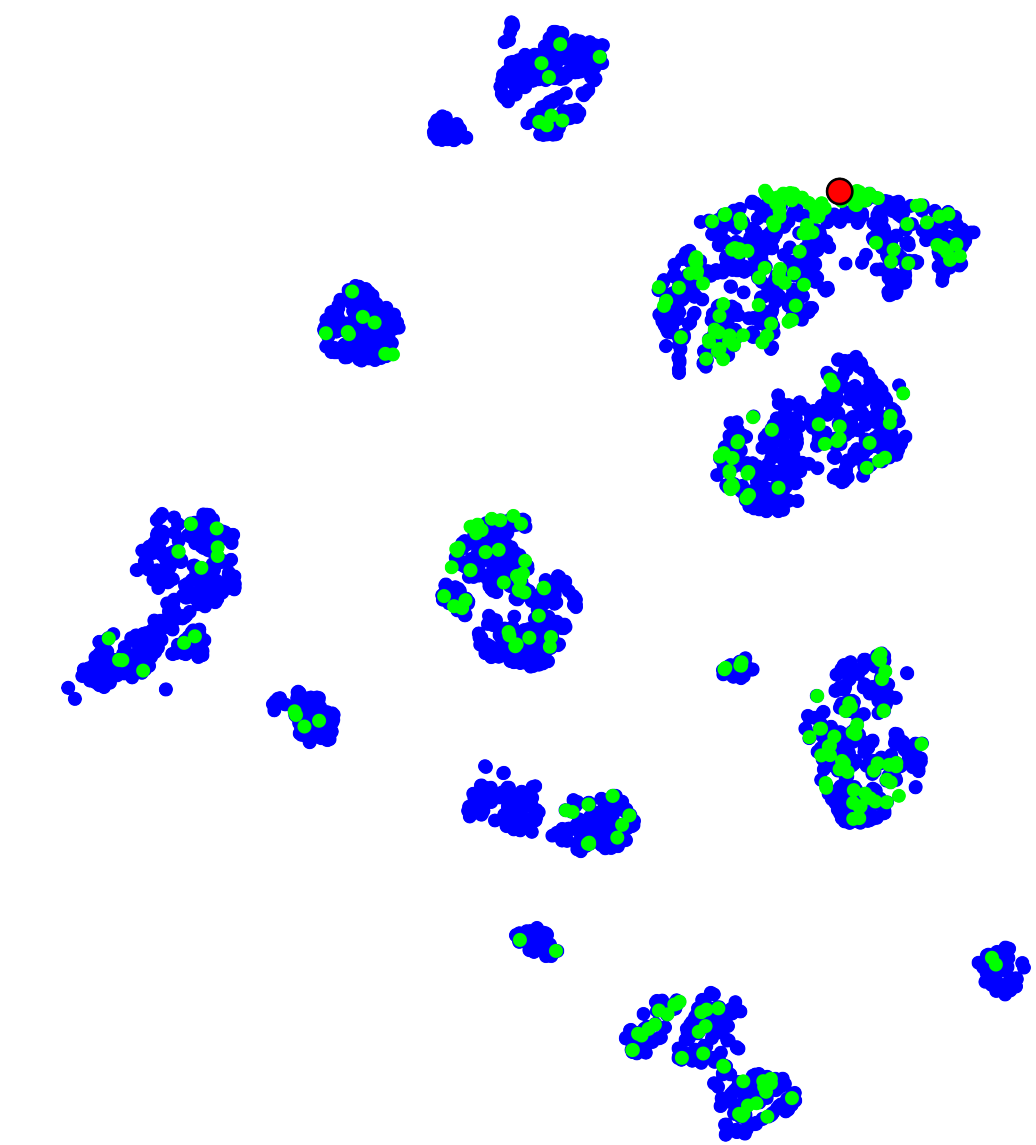
