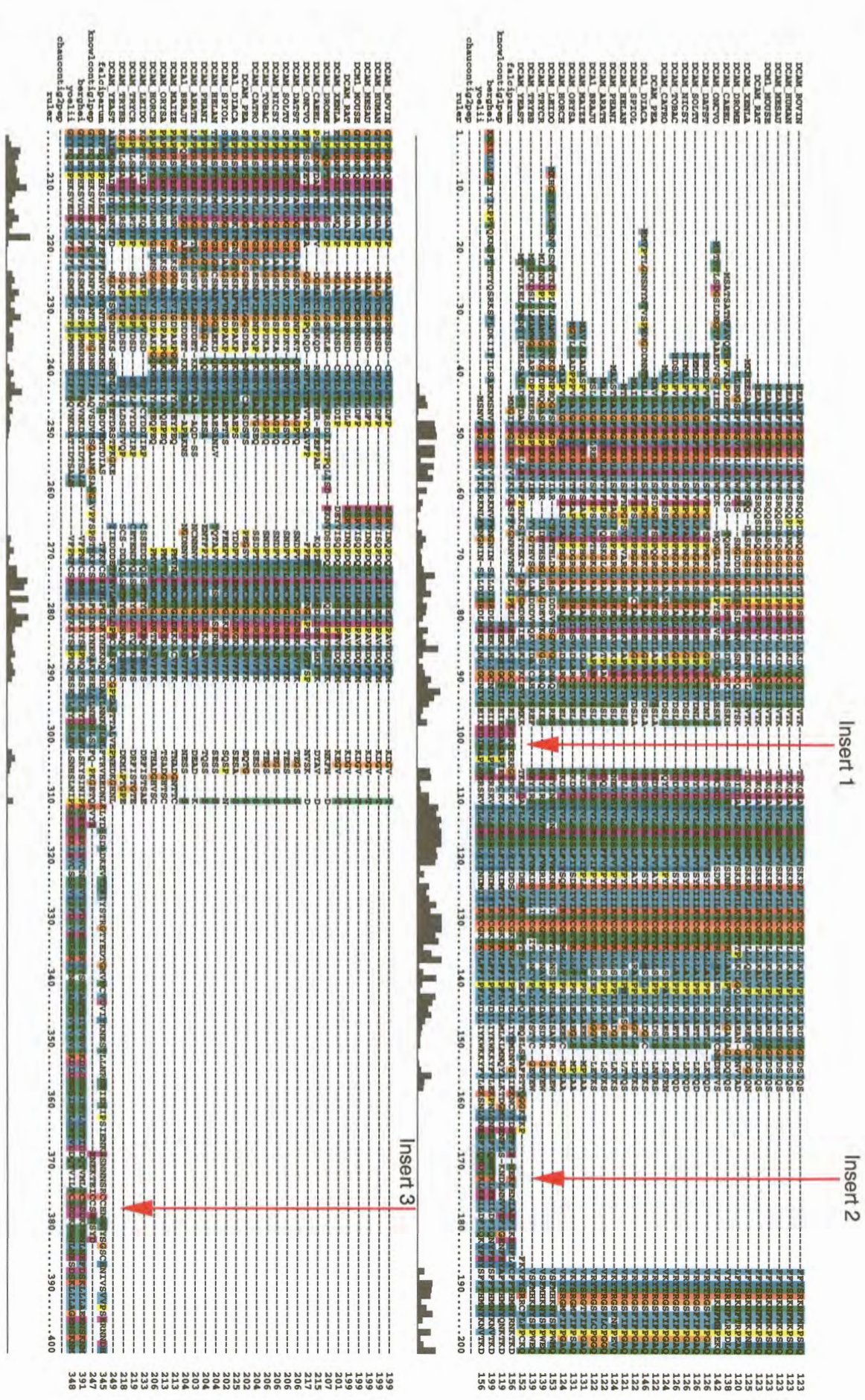


Figure A.1: Multiple alignment. All sequences used are included. Colouring of conserved and similar residues is as according to CLUSTALX defaults.

