SUPPLEMENTAL DATA

DynaFit File

Model used for simulation of cytochrome *b* reduction and semiquinone concentration kinetics (Fig. 9) in a sequential mechanism of quinol oxidation involving a moving semiquinone (15).

REACTION MECHANISM

$E + QH_2$ <===> $E.QH_2$ : $k_{onQH}$ $k_{off}$
$E.QH_2$ <===> EFeS.SQ(d) : $k_1$ $k_{\_1}$
EFeS.SQ(d) <===> EFeS.SQ(p) : $k_{diff}$ $k_{diff}$
EFeS.SQ(p) <===> EFeS.Q(p).b : $k_{2p}$ $k_{\_2p}$
EFeS.SQ(d) <===> EFeS.Q(d).b : $k_{2d}$ $k_{\_2d}$
EFeS.Q(p).b <===> EFeSb + Q : $k_{off}$ $k_{onQ}$
EFeS.Q(d).b <===> EFeSb + Q : $k_{off}$ $k_{onQ}$
$EFeS.QH_2.b$ <===> EFeSb + $QH_2$ : $k_{off}$ $k_{onQH}$

CONSTANTS

$k_{onQH}$ = 500
$k_{off}$ = 5000
$k_{onQ}$ = 50
$k_{diff}$ = (varied between 100000000 and 1000000000000)
$k_1$ = 1300
$k_{\_1}$ = 32500000000
$k_{2d}$ = 90000000000
$k_{\_2d}$ = 3600
$k_{2p}$ = 19000000
$k_{\_2p}$ = 0.76

RESPONSES

EFeS.Q(p).b = 1
EFeS.Q(d).b = 1
EFeSb = 1
$EFeS.QH_2.b$ = 1

PROGRESS

mesh from 0 to 0.01 step 0.00001
monitor EFeS.SQ(d), EFeS.SQ(p)

concentration E = 1, $QH_2$ = 200