

**Sequence Alignment and Secondary Structure (DSSP)**

2A6: secondary structure from 1Z10 (coumarin complex)

2A13: secondary structure from Scott lab structure

2B4: secondary structure from 1SUO (4PI complex)

2E1: secondary structure from ???

2A17: secondary structure from abiraterone structure for mol A/B, C/D, consensus

|         | 1                                   |                             |                    |                            |                            |                            | 50                             |
|---------|-------------------------------------|-----------------------------|--------------------|----------------------------|----------------------------|----------------------------|--------------------------------|
| 2A6     | MLASGMLLVA                          | LLVCLTVMVL                  | MSVWQQRKSK         | G.KLPPGPTP                 | LPFIGN                     | <b>YLQL</b>                |                                |
| 2A13    | MLASGLLLVT                          | LLACLTVMVL                  | MSVWRQRKSR         | G.KLPPGPTP                 | LPFIGN                     | <b>YLQL</b>                |                                |
| 2B4     | MEFSLLLLLA                          | FLAGLLLLLF                  | RG...HPKAH         | G.RLPPGPSP                 | LPVLGNLLQM                 |                            |                                |
| 2E1     | MSALGVT.VA                          | LLVWAAFLLL                  | VSMWRQVHSS         | W.NLPPGPFP                 | LPIIGN                     | <b>LFQL</b>                |                                |
| 17A1    | M...WELVA                           | LLLLTLAYLF                  | ...WPKRRCP         | GAKYPKSLLS                 | LPLVGS                     | LPFL                       | 43                             |
| 17A1Δ19 | M...~~~~~                           | ~~~~~                       | ~~~~~AKKT          | GAKYPKSLLS                 | LPLVGS                     | LPFL                       |                                |
|         |                                     |                             |                    |                            |                            |                            | A'                             |
|         | 51                                  |                             |                    |                            |                            |                            | 100                            |
| 2A6     | <b>NTE.QM</b> YN <b>SL MK</b> ISERY | GPV                         | <b>FTIHLG</b> PRRV | <b>VVLCG</b>               | <b>HDAVREA</b>             | LVDQAE <b>EF</b>           |                                |
| 2A13    | <b>NTE.QM</b> YN <b>SL MK</b> ISERY | GPV                         | <b>FTIHLG</b> PRRV | <b>VVLCG</b>               | <b>GHDAVKEA</b>            | LVDQAE <b>EF</b>           |                                |
| 2B4     | DRK.G <b>LLRSF</b>                  | LRLREKY                     | GDV                | FTVY <b>LGSRPV</b>         | <b>VVLCG</b>               | <b>TDAIREA</b>             | LVDQAE <b>AF</b>               |
| 2E1     | <b>E<b>LK.N</b>IP</b> KS <b>F</b>   | <b>TRLAQRF</b>              | GPV                | <b>FTLYVGS</b> QRM         | <b>VVMHG</b>               | <b>YKAVKEA</b>             | L <b>LDYKDEF</b>               |
| AB17A1  | PRHG <b>H</b> M <b>HNNF</b>         | <b>FKLQ</b> KKY             | G <b>P</b> I       | <b>YSVRMG</b> T <b>KTT</b> | <b>VIVGH</b>               | <b>HQLA</b>                | EV LI <b>KK</b> <b>GKDF</b> 93 |
| CD17A1  | PRHG <b>H</b> M <b>HNNF</b>         | <b>FKLQ</b> KKY             | G <b>P</b> I       | <b>YSVRMG</b> T <b>KTT</b> | <b>VIVGH</b>               | <b>HQLA</b>                | EV LI <b>KK</b> <b>GKDF</b> 93 |
| 17A1    | PRHG <b>H</b> M <b>HNNF</b>         | <b>FKLQ</b> KKY             | G <b>P</b> I       | <b>YSVRMG</b> T <b>KTT</b> | <b>VIVGH</b>               | <b>HQLA</b>                | EV LI <b>KK</b> <b>GKDF</b> 93 |
|         |                                     | A                           | $\beta_{1-1}$      | $\beta_{1-2}$              |                            | B                          |                                |
|         | 101                                 |                             |                    |                            |                            |                            | 150                            |
| 2A6     | <b>SGRGEQ</b> <b>ATFD</b>           | <b>WVF</b> .KGYGVV          | FS.N               | <b>GERAKQ</b>              | <b>LRRFSIATLR</b>          | <b>DFGVGK</b>              | <b>RGIE</b>                    |
| 2A13    | <b>SGRGEQ</b> <b>ATFD</b>           | <b>WLF</b> .KGYGVA          | FS.N               | <b>GERAKQ</b>              | <b>LRRFSIATLR</b>          | <b>GFGVGK</b>              | <b>RGIE</b>                    |
| 2B4     | <b>SGRGKIA</b> VVD                  | <b>PIF</b> .QGYGVI          | FA.N               | <b>GERWRA</b>              | <b>LRRFSLATMR</b>          | <b>DFGMGKRS</b>            | <b>VE</b>                      |
| 2E1     | <b>SGRGDL</b>                       | <b>PAFH</b> .AH             | RDRGII             | FN.N                       | <b>GPTWKD</b>              | <b>IRRFSLTTLR</b>          | <b>NYGMGK</b> <b>QGNE</b>      |
| AB17A1  | SGRPQ <b>M</b> A <b>TLD</b>         | IAS <b>NNR</b> K <b>GIA</b> | FADSG              | <b>AHWQL</b>               | <b>HRRLAMATFA</b>          | <b>LFKDG</b> DQ <b>KLE</b> | 143                            |
| CD17A1  | SGRPQ <b>M</b> A <b>TLD</b>         | IAS <b>NNR</b> K <b>GIA</b> | FADSG              | <b>AHWQL</b>               | <b>HRRLAMA</b> T <b>FA</b> | <b>LFKDG</b> DQ <b>KLE</b> | 143                            |
| 17A1    | SGRPQ <b>M</b> A <b>TLD</b>         | IAS <b>NNR</b> K <b>GIA</b> | FADSG              | <b>AHWQL</b>               | <b>HRRLAMATFA</b>          | <b>LFKDG</b> DQ <b>KLE</b> | 143                            |
|         |                                     | $\beta_{1-5}$               | B'                 |                            | C                          |                            | D                              |
|         | 151                                 |                             |                    |                            |                            |                            | 200                            |
| 2A6     | <b>ERIQEE</b> A <b>GFL</b>          | <b>IDALRG</b>               | T <b>GGA</b>       | <b>NIDP</b>                | <b>TFFLSR</b>              | <b>TVSNVISSIV</b>          | <b>FGDRFDYKD</b> <b>K</b>      |
| 2A13    | <b>ERIQEE</b> A <b>GFL</b>          | <b>IDALRG</b>               | T <b>GTHGA</b>     | <b>NIDP</b>                | <b>TFFLSR</b>              | <b>TVSNVISSIV</b>          | <b>FGDRFDYED</b> <b>K</b>      |
| 2B4     | <b>ERIQEE</b> A <b>RCL</b>          | <b>VEELRK</b>               | <b>SKGA</b>        | <b>LLDN</b>                | <b>TLLFHS</b>              | <b>ITSNIICSIV</b>          | <b>FGKRFDYKD</b> <b>P</b>      |
| 2E1     | <b>SRIQRE</b> A <b>HFL</b>          | <b>LEALRK</b>               | <b>KTQGO</b>       | <b>PFD</b> P               | <b>TFLIGC</b>              | <b>APCNVIADIL</b>          | <b>FRKHFDYND</b> <b>E</b>      |
| AB17A1  | <b>KIICQE</b> I <b>STL</b>          | <b>CDMLA</b> T <b>H</b>     | <b>NGQ</b>         | <b>SIDI</b>                | <b>SFPV</b> FV             | <b>AVTNVISLIC</b>          | <b>FNTSYK</b> NGDP 193         |
| CD17A1  | <b>KIICQE</b> I <b>STL</b>          | <b>CDMLA</b> T <b>H</b>     | <b>NGQ</b>         | <b>SIDI</b>                | <b>SFPV</b> FV             | <b>AVTNVISLIC</b>          | <b>FNTSYK</b> NGDP 193         |
| 17A1    | <b>KIICQE</b> I <b>STL</b>          | <b>CDMLA</b> T <b>H</b>     | <b>NGQ</b>         | <b>SIDI</b>                | <b>SFPV</b> FV             | <b>AVTNVISLIC</b>          | <b>FNTSYK</b> NGDP 193         |
|         |                                     | D                           |                    |                            | E                          |                            |                                |

