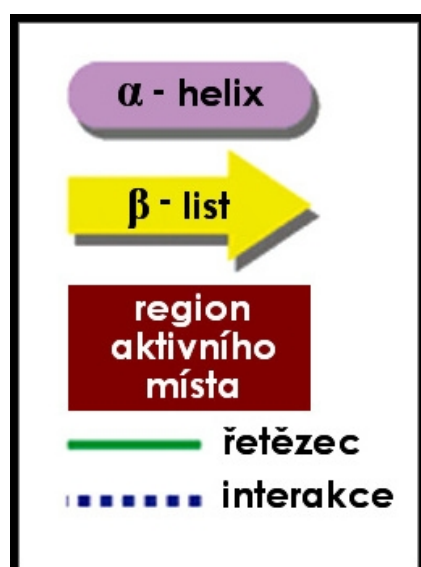


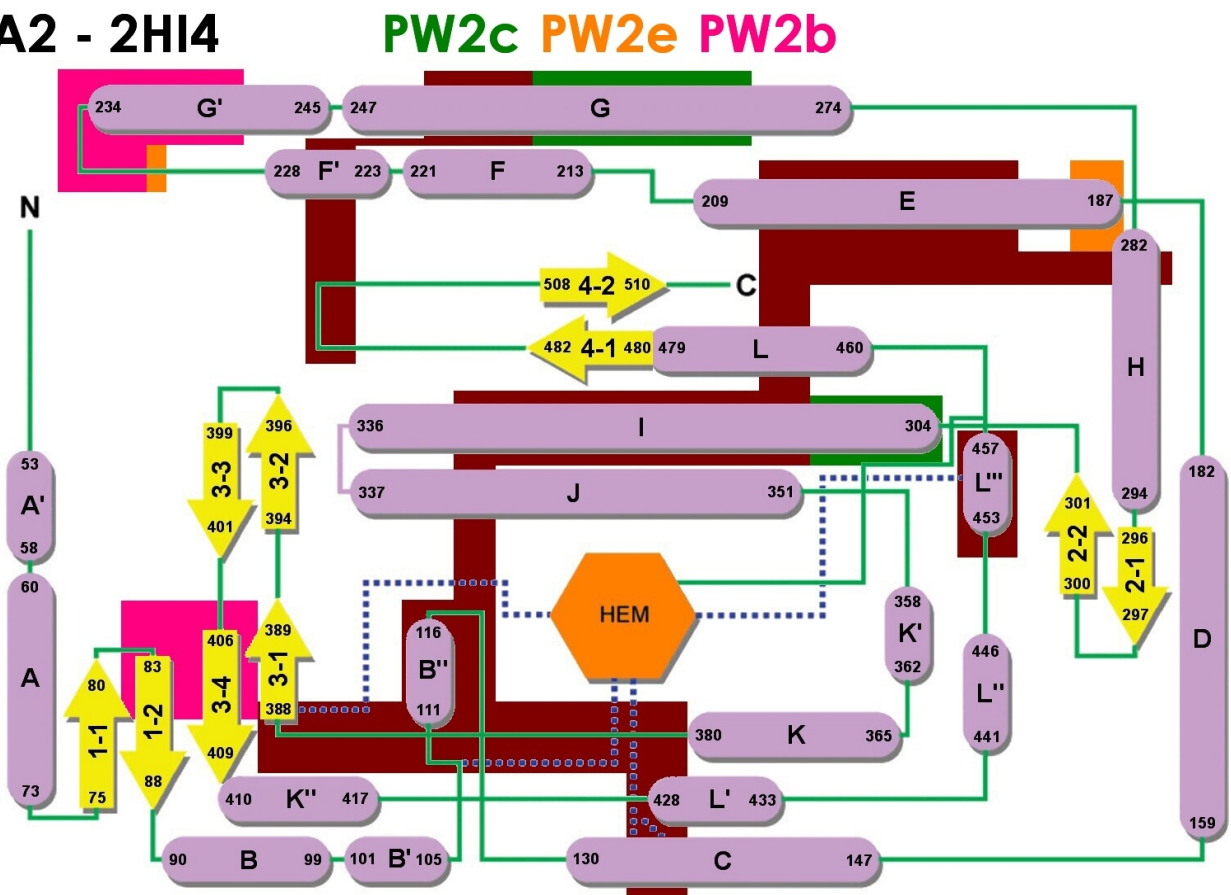
Příloha 1 – Kanálová preference

CYP	Mon	1	2	3	4	5	6	7	8	9	10
1A2	A	PW3	S	PW2c	W	PW2b	PW1	PW2e	PW2ac		
2A6	A	W ₁	S	PW3	PW2c	PW1	PW2e	PW4	W ₂	PW5	
	B	PW2e	W ₁	PW3	PW2c	PW2f	PW1	PW2d	S	W ₂	
	C	PW2e	PW4	W ₁	PW2c	PW1	PW3	S	W ₂		
	D	PW2e	W ₁	PW3	PW2c	PW1	S	W ₂	PW4		
2C8	A	PW2b	PW4	S	PW2c						
	B	PW2b	PW2e	S	PW4	PW2c	PW5				
2C9	A	S	PW2c	PW2f	PW2e	PW2b	PW3	PW4	PW5		
	B	S	PW2c	PW2f	PW3	PW2e	PW2b		PW4	PW5	
2D6	A	S	PW2f	PW2e	PW2c	PW4					
	B	S	PW2e	PW2c	PW4	PW2f	W				
	C	S	PW2e	PW2f	PW2c	PW4	W	PW2b			
	D	S	PW2e	PW2c	PW2f	PW4					
1TQN	A	PW2b	PW2f	PW4	S	PW2e	PW3	PW2ac	PW2d	PW5	PW1
2J0D	A	S	PW2b	PW2e							
	B	S	PW2b	PW2e	PW2c						