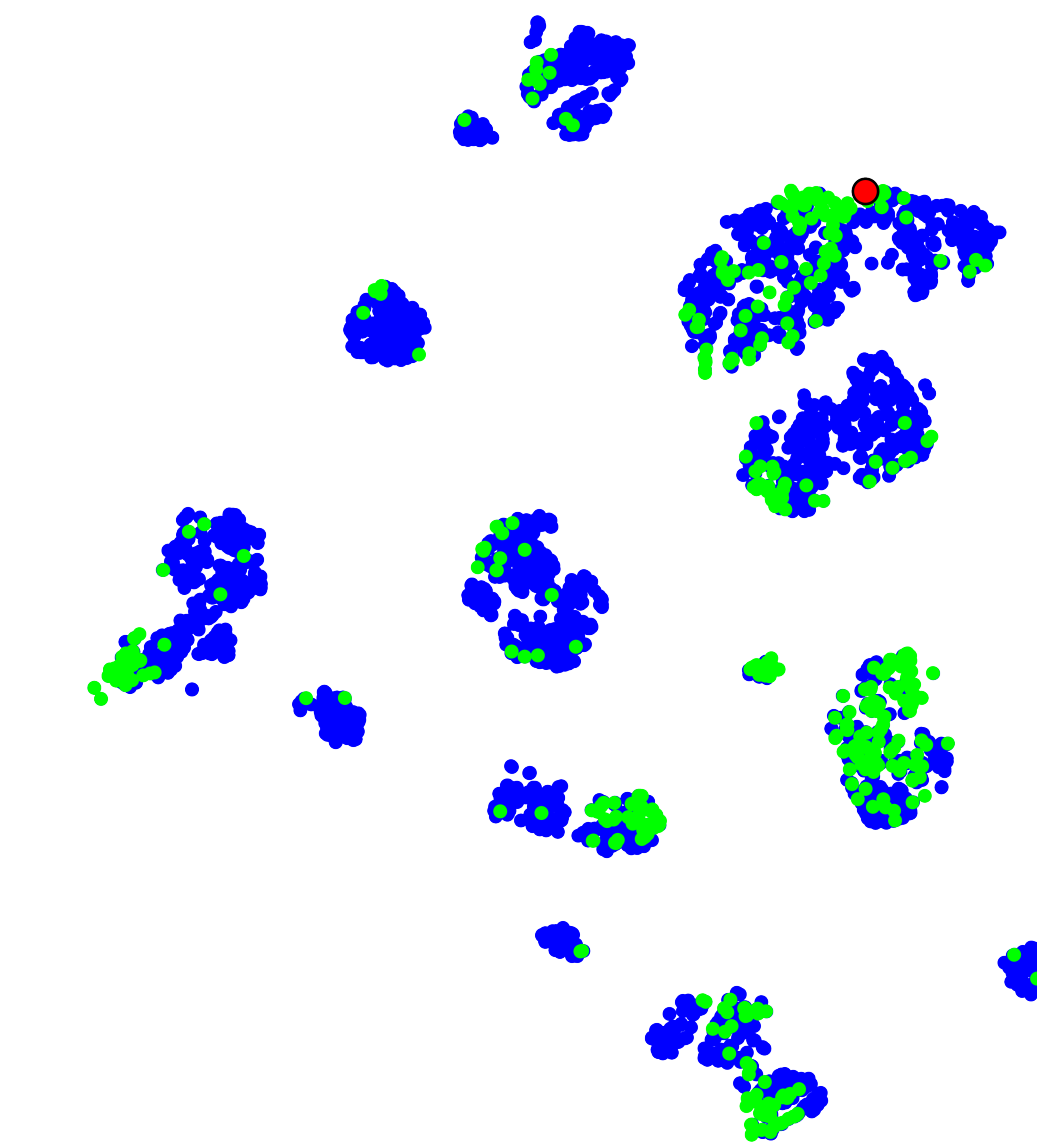


salbutamol (N)