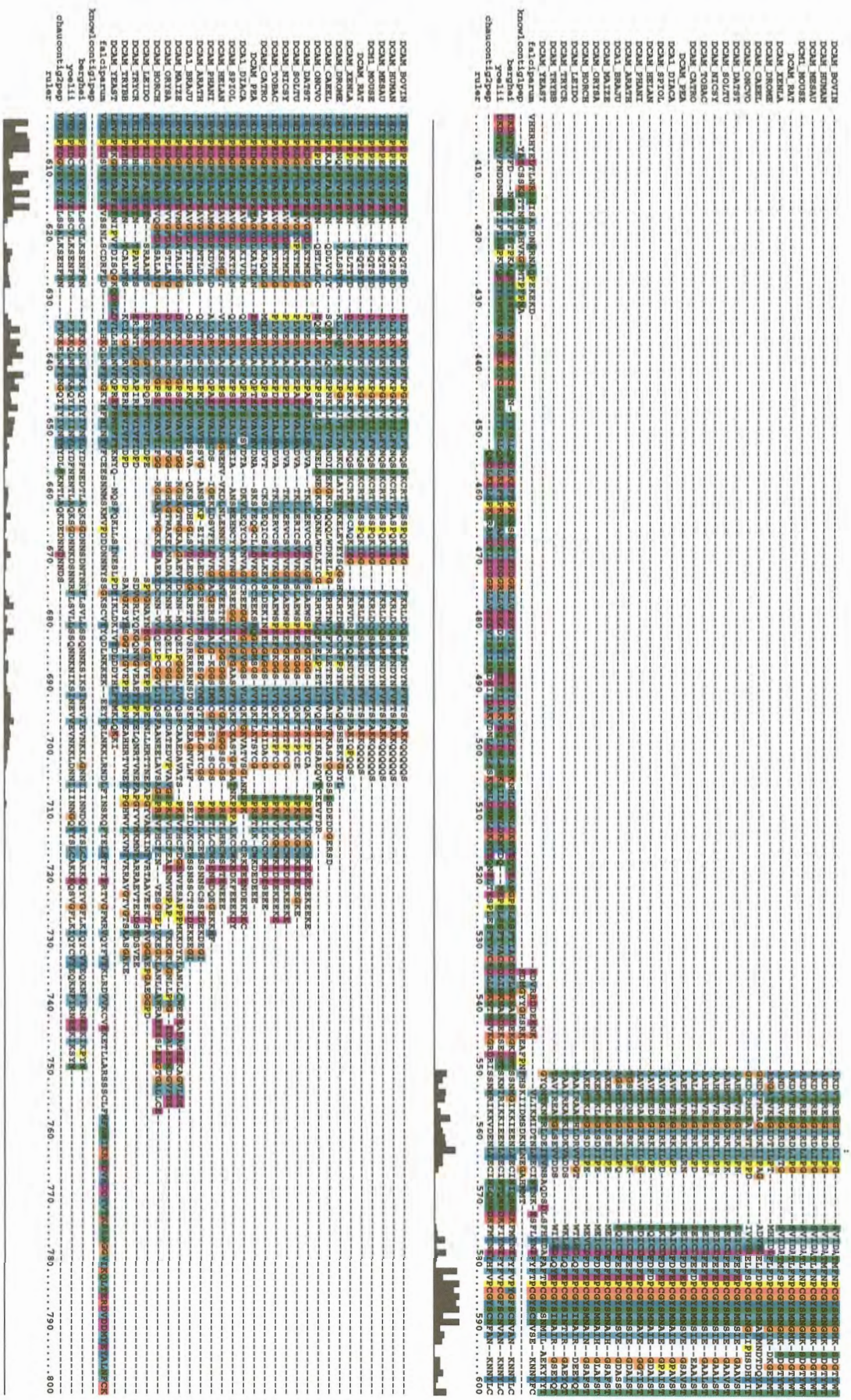


Figure A.1: Mulitiple alignment continued.