Příloha 2 – Topologie enzymů s jejich kanály

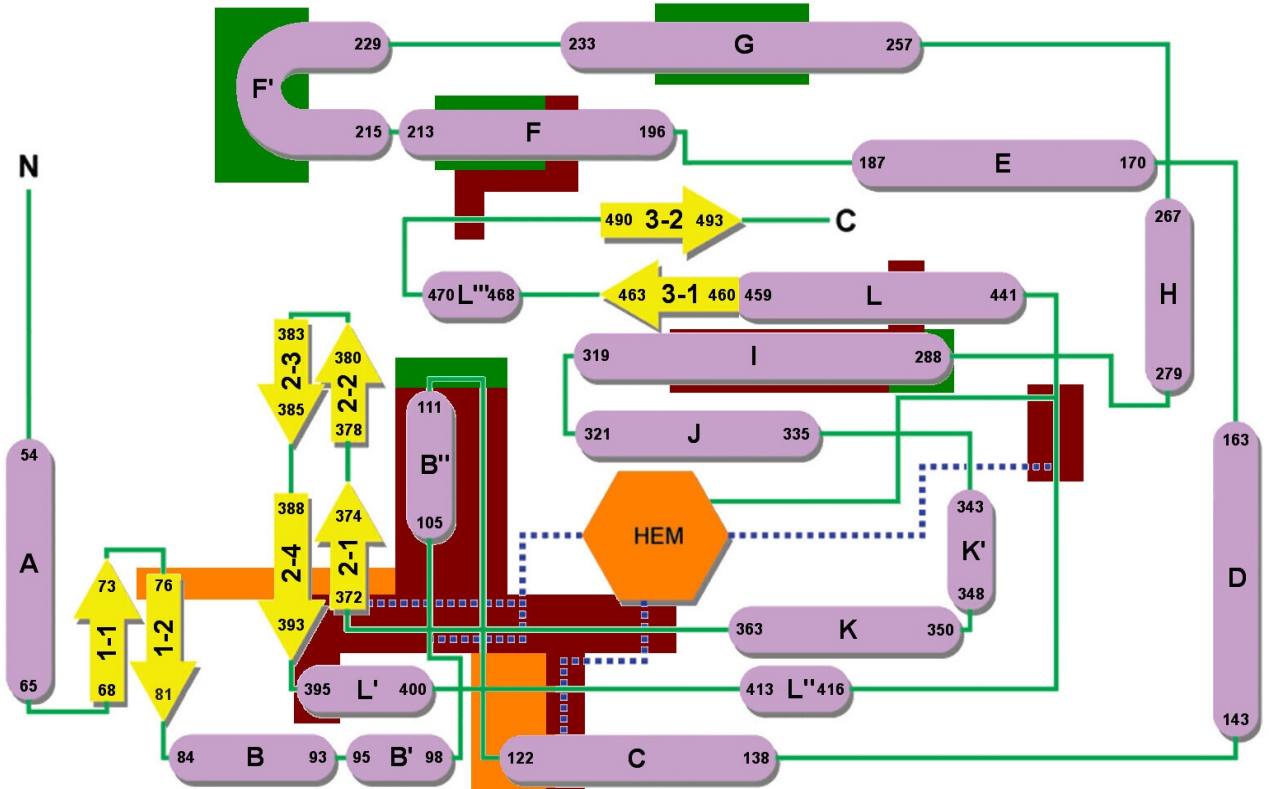


1A2 - 2H14



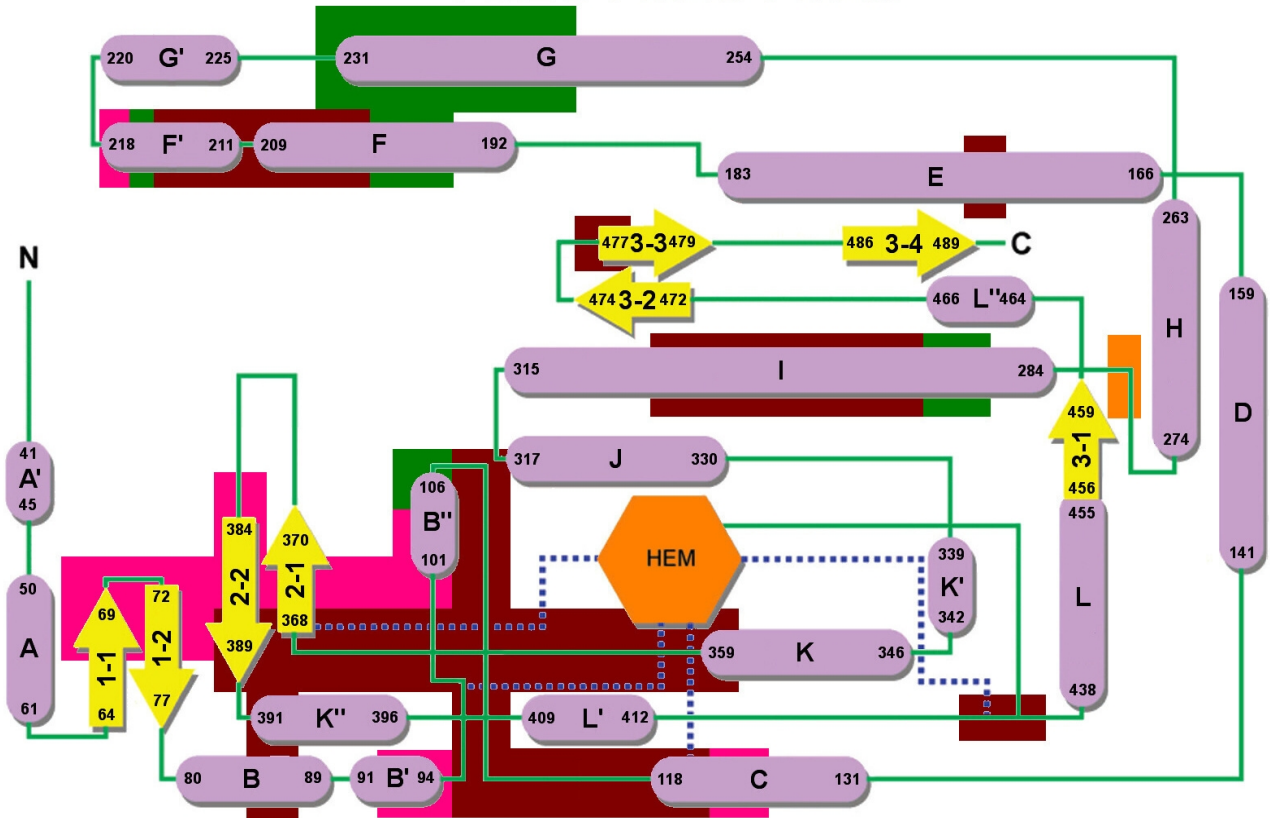
2A6 - 1Z10

PW2c PW2e



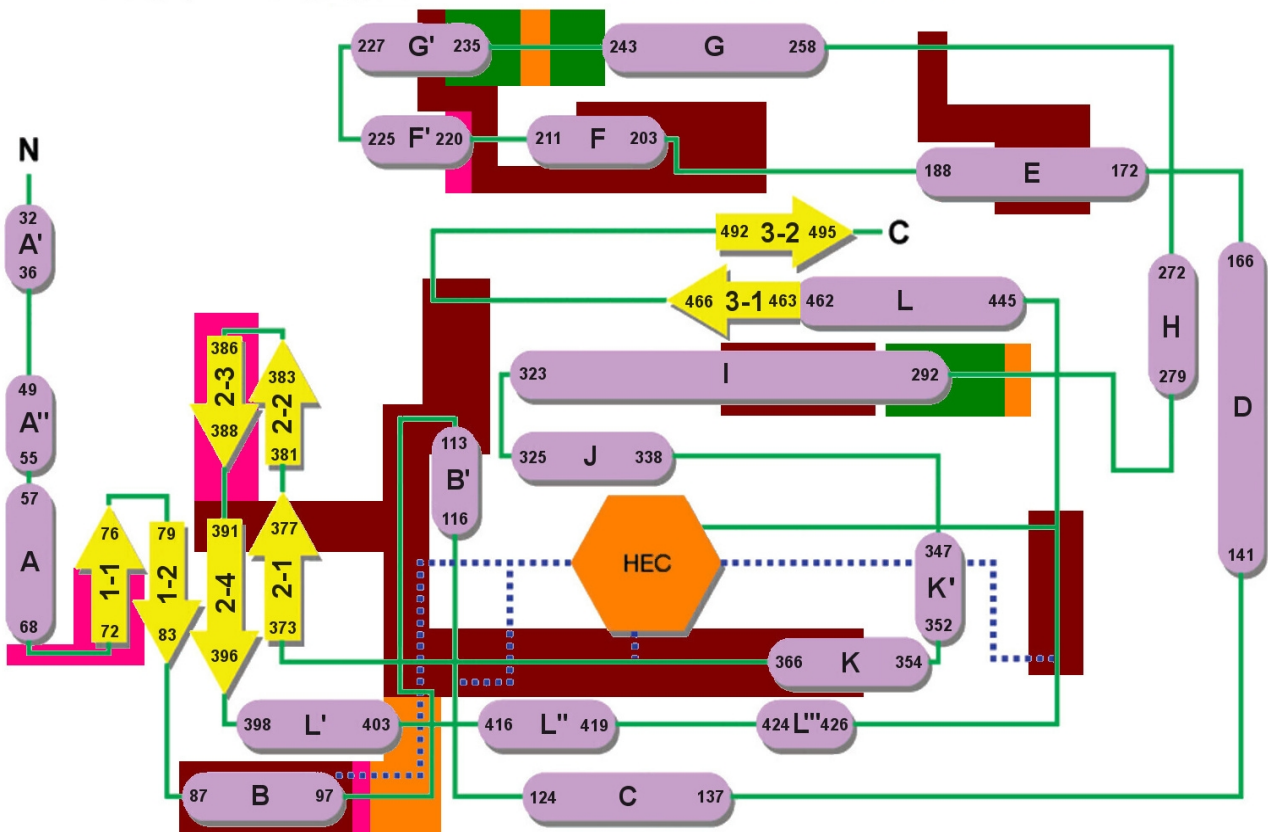
2C8 - 1PQ2

PW2c PW2e PW2b



