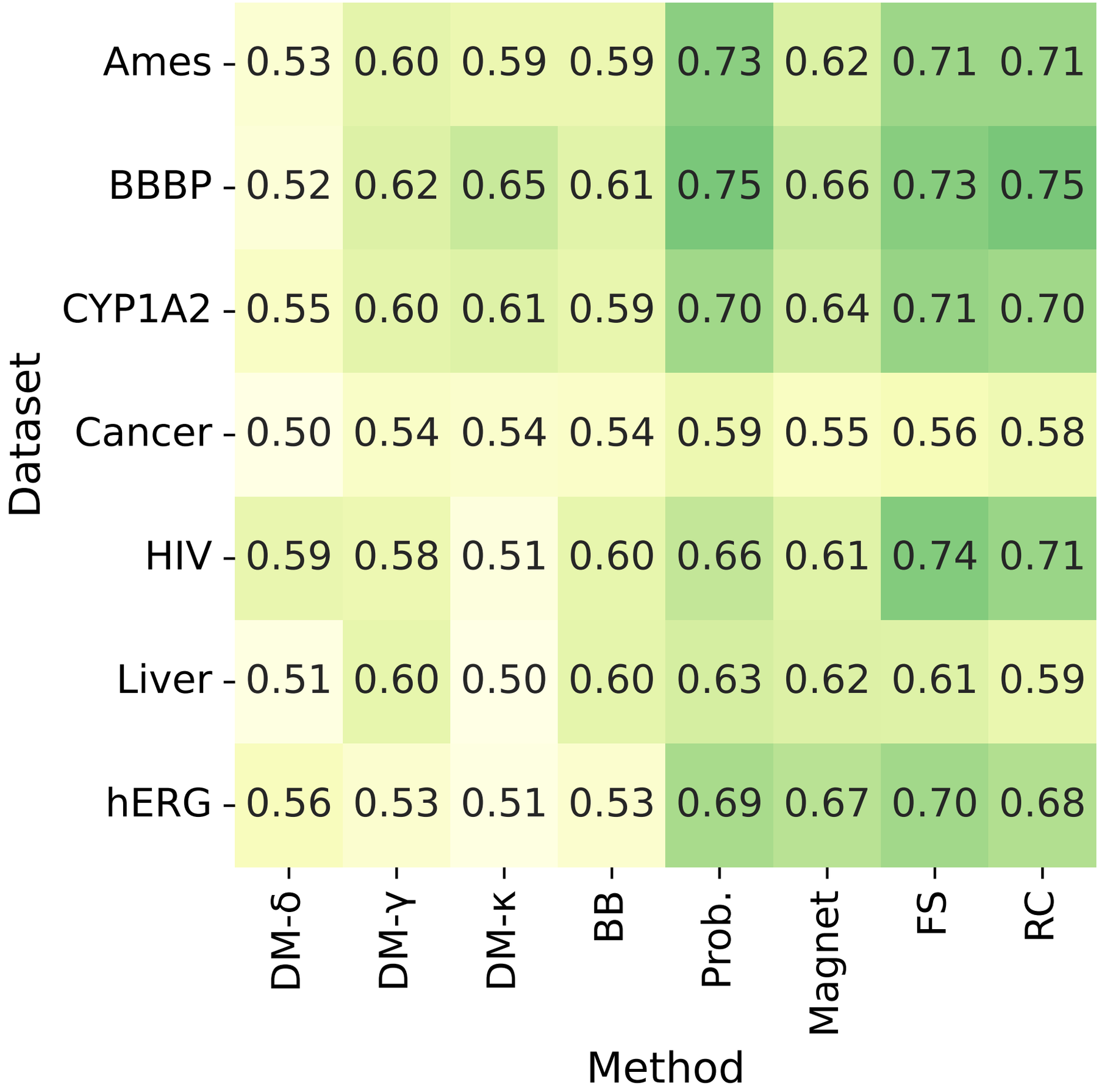
Ames 0.53 0.60 0.59 0.59 0.73 0.62 0.71 0.71
BBBP 0.52 0.62 0.65 0.61 0.75 0.66 0.73 0.75
CYP1A2 0.55 0.60 0.61 0.59 0.70 0.64 0.71 0.70
Cancer 0.50 0.54 0.54 0.54 0.59 0.55 0.56 0.58
HIV 0.59 0.58 0.51 0.60 0.66 0.61 0.74 0.71
Liver 0.51 0.60 0.50 0.60 0.63 0.62 0.61 0.59
hERG 0.56 0.53 0.51 0.53 0.69 0.67 0.70 0.68
Dataset
DM-δ
DM-γ
DM-κ
BB
Prob.
Magnet
FS
RC
Method