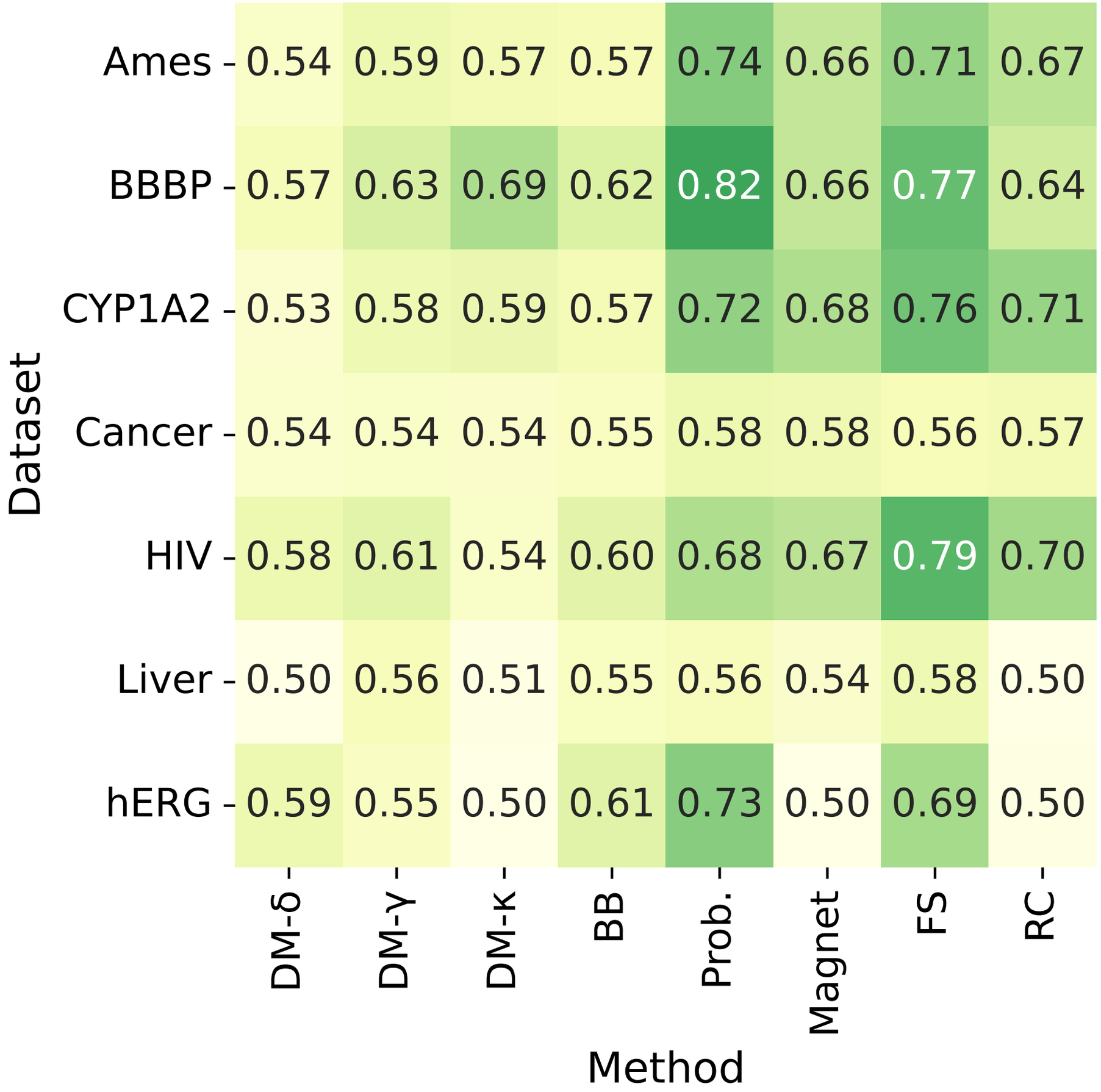
Dataset
Ames
BBBP
CYP1A2
Cancer
HIV
Liver
hERG
0.54 0.59 0.57 0.57 0.74 0.66 0.71 0.67
0.57 0.63 0.69 0.62 0.82 0.66 0.77 0.64
0.53 0.58 0.59 0.57 0.72 0.68 0.76 0.71
0.54 0.54 0.54 0.55 0.58 0.58 0.56 0.57
0.58 0.61 0.54 0.60 0.68 0.67 0.79 0.70
0.50 0.56 0.51 0.55 0.56 0.54 0.58 0.50
0.59 0.55 0.50 0.61 0.73 0.50 0.69 0.50
DM-δ
DM-γ
DM-κ
BB
Prob.
Magnet
FS
RC
Method