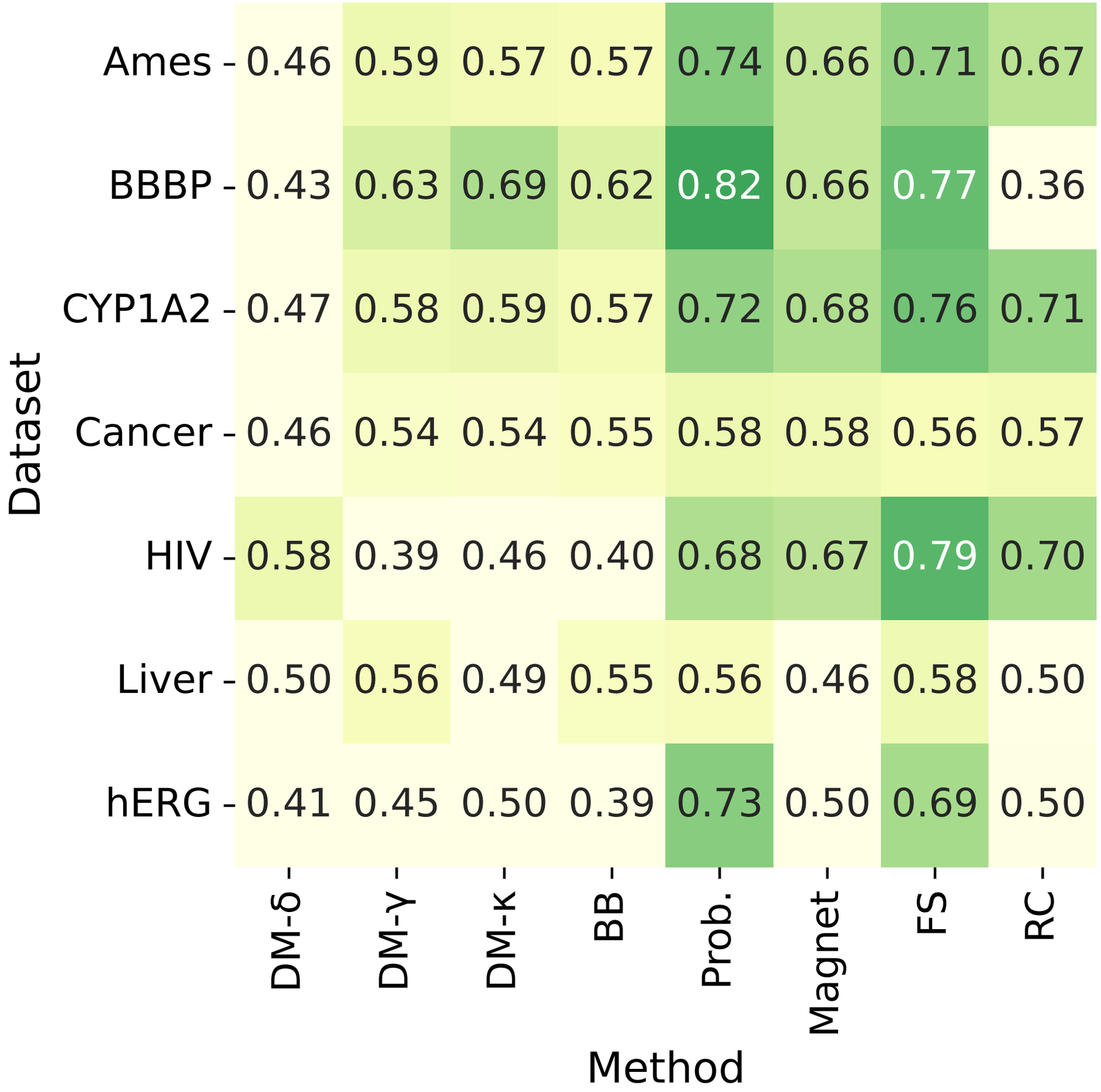
Ames 0.46 0.59 0.57 0.57 0.74 0.66 0.71 0.67
BBBP 0.43 0.63 0.69 0.62 0.82 0.66 0.77 0.36
CYP1A2 0.47 0.58 0.59 0.57 0.72 0.68 0.76 0.71
Cancer 0.46 0.54 0.54 0.55 0.58 0.58 0.56 0.57
HIV 0.58 0.39 0.46 0.40 0.68 0.67 0.79 0.70
Liver 0.50 0.56 0.49 0.55 0.56 0.46 0.58 0.50
hERG 0.41 0.45 0.50 0.39 0.73 0.50 0.69 0.50
Dataset
DM-δ
DM-γ
DM-κ
BB
Prob.
Magnet
FS
RC
Method