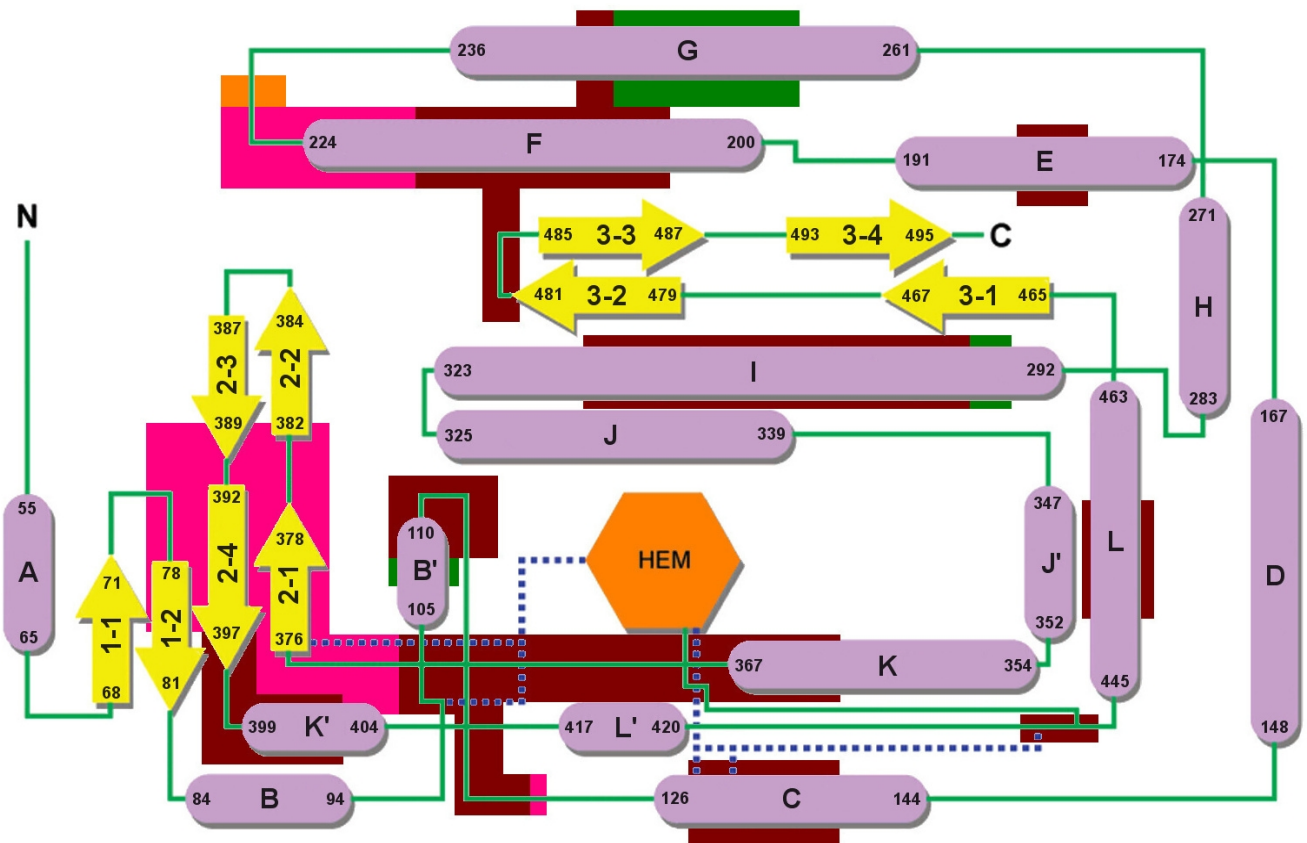
2C9 - 1OG2

PW2c PW2e PW2b



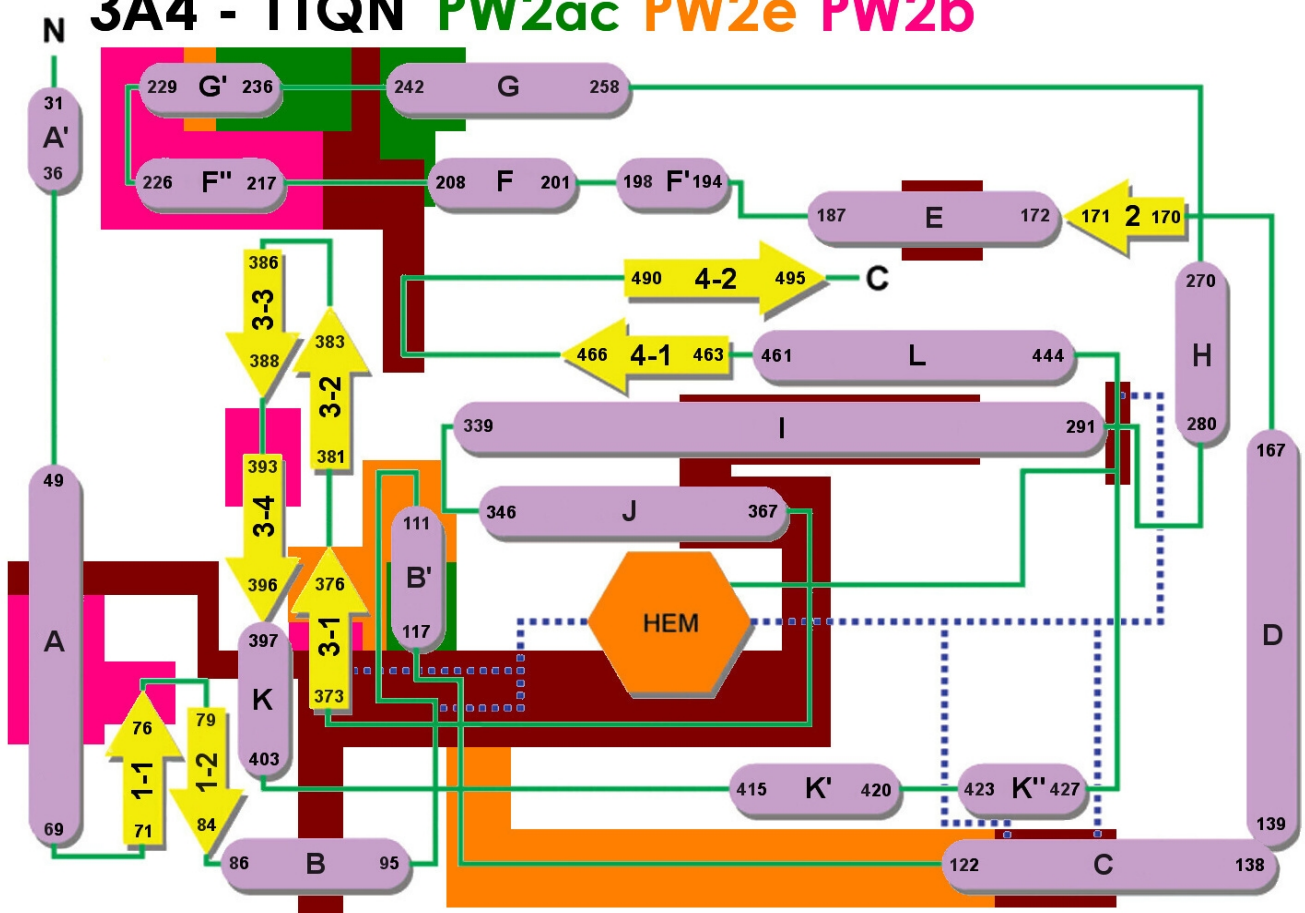
2D6 - 2F9Q

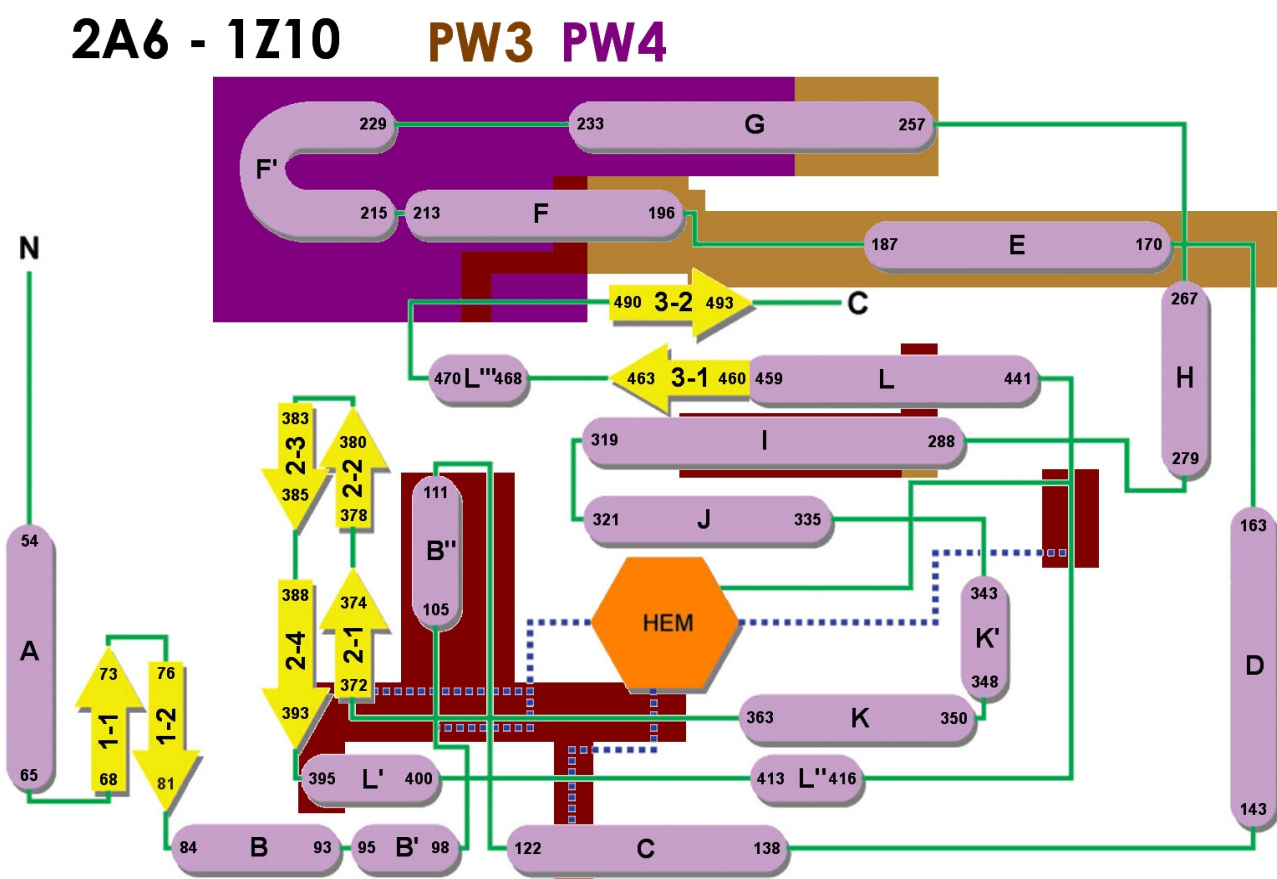
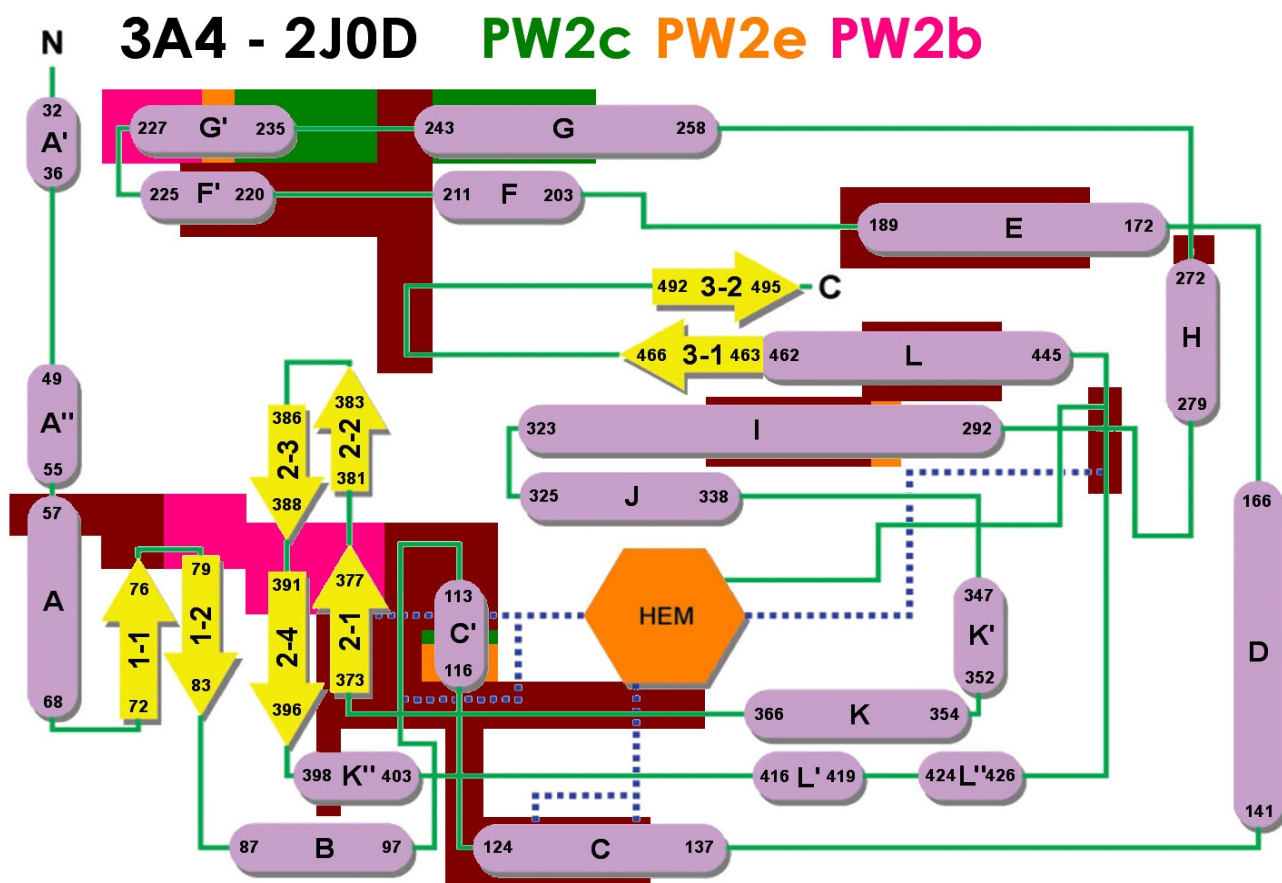
PW2c PW2e PW2b



