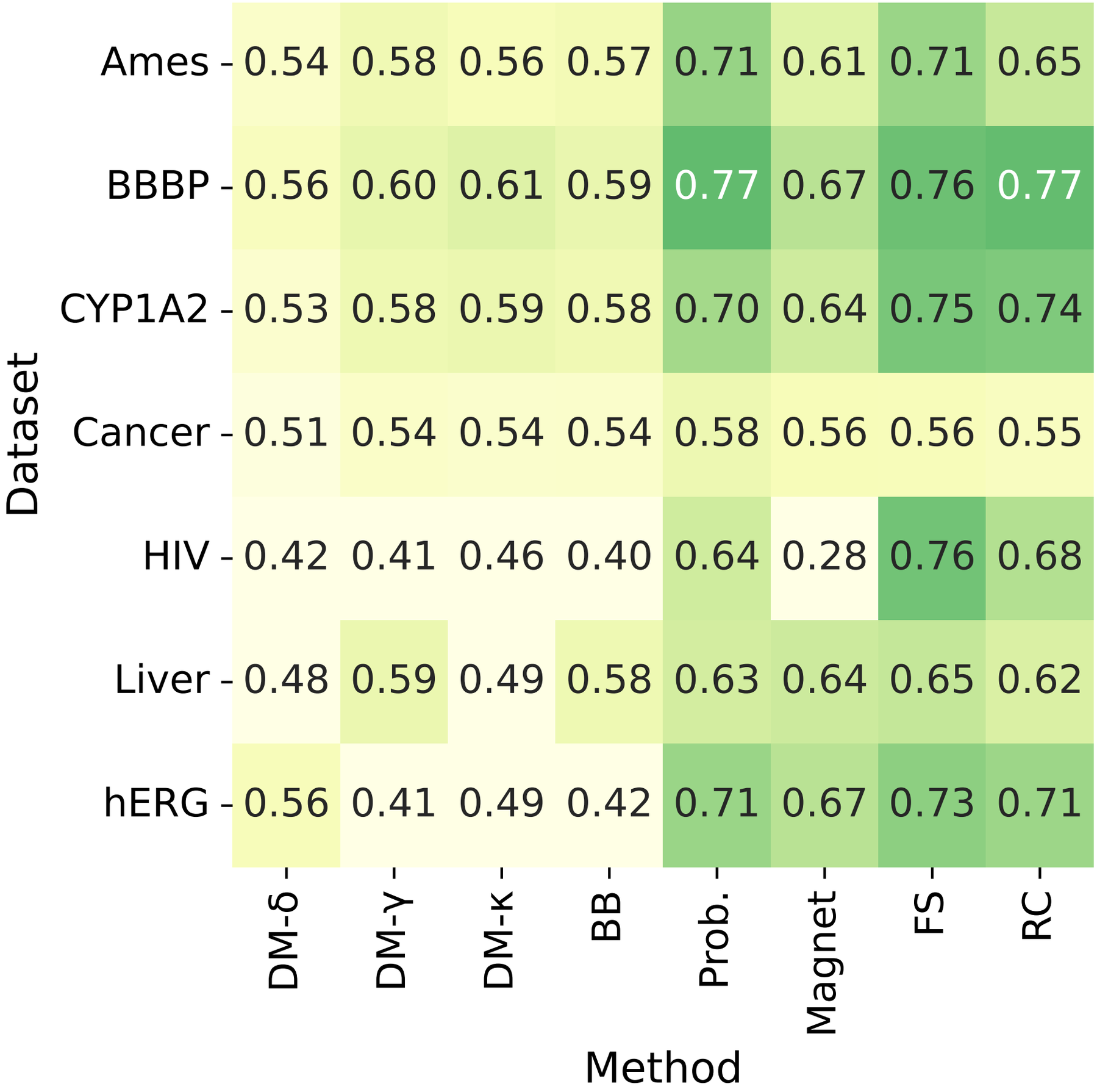
Dataset
Ames 0.54 0.58 0.56 0.57 0.71 0.61 0.71 0.65
BBBP 0.56 0.60 0.61 0.59 0.77 0.67 0.76 0.77
CYP1A2 0.53 0.58 0.59 0.58 0.70 0.64 0.75 0.74
Cancer 0.51 0.54 0.54 0.54 0.58 0.56 0.56 0.55
HIV 0.42 0.41 0.46 0.40 0.64 0.28 0.76 0.68
Liver 0.48 0.59 0.49 0.58 0.63 0.64 0.65 0.62
hERG 0.56 0.41 0.49 0.42 0.71 0.67 0.73 0.71
DM-δ
DM-γ
DM-κ
BB
Prob.
Magnet
FS
RC
Method