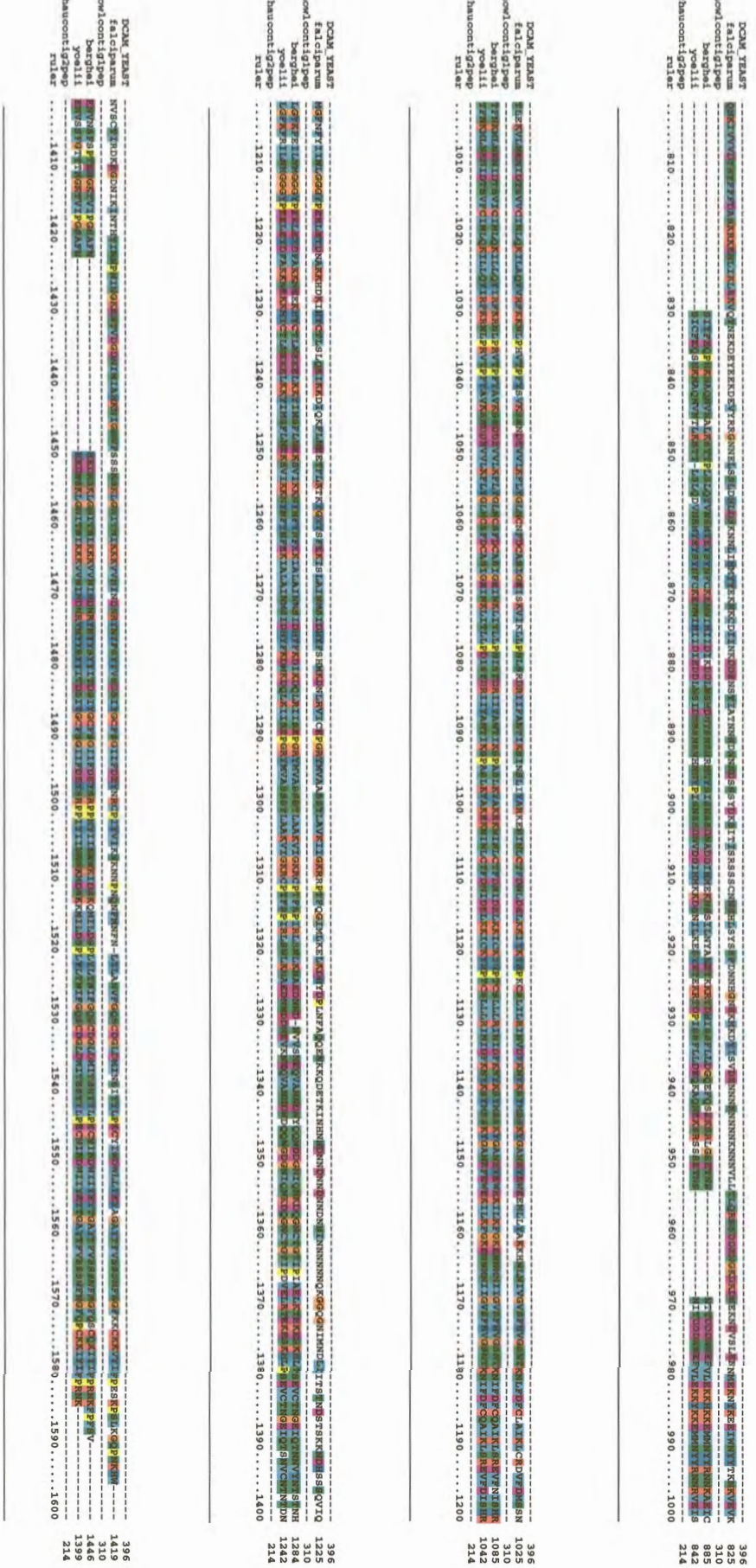


Figure A.1: Mulitiple alignment concluded.

