Supplementary Materials

Ordinary differential equations of the PGHS-1 model

$$\frac{dE_1}{dt} = V_{10} - V_{11} - V_{31} + V_{50} - V_{72} \quad (1)$$

$$\frac{dE_2}{dt} = V_{11} - V_{12} - V_{13} - V_{32} - V_{38} \quad (2)$$

$$\frac{dE_3}{dt} = V_9 - V_{10} + V_{12} - V_{30} \quad (3)$$

$$\frac{dE_4}{dt} = V_{35} - V_{37} - V_{49} + V_{54} - V_{56} \quad (4)$$

$$\frac{dE_5}{dt} = -V_1 + V_4 - V_9 + V_{13} - V_{28} - V_{43} + V_{53} + V_{57} - V_{58} \quad (5)$$

$$\frac{dE_6}{dt} = V_{14} - V_{15} + V_{17} + V_{30} \quad (6)$$

$$\frac{dE_7}{dt} = V_{23} - V_{24} + V_{33} - V_{35} - V_{41} - V_{52} \quad (7)$$

$$\frac{dE_8}{dt} = V_3 - V_4 - V_{22} + V_{24} + V_{49} \quad (8)$$

$$\frac{dE_9}{dt} = V_1 - V_2 - V_{14} + V_{18} - V_{29} - V_{44} - V_{61} \quad (9)$$

$$\frac{dE_{10}}{dt} = V_{15} - V_{16} + V_{31} + V_{50} \quad (10)$$

$$\frac{dE_{11}}{dt} = -V_{47} + V_{52} - V_{53} - V_{54} \quad (11)$$

$$\frac{dE_{12}}{dt} = V_7 - V_8 + V_{22} - V_{23} \quad (12)$$

$$\frac{dE_{13}}{dt} = V_2 - V_3 - V_{19} + V_{21} + V_{48} + V_{56} \quad (13)$$

$$\frac{dE_{14}}{dt} = V_{16} - V_{17} - V_{18} + V_{32} - V_{39} - V_{56} \quad (14)$$

$$\frac{dE_{15}}{dt} = -V_5 + V_8 + V_{28} - V_{45} - V_{50} - V_{60} \quad (15)$$

$$\frac{dE_{16}}{dt} = V_6 - V_7 + V_{19} - V_{20} \quad (16)$$

$$\frac{dE_{17}}{dt} = V_{34} - V_{36} - V_{48} - V_{54} \quad (17)$$

$$\frac{dE_{18}}{dt} = V_{25} - V_{26} + V_{60} + V_{59} \quad (18)$$

$$\frac{dE_{19}}{dt} = V_{47} - V_{64} - V_{65} - V_{66} - V_{67} - V_{68} \quad (19)$$

$$\frac{dE_{20}}{dt} = V_5 - V_6 + V_{29} - V_{46} - V_{51} - V_{59} \quad (20)$$

$$\frac{dE_{21}}{dt} = V_{20} - V_{21} - V_{33} - V_{34} - V_{40} \quad (21)$$

$$\frac{dE_{22}}{dt} = -V_{25} + V_{27} + V_{36} + V_{37} + V_{58} + V_{61} \quad (22)$$

$$\frac{dE_{23}}{dt} = V_{26} - V_{27} - V_{42} \quad (23)$$

$$\frac{dFIE}{dt} = V_{38} + V_{39} + V_{40} + V_{41} + V_{42} + V_{43} + V_{44} + V_{45} + V_{46} + V_{54} \quad (24)$$

$$\frac{dAA}{dt} = -V_1 - V_5 - V_{30} - V_{31} - V_{32} \quad (25)$$

$$\frac{dO_2}{dt} = -2 \cdot V_3 - 2 \cdot V_7 - 2 \cdot V_{33} - 2 \cdot V_{55} \quad (26)$$

$$\frac{dPGH_2}{dt} = V_{11} + V_{16} + V_{20} + V_{23} + V_{26} \quad (27)$$

$$\frac{dRC}{dt} = -V_9 - V_{10} - V_{12} - V_{14} - V_{15} - V_{17} - V_{19} - V_{21} - V_{22} - V_{24} - V_{25} - V_{27} - V_{28} - V_{29} - V_{48} - V_{49} - V_{50} - V_{51} - V_{53} \quad (28)$$

$$\sum_{i=1}^{24} E_i = E_o \quad (29)$$

$$RC + OC = RC_O \quad (30)$$

$$PGH_2 + PGG_2 = AA_0, \quad (31)$$

where rate equations V_i are defined by the following relations:

