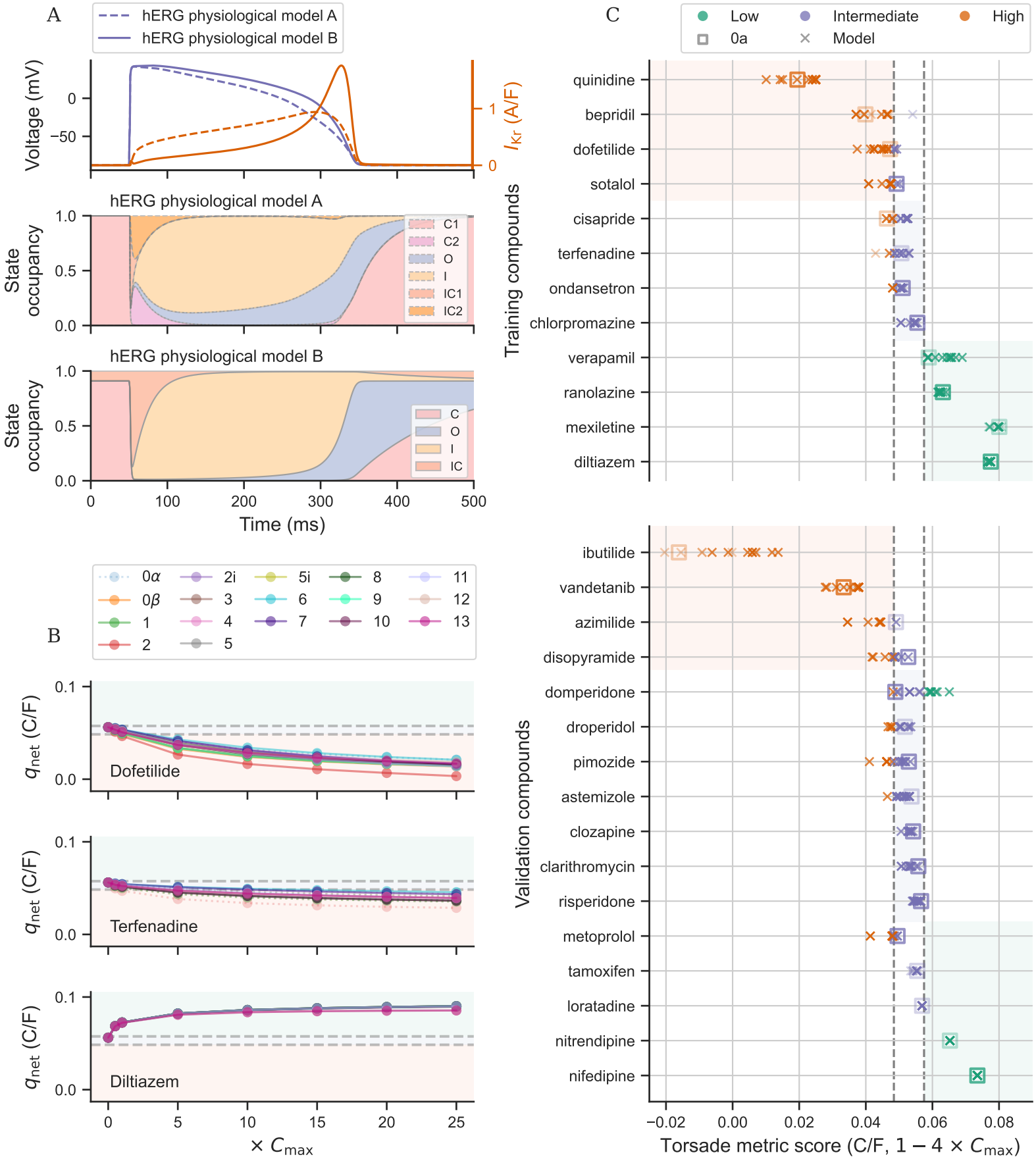
A
hERG physiological model A
hERG physiological model B
Voltage (mV)
0
−50
$I_{Kr}$ (A/F)
1
0
hERG physiological model A
State occupancy
1.0
0.5
0.0
C1
C2
O
I
IC1
IC2
hERG physiological model B
State occupancy
1.0
0.5
0.0
C
O
I
IC
0
100
200
300
400
500
Time (ms)
B
0α
0β
1
2
2i
3
4
5
5i
6
7
8
9
10
11
12
13
$q_{net}$ (C/F)
0.1
0.0
Dofetilide
$q_{net}$ (C/F)
0.1
0.0
Terfenadine
$q_{net}$ (C/F)
0.1
0.0
Diltiazem
0
5
10
15
20
25
× $C_{max}$
C
Low
Intermediate
High
0a
Model
Training compounds
quinidine
bepridil
dofetilide
sotalol
cisapride
terfenadine
ondansetron
chlorpromazine
verapamil
ranolazine
mexiletine
diltiazem
Validation compounds
ibutilide
vandetanib
azimilide
disopyramide
domperidone
droperidol
pimozide
astemizole
clozapine
clarithromycin
risperidone
metoprolol
tamoxifen
loratadine
nitrendipine
nifedipine
−0.02
0.00
0.02
0.04
0.06
0.08
Torsade metric score (C/F, 1 − 4 × $C_{max}$)