201

250

|        |            |          |      |        |        |        |        |           |           |
|--------|------------|----------|------|--------|--------|--------|--------|-----------|-----------|
| 2A6    | EFLSLLRMML | GIFQFTST | ST   | GQLYEM | FSSV   | MKHL   | PGPQQQ | AFQLLOGLE |           |
| 2A13   | EFLSLLRMML | GSFQFTAT | ST   | GQLYEM | FSSV   | MKHL   | PGPQQQ | AFKELQGLE |           |
| 2B4    | VFLRLLDLFF | QSFSLI   | SS   | SQVFEL | FSGF   | LKHFPG | THRQ   | IYRNLQEIN |           |
| 2E1    | KFLRLMYLFN | ENFHL    | LST  | PW     | LQLYNN | FPSF   | LHYLPG | SHRK      | VIKNVAEVK |
| AB17A1 | ELNVIQNYNE | GIIDNL   | SKDS | LVDLVP | WLKI   | FPN..K | TLEK   | LKSHVKIRN | 240       |
| CD17A1 | ELNVIQNYNE | GIIDNL   | SKDS | LVDLVP | WLKI   | FPN..K | TLEK   | LKSHVKIRN | 240       |
| 17A1   | ELNVIQNYNE | GIIDNL   | SKDS | LVDLVP | WLKI   | FPN..K | TLEK   | LKSHVKIRN | 240       |