3A4 - 1TQN

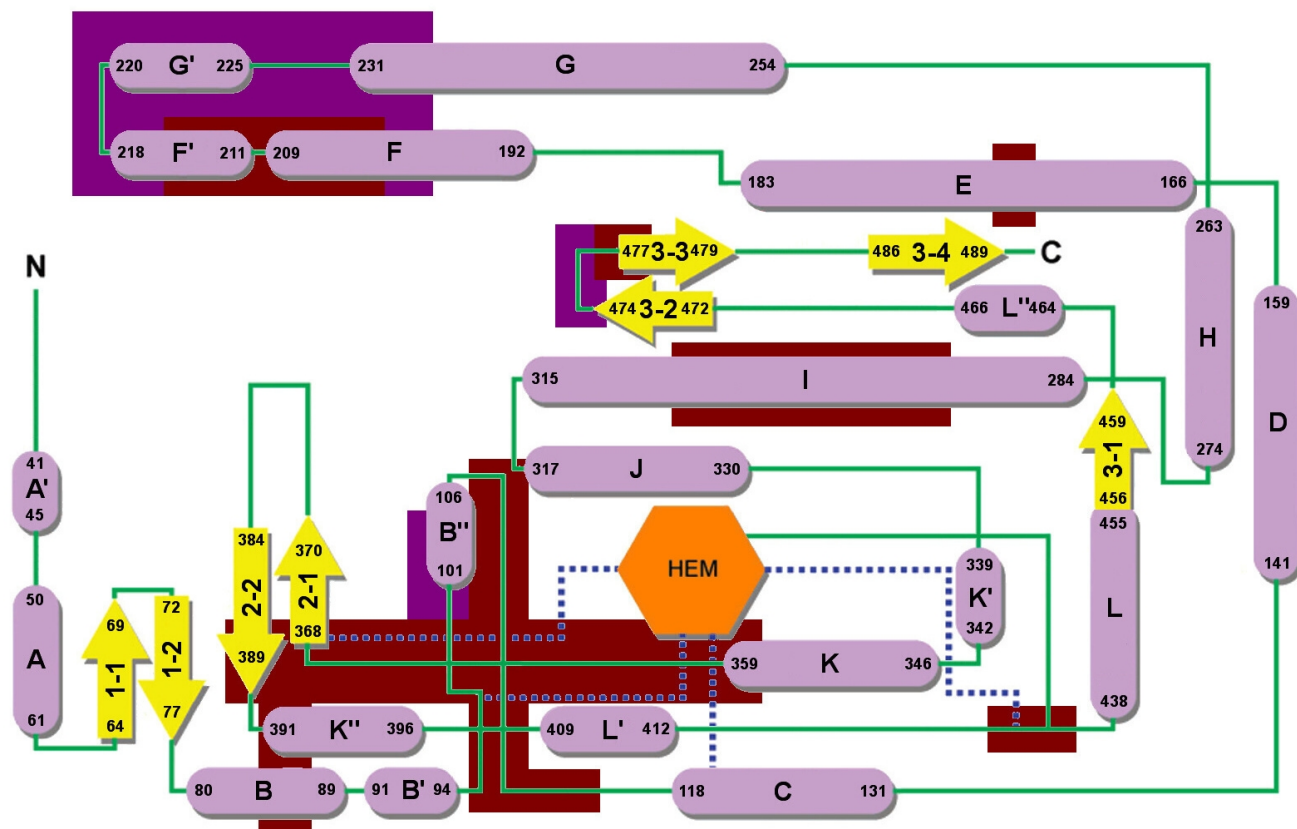
PW2ac PW2e PW2b





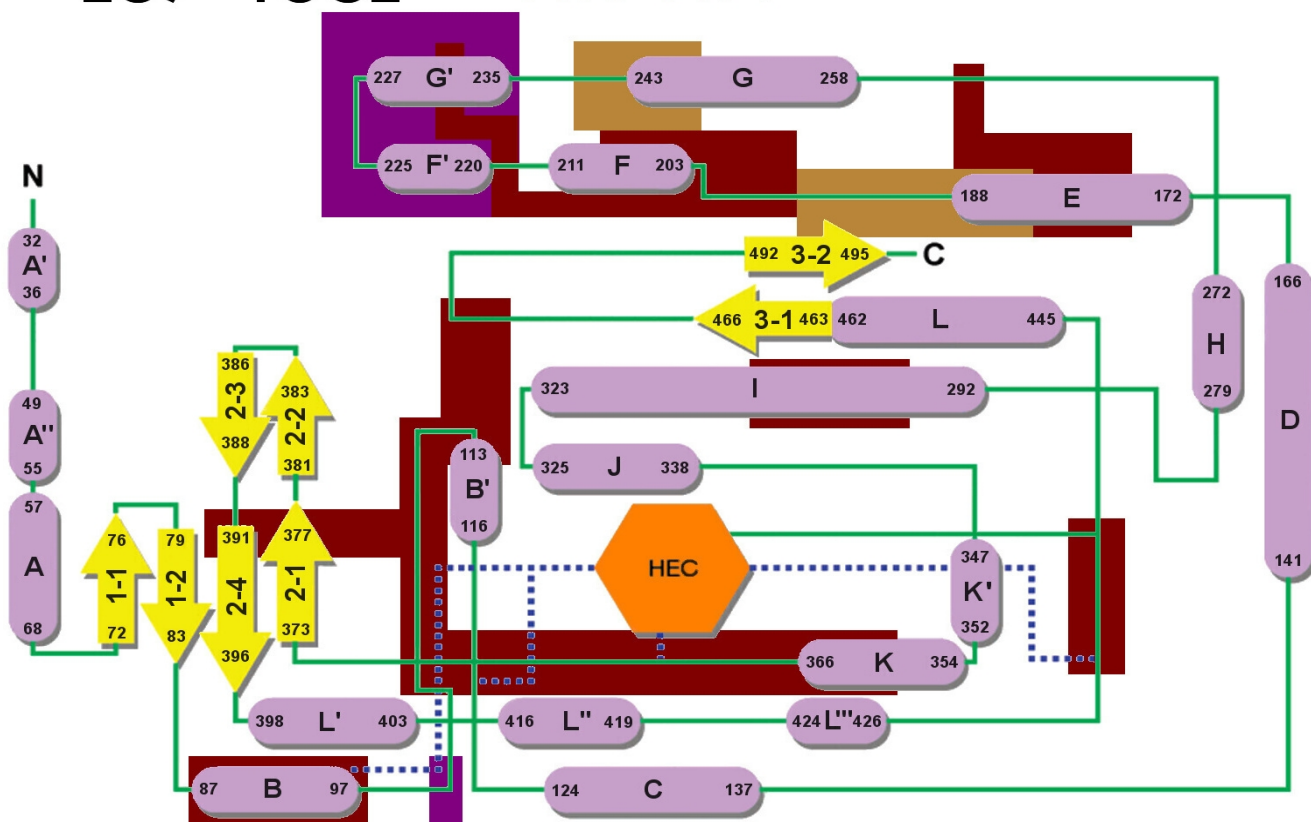
2C8 - 1PQ2

PW4

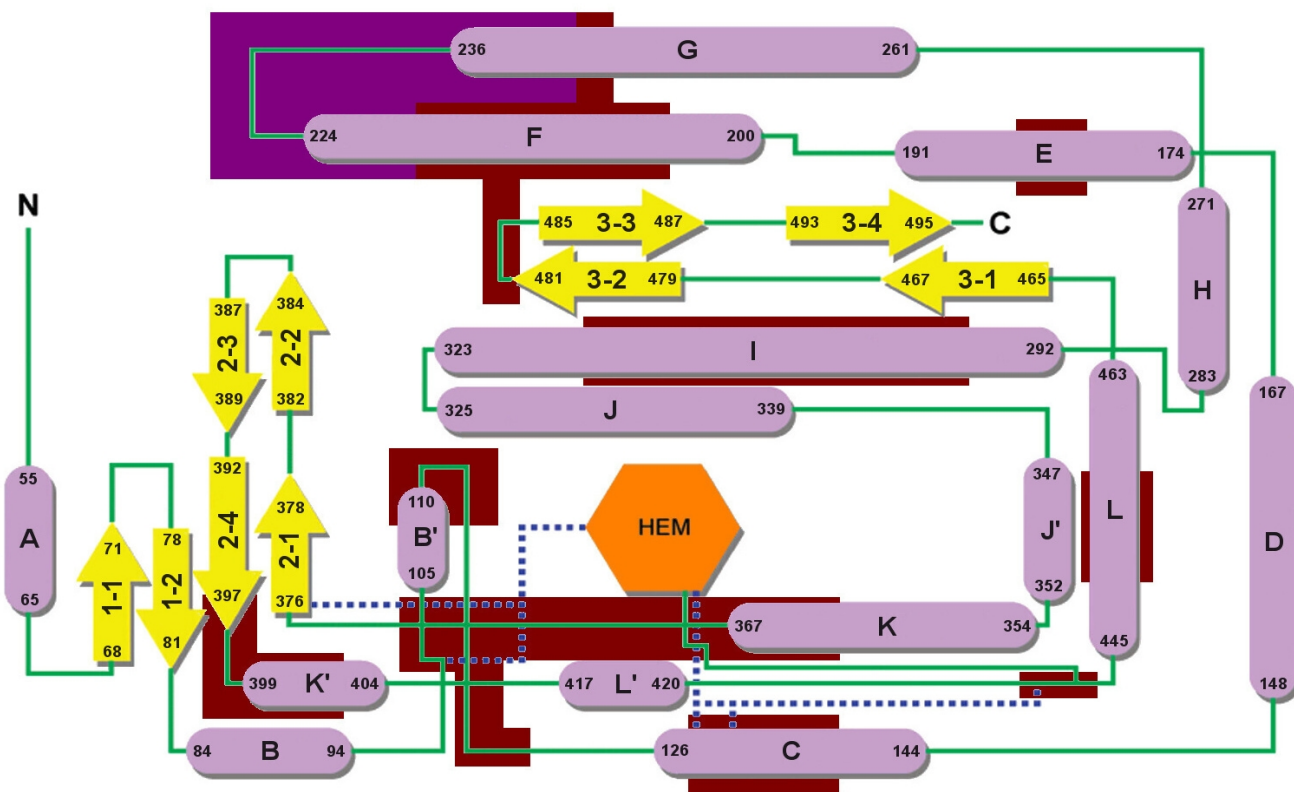


2C9 - 1OG2

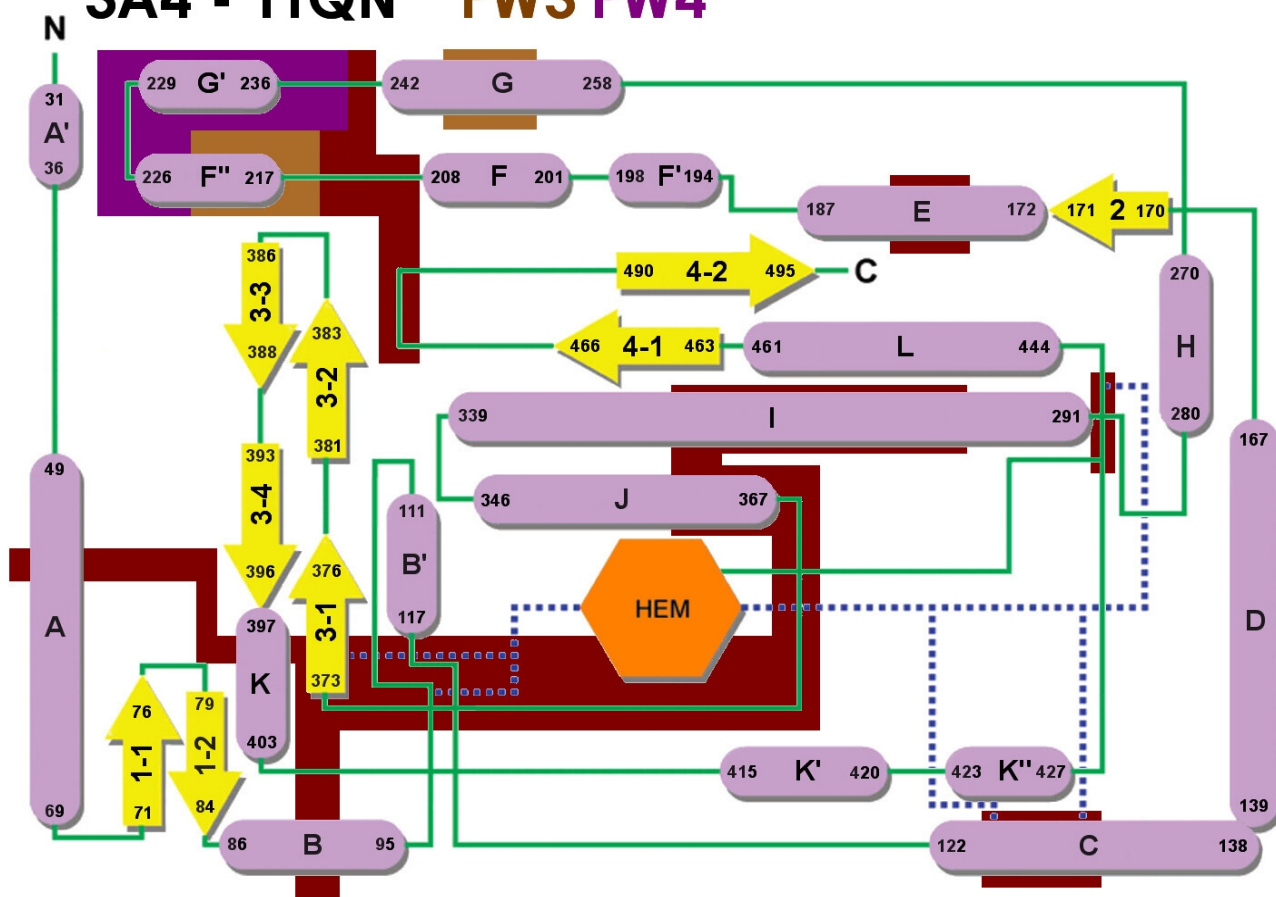
PW3 PW4