$$V_1 = k_1 \cdot (E_5 \cdot AA - K_1 \cdot E_9) \quad (32)$$
$$V_2 = k_2 \cdot E_9 \quad (33)$$
$$V_3 = k_3 \cdot E_{13} \cdot O_2 \cdot O_2 \quad (34)$$
$$V_4 = k_4 \cdot E_8 \quad (35)$$
$$V_5 = k_1 \cdot (E_{15} \cdot AA - K_1 \cdot E_{20}) \quad (36)$$
$$V_6 = k_2 \cdot E_{20} \quad (37)$$
$$V_7 = k_3 \cdot E_{16} \cdot O_2 \cdot O_2 \quad (38)$$
$$V_8 = k_4 \cdot E_{12} \quad (39)$$
$$V_9 = k_5 \cdot E_5 \cdot RC \quad (40)$$
$$V_{10} = k_6 \cdot E_3 \cdot RC \quad (41)$$
$$V_{11} = k_7 \cdot PGG_2 \cdot E_1 \quad (42)$$
$$V_{12} = k_8 \cdot E_2 \cdot RC \quad (43)$$
$$V_{13} = k_9 \cdot E_2 \quad (44)$$
$$V_{14} = k_{10} \cdot E_9 \cdot RC \quad (45)$$
$$V_{15} = k_6 \cdot E_6 \cdot RC \quad (46)$$
$$V_{16} = k_7 \cdot PGG_2 \cdot E_1 \quad (47)$$
$$V_{17} = k_8 \cdot E_{14} \cdot RC \quad (48)$$
$$V_{18} = k_{11} \cdot E_{14} \quad (49)$$
$$V_{19} = k_6 \cdot E_{13} \cdot RC \quad (50)$$
$$V_{20} = k_7 \cdot PGG_2 \cdot E_{16} \quad (51)$$
$$V_{21} = k_8 \cdot E_{21} \cdot RC \quad (52)$$
$$V_{22} = k_6 \cdot E_8 \cdot RC \quad (53)$$
$$V_{23} = k_7 \cdot PGG_2 \cdot E_{12} \quad (54)$$
$$V_{24} = k_8 \cdot E_7 \cdot RC \quad (55)$$
$$V_{25} = k_6 \cdot E_{22} \cdot RC \quad (56)$$
$$V_{26} = k_7 \cdot PGG_2 \cdot E_{18} \quad (57)$$
$$V_{27} = k_8 \cdot E_{23} \cdot RC \quad (58)$$
$$V_{28} = k_6 \cdot E_5 \cdot RC \quad (59)$$
$$V_{29} = k_6 \cdot E_9 \cdot RC \quad (60)$$
$$V_{30} = k_{12} \cdot (E_3 \cdot AA - K_{12} \cdot E_6) \quad (61)$$
$$V_{31} = k_{12} \cdot (E_1 \cdot AA - K_{12} \cdot E_{10}) \quad (62)$$
$$V_{32} = k_{12} \cdot (E_2 \cdot AA - K_{12} \cdot E_{14}) \quad (63)$$
$$V_{33} = k_3 \cdot E_{21} \cdot O_2 \cdot O_2 \quad (64)$$
$$V_{34} = k_{13} \cdot E_{21} \quad (65)$$
$$V_{35} = k_{14} \cdot E_7 \quad (66)$$
$$V_{36} = k_{15} \cdot E_{17} \quad (67)$$
$$V_{37} = k_{16} \cdot E_4 \quad (68)$$
$$V_{38} = k_{in1} \cdot E_2 \quad (69)$$
$$V_{39} = k_{in1} \cdot E_{14} \quad (70)$$
$$V_{40} = k_{in1} \cdot E_{21} \quad (71)$$
$$V_{41} = k_{in1} \cdot E_7 \quad (72)$$
$$V_{42} = k_{in1} \cdot E_{23} \quad (73)$$
$$V_{43} = k_{in2} \cdot E_5 \quad (74)$$
$$V_{44} = k_{in2} \cdot E_9 \quad (75)$$
$$V_{45} = k_{in2} \cdot E_{15} \quad (76)$$
$$V_{46} = k_{in2} \cdot E_{20} \quad (77)$$
$$V_{47} = k_1 \cdot (AA \cdot E_{11} - K_1 \cdot E_{19}) \quad (78)$$
$$V_{48} = k_5 \cdot E_{17} \cdot RC \quad (79)$$
$$V_{49} = k_5 \cdot E_4 \cdot RC \quad (80)$$
$$V_{50} = k_5 \cdot E_{15} \cdot RC \quad (81)$$
$$V_{51} = k_{10} \cdot E_{20} \cdot RC \quad (82)$$
$$V_{52} = k_4 \cdot E_7 \quad (83)$$
$$V_{53} = k_8 \cdot E_{11} \cdot RC \quad (84)$$
$$V_{54} = k_{in1} \cdot E_{11} \quad (85)$$
$$V_{55} = k_3 \cdot E_{17} \cdot O_2 \cdot O_2 \quad (86)$$
$$V_{56} = k_{13} \cdot E_{14} \quad (87)$$
$$V_{57} = k_{14} \cdot E_4 \quad (89)$$
$$V_{58} = k_{in} \cdot E_5 \quad (90)$$
$$V_{59} = k_{in} \cdot E_{20} \quad (91)$$
$$V_{60} = k_{in} \cdot E_{15} \quad (92)$$
$$V_{61} = k_{in} \cdot E_9 \quad (93)$$
$$V_{62} = k_{in} \cdot E_{11} \quad (94)$$
$$V_{63} = k_7 \cdot PGG_2 \cdot E_{15} \quad (95)$$
$$V_{64} = k_2 \cdot E_{19} \quad (96)$$
$$V_{65} = k_5 \cdot E_{19} \cdot RC \quad (97)$$
$$V_{66} = k_8 \cdot E_{19} \cdot RC \quad (98)$$

SBML file of the model can be downloaded from

https://www.researchgate.net/project/COX-1-2-and-NSAIDs