F                      F'                      G'                      G

251

300

|        |            |            |   |           |     |          |          |         |     |
|--------|------------|------------|---|-----------|-----|----------|----------|---------|-----|
| 2A6    | DFIAKKVEHN | QRTLDPNSPR | D | FIDSFLIRM | QE  | EENP...  | ...NTEFY | LK      |     |
| 2A13   | DFIAKKVEHN | QRTLDPNSPR | D | FIDSFLIRM | QE  | EENP...  | ...NTEFY | LK      |     |
| 2B4    | TFIQSVEKH  | RATLDPNSPR | D | FIDVYLLRM | EK  | DKSDP... | ...SSEFH | HQ      |     |
| 2E1    | EYVSERVKEH | HQSLDPNCPR | D | LTDCLLVEM | E   | KEKHA... | ...ERLYT | MD      |     |
| AB17A1 | DLLNKILENY | KEKFRSDSIT | N | MLDTLMQAK | MNS | SDNGNAGP | DQDSE    | SELLSDN | 290 |
| CD17A1 | DLLNKILENY | KEKFRSDSIT | N | MLDTLMQAK | MNS | SDNGNAGP | DQDSE    | SELLSDN | 290 |
| 17A1   | DLLNKILENY | KEKFRSDSIT | N | MLDTLMQAK | MNS | SDNGNAGP | DQDSE    | SELLSDN | 290 |

H

301

350

|        |            |            |            |   |           |        |       |     |
|--------|------------|------------|------------|---|-----------|--------|-------|-----|
| 2A6    | NLVMTTLNLF | IGGTETVSTT | LRYGFLLLMK | H | PEVEAKVHE | EIDRV  | IGKNR |     |
| 2A13   | NLVMTTLNLF | FAGTETVSTT | LRYGFLLLMK | H | PEVEAKVHE | EIDRV  | IGKNR |     |
| 2B4    | NLILTVLSLF | FAGTETTSTT | LRYGFLLLMK | Y | PHVTERVQK | EIEQV  | IGSHR |     |
| 2E1    | GITVTVADLF | FAGTETTSTT | LRYGLLILMK | Y | PEIEEKLHE | EIDRV  | IGPSR |     |
| AB17A1 | HILTTIGDIF | GAGVETTTSV | VKWTLAFLH  | N | PQVKKKLYE | EIDQNV | VGFSR | 340 |
| CD17A1 | HILTTIGDIF | GAGVETTTSV | VKWTLAFLH  | N | PQVKKKLYE | EIDQNV | VGFSR | 340 |
| 17A1   | HILTTIGDIF | GAGVETTTSV | VKWTLAFLH  | N | PQVKKKLYE | EIDQNV | VGFSR | 340 |

I                                      J

351

400

|        |      |         |            |      |         |            |            |      |
|--------|------|---------|------------|------|---------|------------|------------|------|
| 2A6    | QPK  | FEDRAKM | PYMEAVIHEI | QRFG | DVIPMS  | LARRVKKDTK | FRDFFL     | PKGT |
| 2A13   | QPK  | FEDRAKM | PYTEAVIHEI | QRFG | DMLPMG  | LAHRVNKDTK | FRDFFL     | PKGT |
| 2B4    | PPAL | DDRAKM  | PYTDAVIHEI | QRLG | DLIPFG  | VPHTVTKDTQ | FRGYVIPKNT |      |
| 2E1    | IPAI | IKDRQEM | PYMDAVVHEI | QRFI | TLVPSN  | LPHEATRDTI | FRGYLIPKGT |      |
| AB17A1 | TPT  | ISDRNRL | LLLEATIREV | LRL  | RPVAPML | IPHKANVDSS | IGFAVDKGT  | 390  |
| CD17A1 | TPT  | ISDRNRL | LLLEATIREV | LRL  | RPVAPML | IPHKANVDSS | IGFAVDKGT  | 390  |
| 17A1   | TPT  | ISDRNRL | LLLEATIREV | LRL  | RPVAPML | IPHKANVDSS | IGFAVDKGT  | 390  |