2D6 - 2F9Q PW4



3A4 - 1TQN PW3 PW4

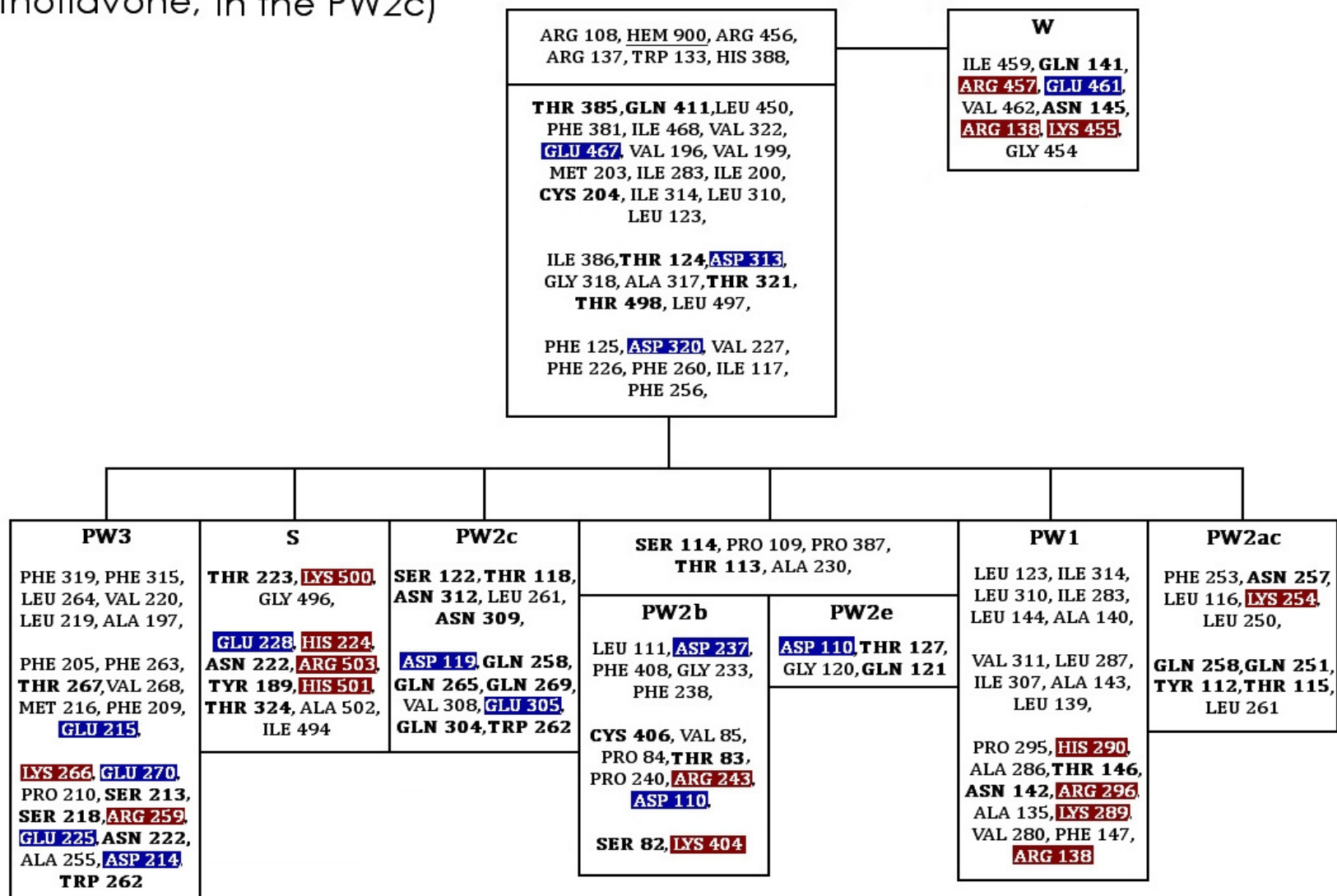


Příloha 3 – Schémata kanálů a aminokyselinových zbytků v nich

CYP 1A2

PDB ID: 2HI4

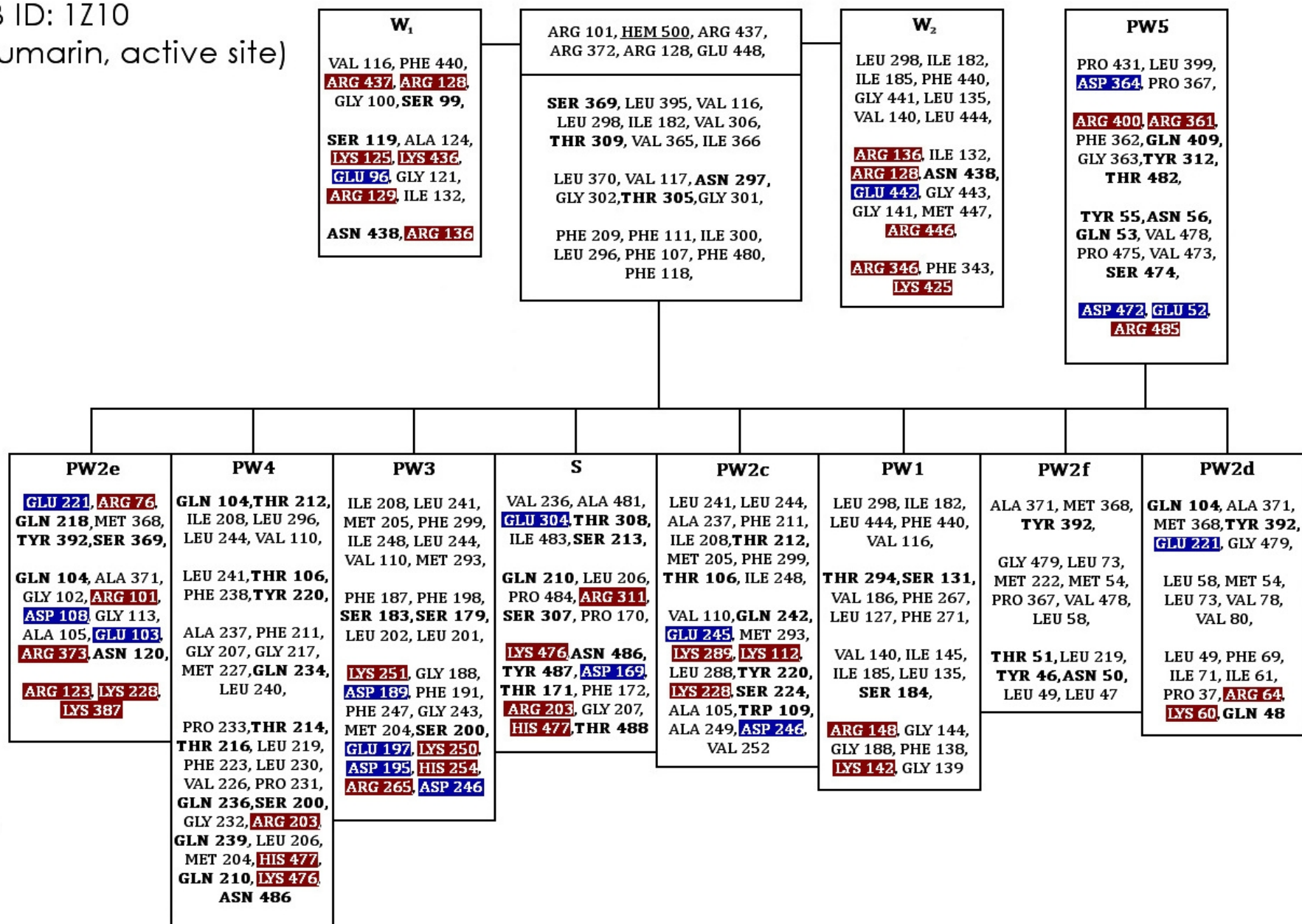
(a - naphthoflavone, in the PW2c)