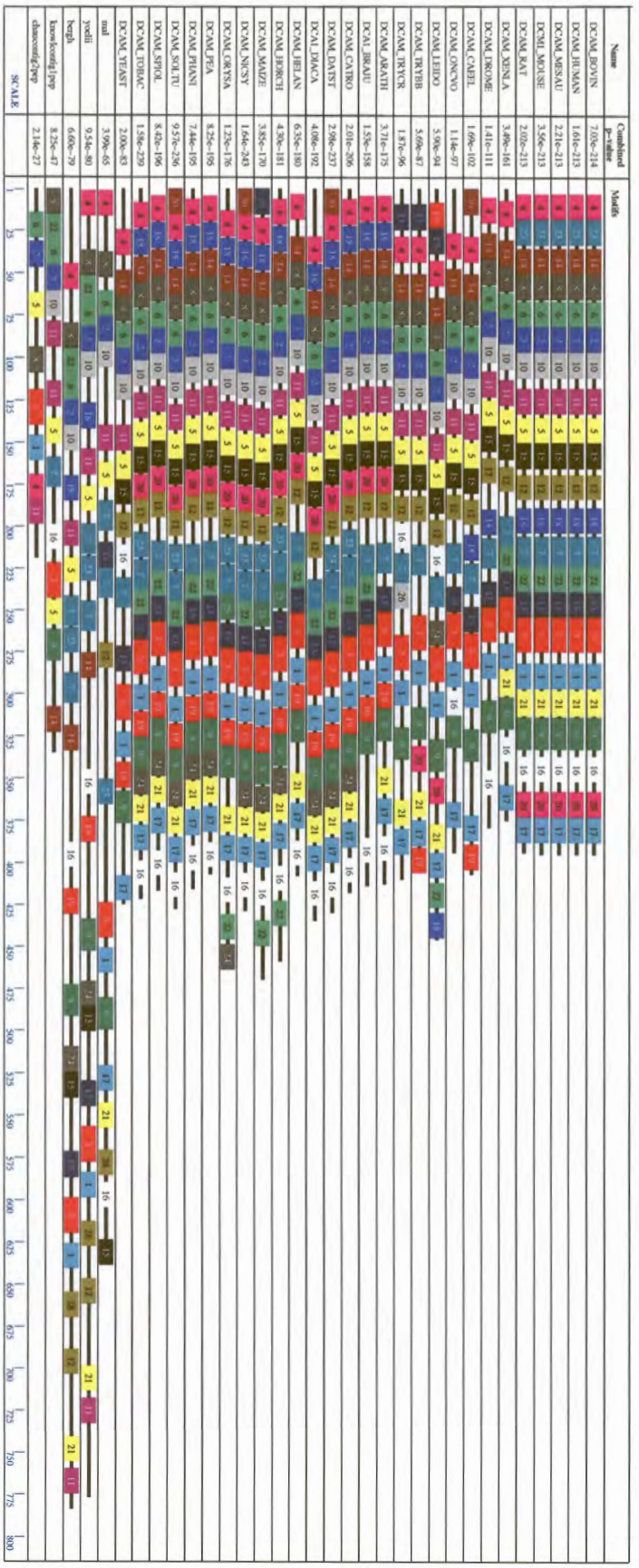


Figure A.2: Meme motifs of the set of unaligned sequences. Homologous motifs are numbered and coloured the same. Higher numbers indicate greater conservation. Motif 5 which roughly corresponds to helix 6 of the human enzyme was used to adjust the alignment.

Appendix B

Supplementary data for chapter 4

Table B.1: Hits identified from virtual screening against the internal LUDI BIOSYM database