J'                      K                       $\beta_{1-4}$                        $\beta_{2-1}$                        $\beta_{2-2}$

401

450

|        |                                   |            |     |                        |            |            |                |
|--------|-----------------------------------|------------|-----|------------------------|------------|------------|----------------|
| 2A6    | <u>EVYPM</u> <u>LG</u> <u>SVL</u> | RDPSFFSNPQ | DFN | <u>PQHFL</u> <u>NE</u> | KGQ..FKKSD | AFVPFSIGKR |                |
| 2A13   | <u>EVFPM</u> <u>LG</u> <u>SVL</u> | RDPRFFSNPR | DFN | <u>PQHFL</u> <u>DK</u> | KGQ..FKKSD | AFVPFSIGKR |                |
| 2B4    | <u>EVFPV</u> <u>LSSAL</u>         | HDPRYFETPN | TFN | <u>PGHF</u> <u>LDA</u> | NGA..LKRNE | GFMPFSL    | <u>GKR</u>     |
| 2E1    | <u>VVVPTL</u> <u>DSVL</u>         | YDNQEFDPDE | KFK | <u>PEHF</u> <u>LNE</u> | NGK..FKYSD | YFKPFSTGKR |                |
| AB17A1 | <u>EVIIN</u> <u>LWALH</u>         | HNEKEWHQPD | QFM | <u>PERF</u> <u>LNP</u> | AGTQLISPSV | SYLPFGA    | <u>GPR</u> 440 |
| CD17A1 | <u>EVIIN</u> <u>LWALH</u>         | HNEKEWHQPD | QFM | <u>PERF</u> <u>LNP</u> | AGTQLISPSV | SYLPFGA    | <u>GPR</u> 440 |
| 17A1   | <u>EVIIN</u> <u>LWALH</u>         | HNEKEWHQPD | QFM | <u>PERF</u> <u>LNP</u> | AGTQLISPSV | SYLPFGA    | <u>GPR</u> 440 |

$\beta_{1-3}$       K'                                      K''                                      K'''

451

500

|        |      |               |                           |    |                         |            |                        |                                    |     |
|--------|------|---------------|---------------------------|----|-------------------------|------------|------------------------|------------------------------------|-----|
| 2A6    | NCFG | <u>EGLARM</u> | <u>ELFLFFT</u> <u>TVM</u> | QN | <u>FRLKSSQS</u>         | <u>PKD</u> | <u>IDVSPKH</u>         | <u>VG</u> <u>FATIP</u> <u>PRNY</u> |     |
| 2A13   | YCFG | <u>EGLARM</u> | <u>ELFLFFT</u> <u>TIM</u> | QN | <u>FRFKSPQS</u>         | <u>PKD</u> | <u>IDVSPKH</u>         | <u>VG</u> <u>FATIP</u> <u>PRNY</u> |     |
| 2B4    | ICLG | <u>EGIART</u> | <u>ELFLFFT</u> <u>TIL</u> | QN | <u>FSIASPVP</u>         | <u>PED</u> | <u>IDLTPRE</u>         | <u>SGVGNV</u> <u>PPSY</u>          |     |
| 2E1    | VCAG | <u>EGLARM</u> | <u>ELFLL</u> <u>CAIL</u>  | QH | <u>FN</u> <u>LKPLVD</u> | PKD        | <u>IDLSP</u> <u>IH</u> | <u>IG</u> <u>FGC</u> <u>IPPRY</u>  |     |
| AB17A1 | SCIG | <u>EILARQ</u> | <u>ELFLIMAWLL</u>         | QR | <u>FDLEVPDD</u>         | GQLPSLEG.  | <u>I</u>               | <u>PKVV</u> <u>FLIDSF</u>          | 489 |
| CD17A1 | SCIG | <u>EILARQ</u> | <u>ELFLIMAWLL</u>         | QR | <u>FDLEVPDD</u>         | GQLPSLEG.  | <u>I</u>               | <u>PKVV</u> <u>FLIDSF</u>          | 489 |
| 17A1   | SCIG | <u>EILARQ</u> | <u>ELFLIMAWLL</u>         | QR | <u>FDLEVPDD</u>         | GQLPSLEG.  | <u>I</u>               | <u>PKVV</u> <u>FLIDSF</u>          | 489 |

   L                                       $\beta_{3-3}$                                       L'                                       $\beta_{4-1}$                                        $\beta_{4-2}$

2A6 TMSFLPR 4942A13 TMSFLPR 4942B4 QIRFLAR2E1 KLCVIPRSAB17A1 KVKIKVRQAW REAQAEGST 508CD17A1 KVKIKVRQAW REAQAEGST 508CD17A1 KVKIKVRQAW REAQAEGST 508 $\beta_{3-2}$