CYP 2A6

PDB ID: 1Z10

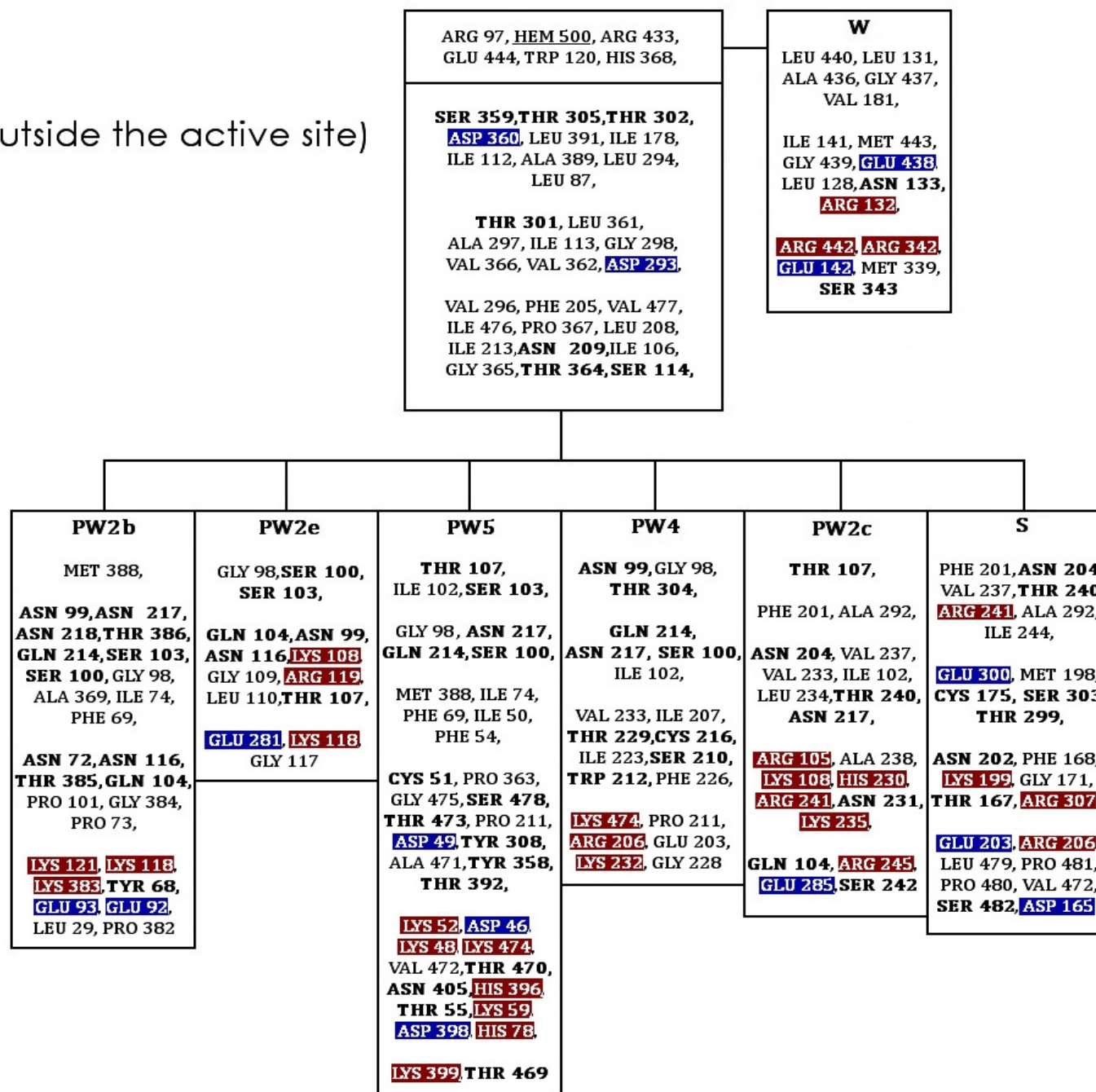
(coumarin, active site)



CYP 2C8

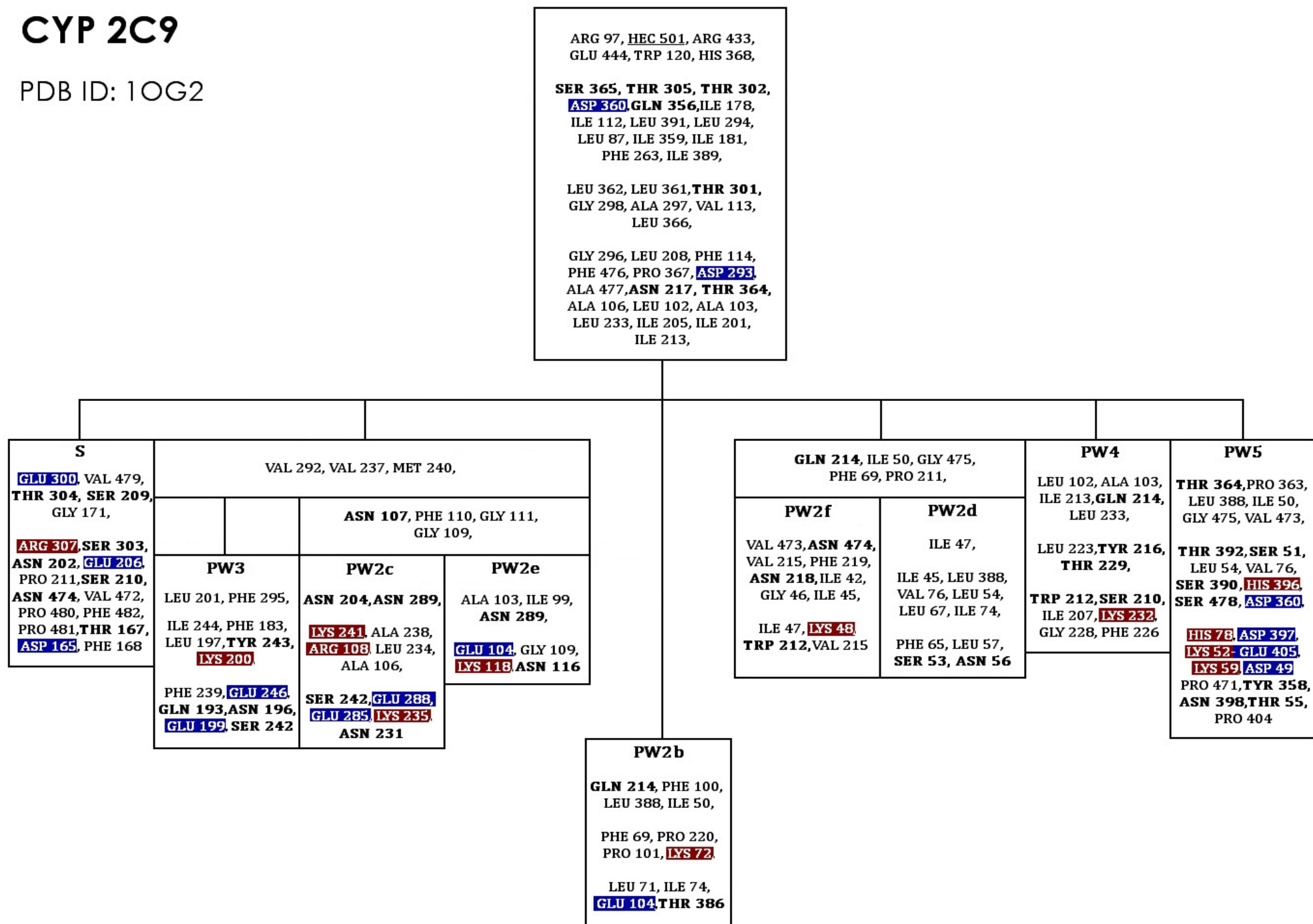
PDB ID: 1PQ2

(palmitic acid, outside the active site)