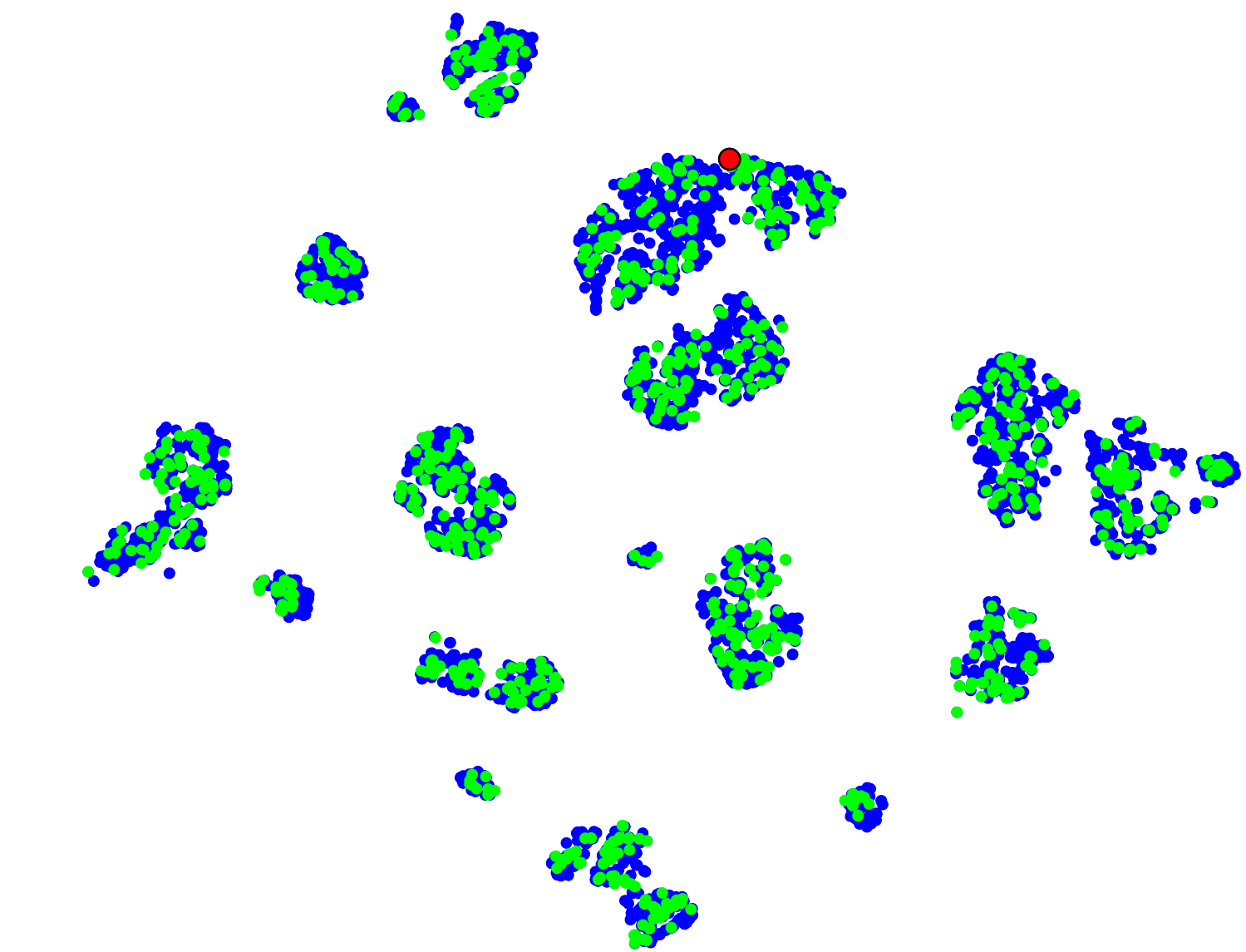
(a) ILP(p=0)