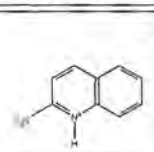
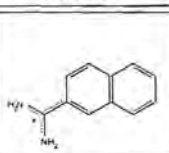
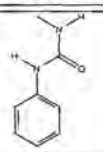
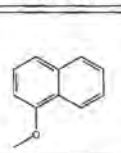
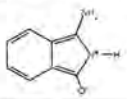
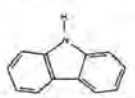
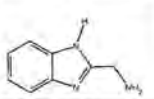
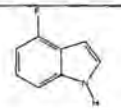
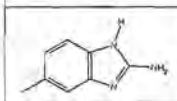
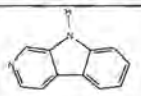
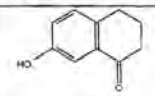
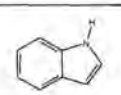
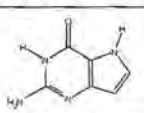
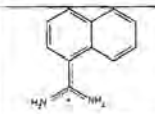
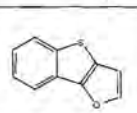
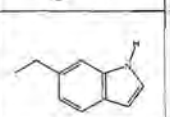
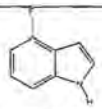
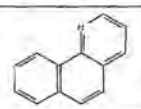
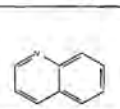
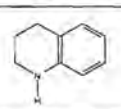
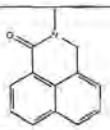
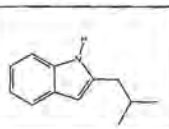
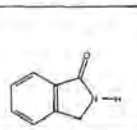
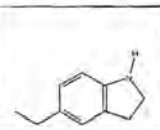
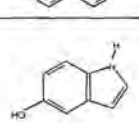
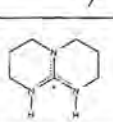
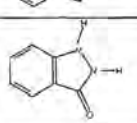
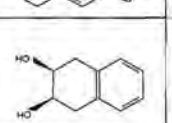
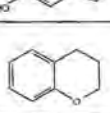
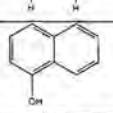
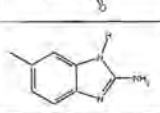
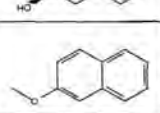
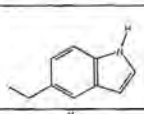
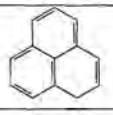
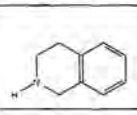
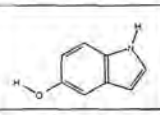
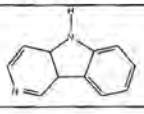
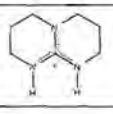
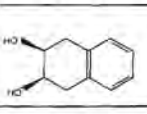
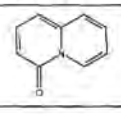
Human	Score	Model	Score	Human	Score	Model	Score
	638		680		524		549
	614		676		521		545
	585		667		518		538
	577		658		505		530
	563		625		503		524
	547		581		500		519
	544		574		500		515
	542		563		498		512
	534		563		487		508
	530		561		486		508

