Supplemental Materials

Supplemental Table 1: The alignment of the target sequence of UGT1A6 to the template sequences (2IYF and 1IIR) by Fugue tool.

```
                 1         11        21        31        41

gi|89276780|ref  MACLLPAARLPAGFLFLVLWGSVLGDKLLVVPQDGSHWLSMKEIVEHLSE

model_s4_1       --------------------------KLLVVPQDGSHWLSMKEIVEHLSE

1iira            -------------MRVLLATCG-----------SRGDTEPLVALAVRVRD

hs2iyfa          -------------AHIAMFSIA-----------AHGHVNPSLEVIRELVA

                 51        61        71        81        91

gi|89276780|ref  R--GHDIVVLVPEVNLLLGESKYYRR-----KSFPVPYNLEELRTRYRSF

model_s4_1       R--GHDIVVLVPEVNLLLGESKYYRR-----KSFPVPYNLEELRTRYRSF
```

```
1iira             L--GADVRMCAP--PD--CA-ERLAEV--G---VPHV-PV-GPRAKPLT-

hs2iyfa           R--GHRVTYAIP--PV--FA-DKVAAT--GPRPVLYHSTLPGPDADPEAW

                  101       111       121       131       141

gi|89276780|ref   GNNHFAASSPLMAPLREYRNNMIVIDMCFFSCQSLLKDSATLSFLRENQF

model_s4_1        GNNHF---------------------------------------------

1iira             -AEDVR----------RFTT--EAIATQFDEIPAAAE--GC-AAVVTTGL

hs2iyfa           GSTLLD----------NVEPFLNDAIQALPQLADAYADDIP-DLVLHD--

                  151       161       171       181       191

gi|89276780|ref   DALFTDPAMPCGVILAEYLKLPSVYLFRGFPCSLEHMLGQSPSPVSYV--

model_s4_1        ---FTDPAMPCGVILAEYLKLPSVYLFRGFPCSLEHMLGQSPSPVSYV--
```

```
1iira            -LAAAIGVR----SVAEKLGIPYFYAFH-CPSYVPSPYY-PPPPID-I--

hs2iyfa          --ITSYPAR----VLARRWGVPAVSLSP-N--LVAWKGYEEE-----V-A

                 201       211       221       231       241

gi|89276780|ref  PRFYTKFSDHMTFPQRLANFIANILENYLYHCLYSKYEILASDLLKRDVS

model_s4_1       PRFYTK---HMTFPQRLANFIANILENYLYHCLYSKYEILASDLLKRDVS

1iira            PAQWERN--NQSAYQR---YGGLLNSHRDAIGL-PPVEDIFT-FGYTDHP

hs2iyfa          EPMWREP--RQTERGRA--YYARFEAWLKENGI-T--EHPDTFASHPPRS

                 251       261       271       281       291

gi|89276780|ref  L----PALHQNSLW-LLRYDFVFEYPRPVMPNMIFIGGTNCKKKGNLSQE

model_s4_1       L----PALHQNSLW-LLRYDFVFEYPRPVMPNMIFIGGTNCKKKGNLSQE
```

```
1iira           WVAADPVLAP--LQPT-D----L-DAVQTGAWI-LP-DERP-LS----PE

hs2iyfa         LVLIPKALQPH-ADRVDE-----DVYTFVGACQ-EGGWQRPA--------

                301       311       321       331       341

gi|89276780|ref FEAYVNASGEHGIVVFSLGSMVSEIPEKKAMEIAEALGRI--PQTVLWRY

model_s4_1      FEAYVNASGEHGIVVFSLG---SEIPEKKAMEIAEALGRI--PQTVLWRY

1iira           LAAFLD--AGPPPVYLGFG----AP-ADAVRVAIDAIRA-HG--RRVILS

hs2iyfa         --------GAEKVVLVSLGS--AFTQPAFYRECVRAFGN-LP-GWHLVLQ

                351       361       371       381       391

gi|89276780|ref TGT-----------RPSNLAKNTILVKWL-PQNDLLGHPKARAFITHSGS

model_s4_1      TGT-----------RPSNLAKNTILVKWL-PQNDLLGHPKARAFITHSGS
```

```
1iira             --RGWA-DL-V-LPDD---GADCFAIGEV-NHQVLFG-R-VAAVIHHGGA
hs2iyfa           IGT--PAELGE-LPD------NVEVHDWV-PQLAILR-Q-ADLFVTHAGA

                  401       411       421       431       441
gi|89276780|ref   HGIYEGICNGVPMVMMPLF---GDQMDNAKRMETR-GAGVTLNV------
model_s4_1        HGIYEGICNGVPMVMMPLF---GDQMDNAKRMETR-GAGVTLNV------
1iira             GTTHVAARAGAPQILLP-QM--ADQPYYAGRVAE-LGVGVAHD------G
hs2iyfa           GGSQEGLATATPMIAVP-QA--VDQFGNADMLQG-LGVARKLAT------
                  451       461       471       481       491
gi|89276780|ref   LEMTADDLENALKTVINNKSYKENIMRLSSLHKDRPIEPLDLAVFWVEYV
```

```
model_s4_1        LEMTADDLENALKTVINNKSYKENIMRLSSLHKDRPIEPLDLAVFWVEYV
1iira             PIPTFDSLSAALATALT-P-ETHARATAVAGTIRT-----DGAAVAARLL
hs2iyfa           -EATADLLRETALALVDDP-EVARRLRRIQAEMAQE----GGTRRAADLI
                  501       511       521       531       541
gi|89276780|ref   MRHKGAPHLRPAAHDLTWYQYHSLDVIGFLLAIVLTVVFIVYKSCAYGCR
model_s4_1        MRHKGAPHLRP---------------------------------------
1iira             LDAVSRE-------------------------------------------
hs2iyfa           EAELPA--------------------------------------------
                  551       561
gi|89276780|ref   KCFGGKGRVKKSHKSKTH
```

```
model_s4_1       ------------------

1iira            ------------------

hs1iira          ------------------

hs2iyfa          ------------------
```