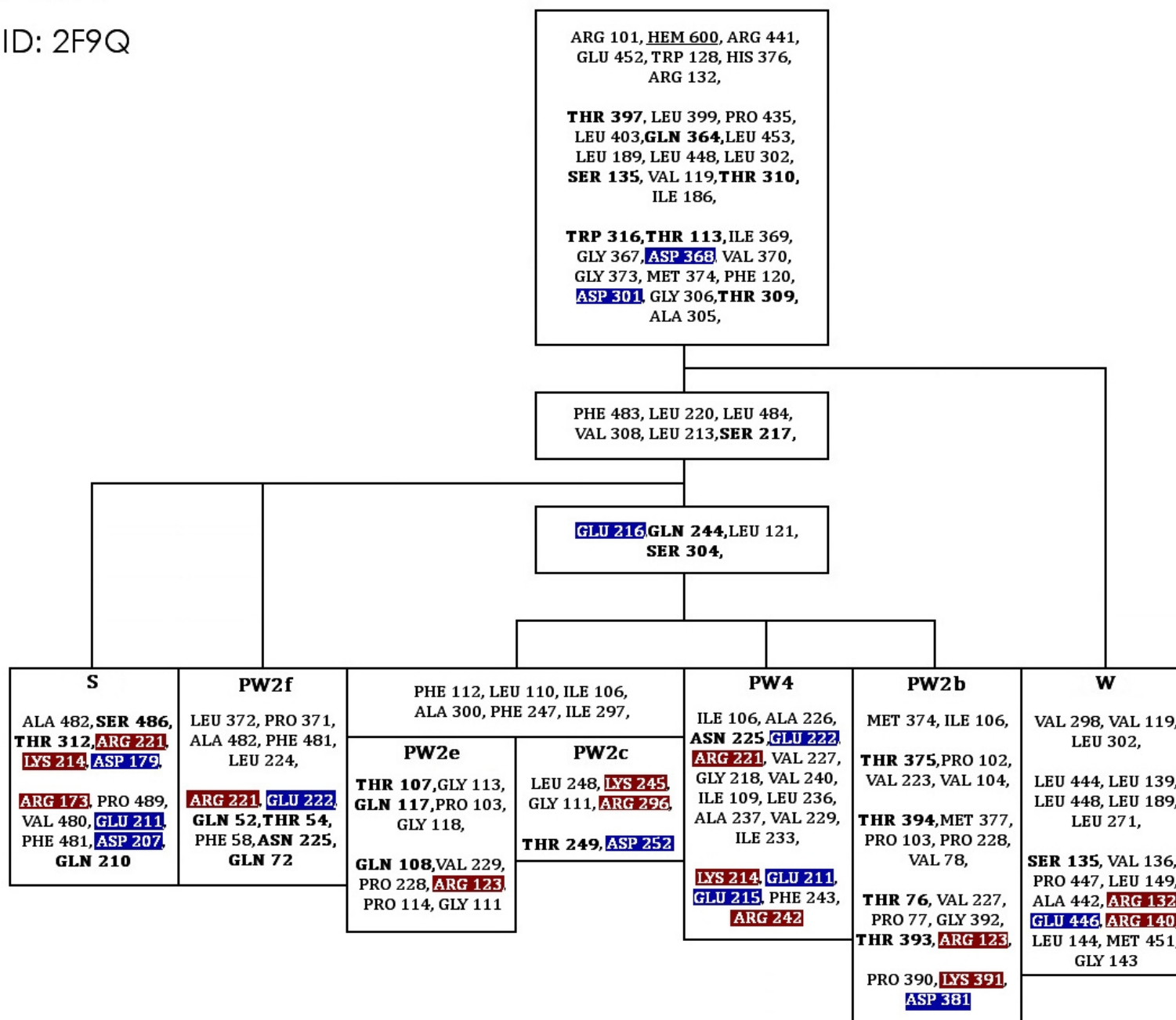
CYP 2C9

PDB ID: 1OG2



CYP 2D6

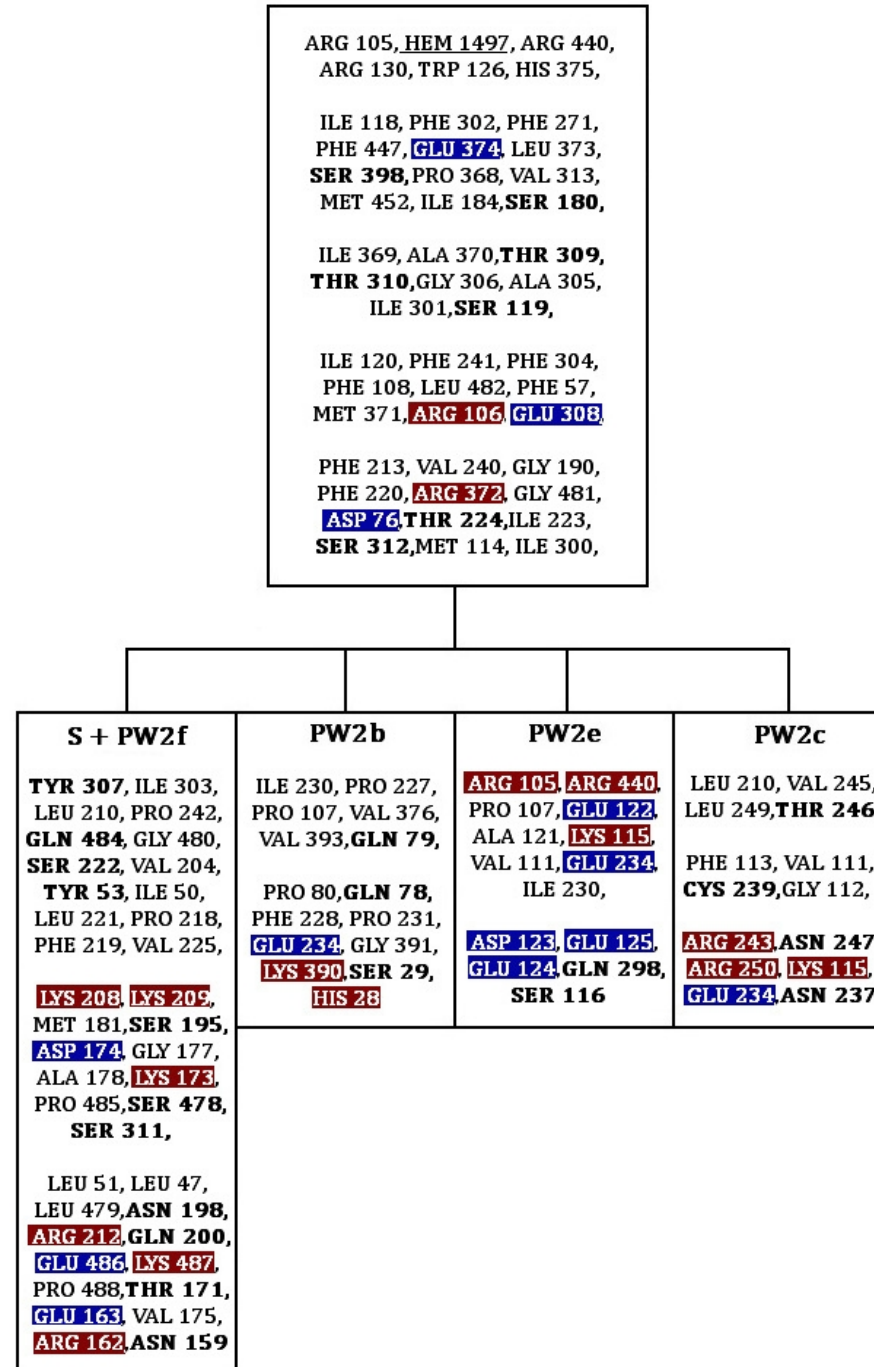
PDB ID: 2F9Q



CYP 3A4

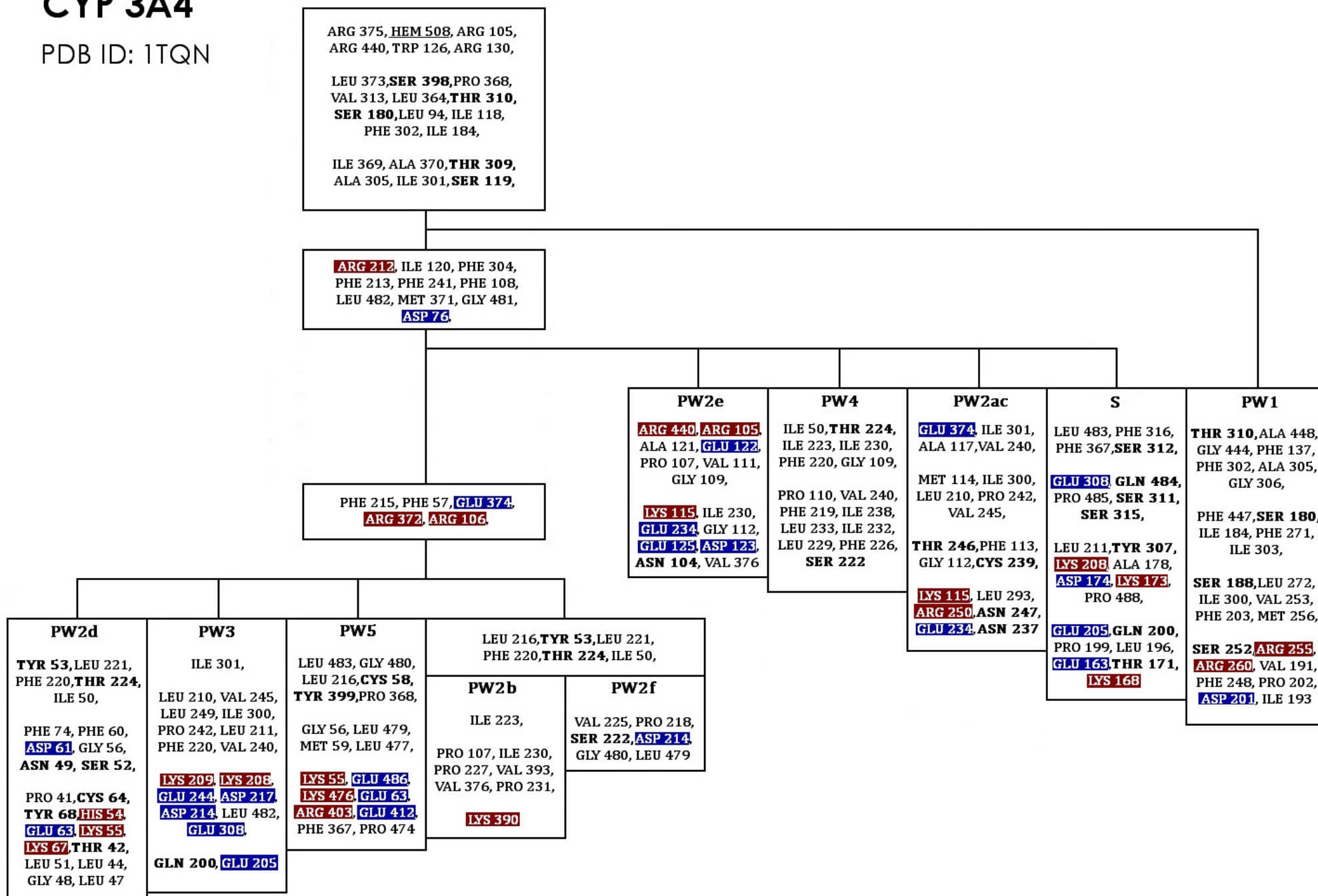
PDB ID: 2J0D

(erythromycin, active site)