Table B.2: Hits identified from virtual screening against the ACD database

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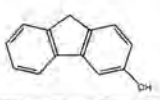
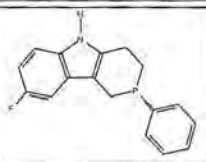
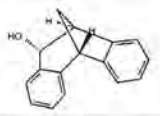
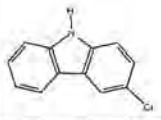
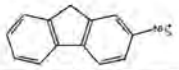
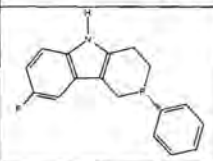
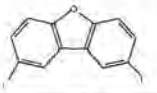
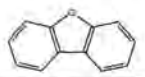
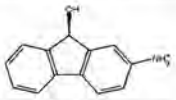
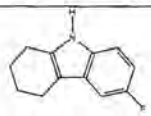
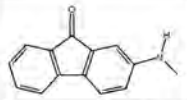
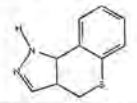
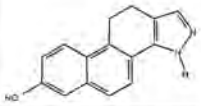
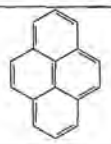
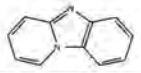
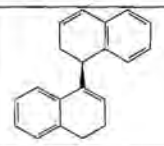
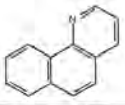
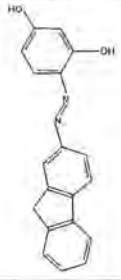
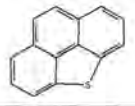
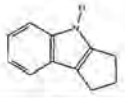
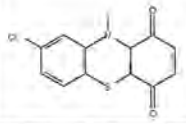
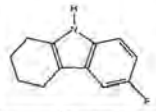
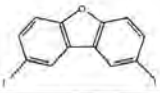
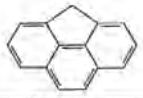
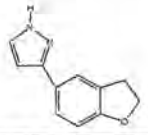
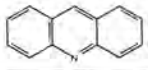
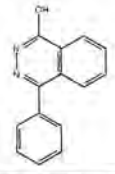
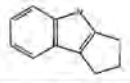
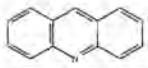
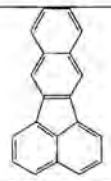
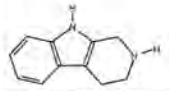
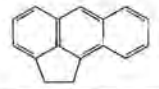
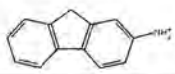
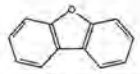
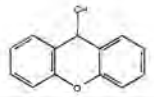
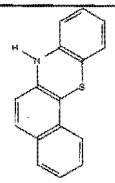
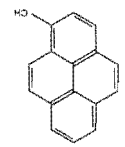
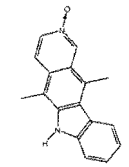
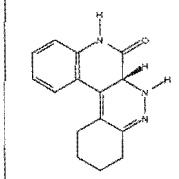
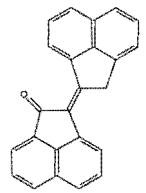
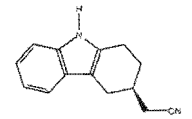
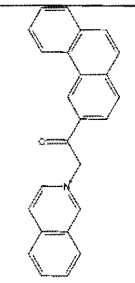
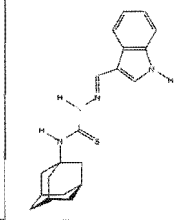
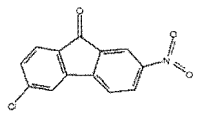
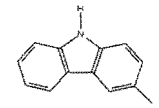
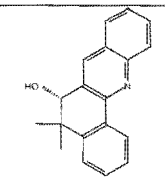
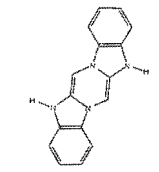
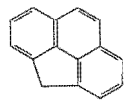
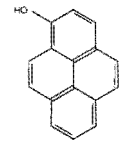
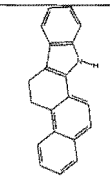
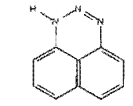
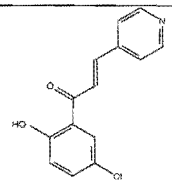
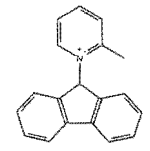
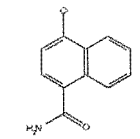
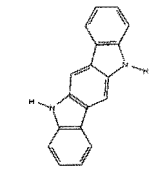
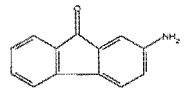
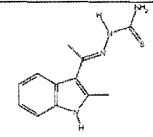
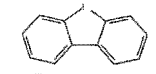
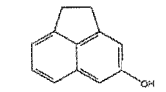
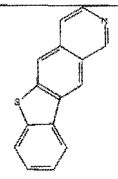
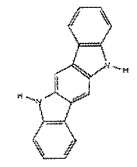
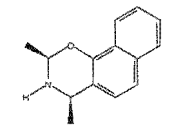
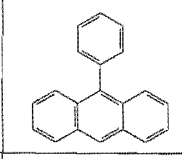
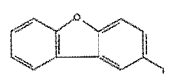
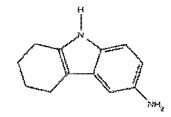
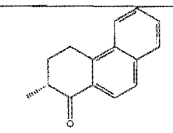
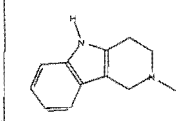
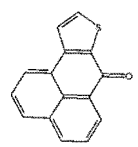
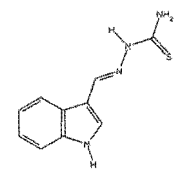
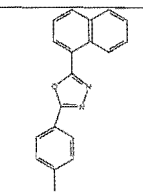
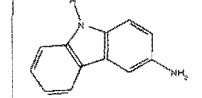
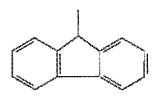
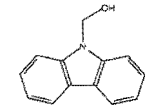
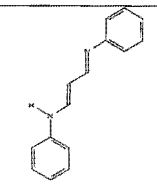
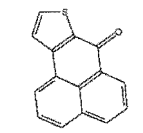
	718		832		674		709
	711		817		670		702
	709		747		668		698
	701		731		658		693
	698		729		655		692
	692		725		648		689
	688		722		646		687
	685		722		645		684
	683		714		643		676
	683		710		643		676

Table B.3: Hits identified from virtual screening against the NCI database

Human - NCI	Score	Model - NCI	Score	Human - NCI	Score	Model - NCI	Score
	717		832		649		709
	701		817		645		702
	690		747		645		698
	673		731		643		693
	672		729		641		692
	665		725		636		689
	661		722		636		687
	658		722		635		684
	656		714		635		676
	655		710		628		676