CYP 3A4

PDB ID: 1TQN



Příloha 4 – Přehled reziduí v primárních sekvencích

CLUSTAL W (1.81) multiple sequence alignment

Amino acid residues of channels:

SOLVATION PW2b PW2c PW2e PW3 PW4 PW5 WATER

```

1PQ2  -----MAKKTSSKGKLP PGPTPLPIIGNMLQIDVKDICKSFTNFSKVYG
1OG2  -----MAKKTSSKG-RPPGPTPLPVIGNILQIGIKDISKSLTNLSKVYG
1Z10  -----MAKKTSSKGKLP PGPTPLPFIGNYLQNLNT EOMYNLSMKISERYG
2F9Q  -----MAKKTSSKGKLP PGPLPLPGLGNLLHVDFQNTPYCFDQLRRRFG
1TON  -MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKG-FCMFDMECHKKYG
2J0D  --MAYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKG-FCMFDMECHKKYG
2HI4  MAVLKGLRPRVPKGLKSPPEPWGWPLLGHVLT LGKN-PHLALS RMSQRYG
1OG2  -----

```

```

1PQ2  PVFTVYFGMNPIVVFHGYEAVKEALIDNGE-EFSGRGNSPISORITKGLG
1OG2  PVFTLYFGLKPIVVVHGYEAVKEALIDLGE-EFSGRGIFPLAERANRGFG
1Z10  PVFTIHLGPRRVVVL CGHDAVREALVDOAE-EFSGRGEQATFDWVFKGYG
2F9Q  DVFSLQLAWTPVVVLNGLAAVREALVTHGE-DTADRPPVPITQILGFGPR
1TON  KVGWGFYDGOQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAIS
2J0D  KVGWGFYDGOQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAIS
2HI4  DVLQIRIGSTPVLVLSRLDTIRQALVRQGD-DFKGRPDLYTSTLITDGQS
1OG2  -----

```

```

1PQ2  ----IISSNGKRWKEIRRFSLTTLRNFGMGKR-----SIEDRVQEEAH
1OG2  ----IVFSNGKKWKEIRRFSLMTLRNFGMGKR-----SIEDRVQEEAR
1Z10  ----VVFSNGERAKQLRRFSIATLRDFGVGKR-----GIEERIQEEAG
2F9Q  SQGVFLARYGPAWREORRFSVSTLRNLGLGKK-----SLEQWVTEEAA
1TON  -----IAEDEEWKRLRSLLSPTFTSGKLKEM-----VPIIAQYGDVL
2J0D  -----IAEDEEWKRLRSLLSPTFTSGKLKEM-----VPIIAQYGDVL
2HI4  --LTFSTDSGPVWAARRBLAQNALNTFSIASDPASSSSCYLEEHVSKAK
1OG2  -----

```

```

1PQ2  CLVEELRKTASP--CDPTFILGCAPCNVICSVVFQKRFDYKDQONFLTLM
1OG2  CLVEELRKTASP--CDPTFILGCAPCNVICSIIFHKRFDYKDQOFLNLM
1Z10  FLIDALRGTTGAN--IDPTFFLSRTVSNVISSIVFGDRFDYKDKEEFLSLL
2F9Q  CLCAAFANHSGRP--FRPNGLLDKAVSNVIASLT CGRRFEYDDPRFLRLL
1TON  VRNLRREAETGKP--VTLKDVFGAYSMDVITSTSFVGNIDSLNPNQDPFV
2J0D  VRNLRREAETGKP--VTLKDVFGAYSMDVITSTSFVGNIDSLNPNQDPFV
2HI4  ALISRLQELMAGPGHFDPYNQVVSVANVIGAMCFGQHFPESSEMLSLV
1OG2  -----

```

```

1PQ2  KRFNENFRILNS-PWIOVCNNEPPLLIDCFPGTHNKKVLKNVALTRSYIREK
1OG2  EKLNENIEILSS-PWIOVYNNFPALLDYFPGTHNKKLVAFMKSYILEK
1Z10  RMMLGIFQFTST-STGQLYEMFSSVMKHLPGPOQOAFOLLOGLED FIAKK
2F9Q  DLAQEGLEESG-FLREVLNAV-VDRHIPALAGKVLRFQKAFLTOLDEL
1TON  ENTKKLLRFDFLD PFFLSITVFPFLIPILEVLNICVFPR E VTNFLRKSVK
2J0D  ENTKKLLRFDFLD PFFLSITVFPFLIPILEVLNICVFPR E VTNFLRKSVK
2HI4  KNTHEFVETASS----GNPLDFFPILRYLPNPALQRFKAFNQRF LWFLQK
1OG2  -----

```

1PQ2 VKEHQASLDVNNP-RDFIDCFLIKMEQEKDNQKSEFNIEENLVGTVA^{DL}FV
 1OG2 VKEHQESMDMNNP-QDFIDCFLMKMEKEKHNPSEFTIESLENTAV^{DL}FG
 1Z10 VEHNQRTLDPNSP-RDFIDSFLIRMQEEEEKNPNTEFYLNKLVMTTLNLF
 2F9Q LTEHRMTWDPAQPPRDLTEAFLAEMEKAKGNPESSEFNENLRIVVA^{DL}FS
 1TON RMKESRLEDTOKHRVDFLOLMIDSONSKETESHKALSDLELVAQSIIFIF
 2J0D RMKESRLEDTOKHRVDFLOLMIDSONSKETESHKALSDLELVAQSIIFIF
 2HI4 TVQEHYQDFDKNSVRDITGALFKHSHKKGPRASGNLIPQEKIVNLVNDIFG
 1OG2 -----

1PQ2 AGT^ETTSTTLRYGLLLLLLKHPVTAKEVQEEIDHVIGRHRSPCMQDRSHMP
 1OG2 AGT^ETTSTTLRYALLLLLLLKHPVTAKEVQEEIERVIGRNRSPCMQDRSHMP
 1Z10 GGT^ETVSTTLRYGFLLLMKHPEVEAKVHEEIDRVIGKNRQPKFEDRAKMP
 2F9Q AGMVTSTTLAWGLLLMILHPDVQRRVQEEIDDVIGQVRRPEMGDQAHMP
 1TON AGY^ETTSSVLSFIMYELATHPDVQOKLQEEIDAVLPNKAPPTYDTVLQME
 2J0D AGY^ETTSSVLSFIMYELATHPDVQOKLQEEIDAVLPNKAPPTYDTVLQME
 2HI4 AGFDTVTTAISWSLMYLVTKEPIQRKIQKELDTVIGRERRPRLSDRPQLP
 1OG2 -----

1PQ2 YTDAVVHEIQORYS^{DL}VPTGVPHAVTTDTKFRNYLIP^KGTTIMALLTSVLH
 1OG2 YTDAVVHEVQRYI^{DL}LPTSLPHAVTCDIKFRNYLIPKGTTILISLTSVLH
 1Z10 YMEAVIHEIQRF^{GD}VIPMSLARVKKDTKFRDFFLPKGTEVYPMLGSLV^R
 2F9Q YTTAVIHEVQRF^{GD}IVPLGMTHMTSRDIEVQGFRI^PKGTTLITNLSSVLK
 1TON YLDMVVNETLRLFP^{IA}MR-LERVCKKDVEINGMFIP^KGVVVMIPSYALH^R
 2J0D YLDMVVNETLRLFP^{IA}MR-LERVCKKDVEINGMFIP^KGVVVMIPSYALH^R
 2HI4 YLEAFILETFRHSSFLPFTIPHSTTRDTTLNGFYIPK^KCCVFVNQWQVNH
 1OG2 -----

1PQ2 DDKEFPNPNI^FDPGHFLDKNGNFK---KSDYFMPFSAGKRICAGEGLARM
 1OG2 DNKEFPNP^EMFDPHHFLDEGGNFK---KSKYFMPFSAGKRICVGEALAGM
 1Z10 DPSFFSNPODFNPQHFLNEKGQFK---KSDAFVPFSIG^{KR}NCFGEGGLARM
 2F9Q DEAVWEKPF^RFRHPEHFLDAQGHFV---KPEAFLPFSAGRRACLG^EPLARM
 1TON DPKYWTEP^EKFLPERFSKKNKDNI---DPYIYTPFGSGPRNCIGMRFALM
 2J0D DPKYWTEP^EKFLPERFSKKNKDNI---DPYIYTPFGSGPRNCIGMRFALM
 2HI4 DP^ELWEDPSEFRPERFLTADGTAINKPLSEKMMLFGMG^{KR}RCIG^EVLAKW
 1OG2 -----

1PQ2 ELFLFLTTILQNFNLKSVDDLKN-----LNTTAVTKGIVSLPPSYQICF
 1OG2 ELFLFLTSILQNFNLKSLVDPKN-----LDTPPVVNGFASVPPFYQLCF
 1Z10 ELFLFFTVMQNFRLKSSQSPKD-----IDVSPKHVGFATIPRNYTMSF
 2F9Q ELFLFFTSLLOHFSFS-VPTGQP-----RPSHHGVFAFLVSPSPYELCA
 1TON NMKLALIRVLQNF^SFKPCKETOIPLKLSLGGLLOPEKPVVLKVESRDGT
 2J0D NMKLALIRVLQNF^SFKPCKETOIPLKLSLGGLLOPEKPVVLKVESRDGT
 2HI4 EIFLFLAILLQQL^EFSVPPGVKVD----LTPIYGLTMKHARCEHVQARRF
 1OG2 -----

1PQ2 IPVHHHH
 1OG2 IPVHHHH
 1Z10 LPRHHHH
 2F9Q VPRHHHH
 1TON SGHHHH
 2J0D SGHHHH
 2HI4 SINHHHH
 1OG2 -----