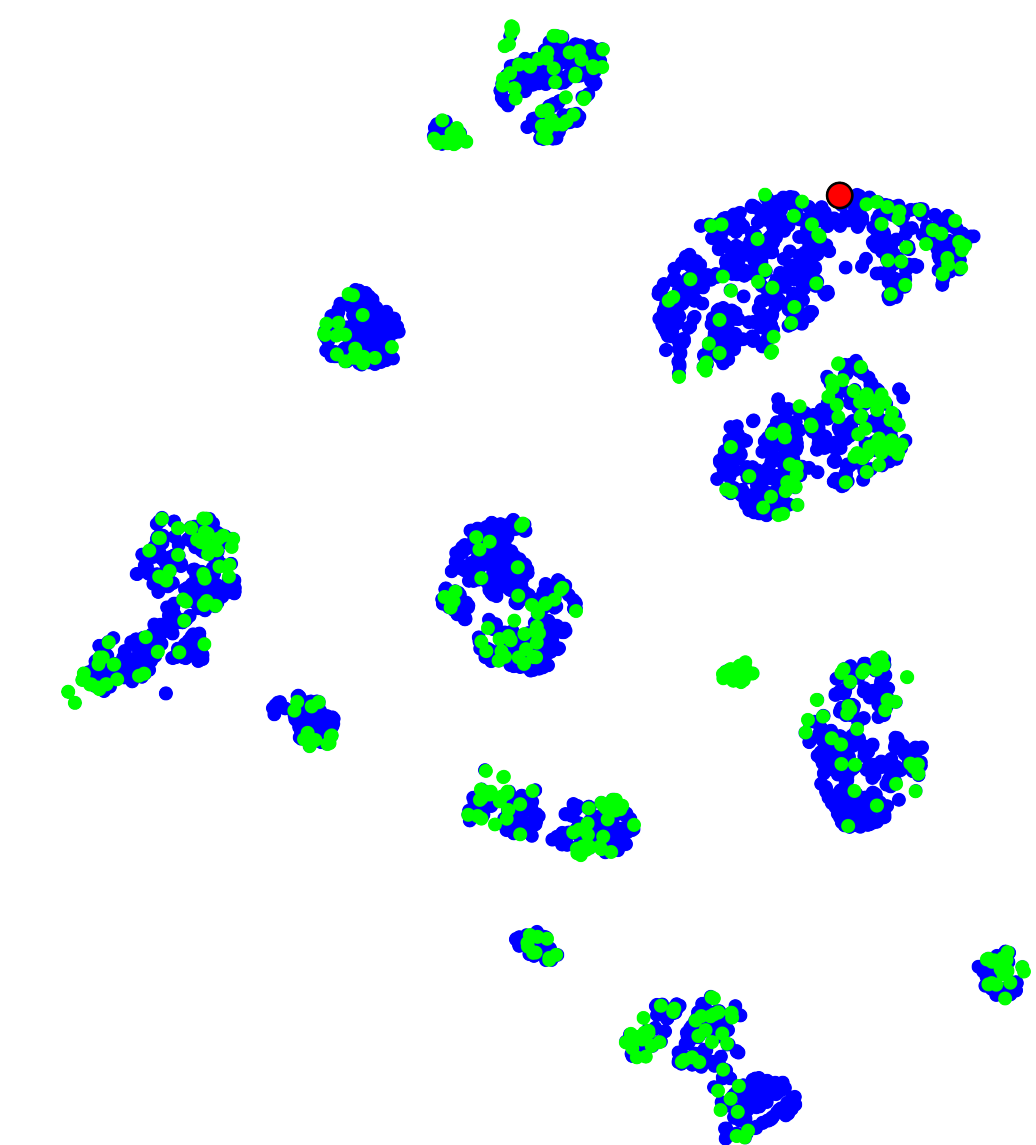
(b) ILP(p=1)



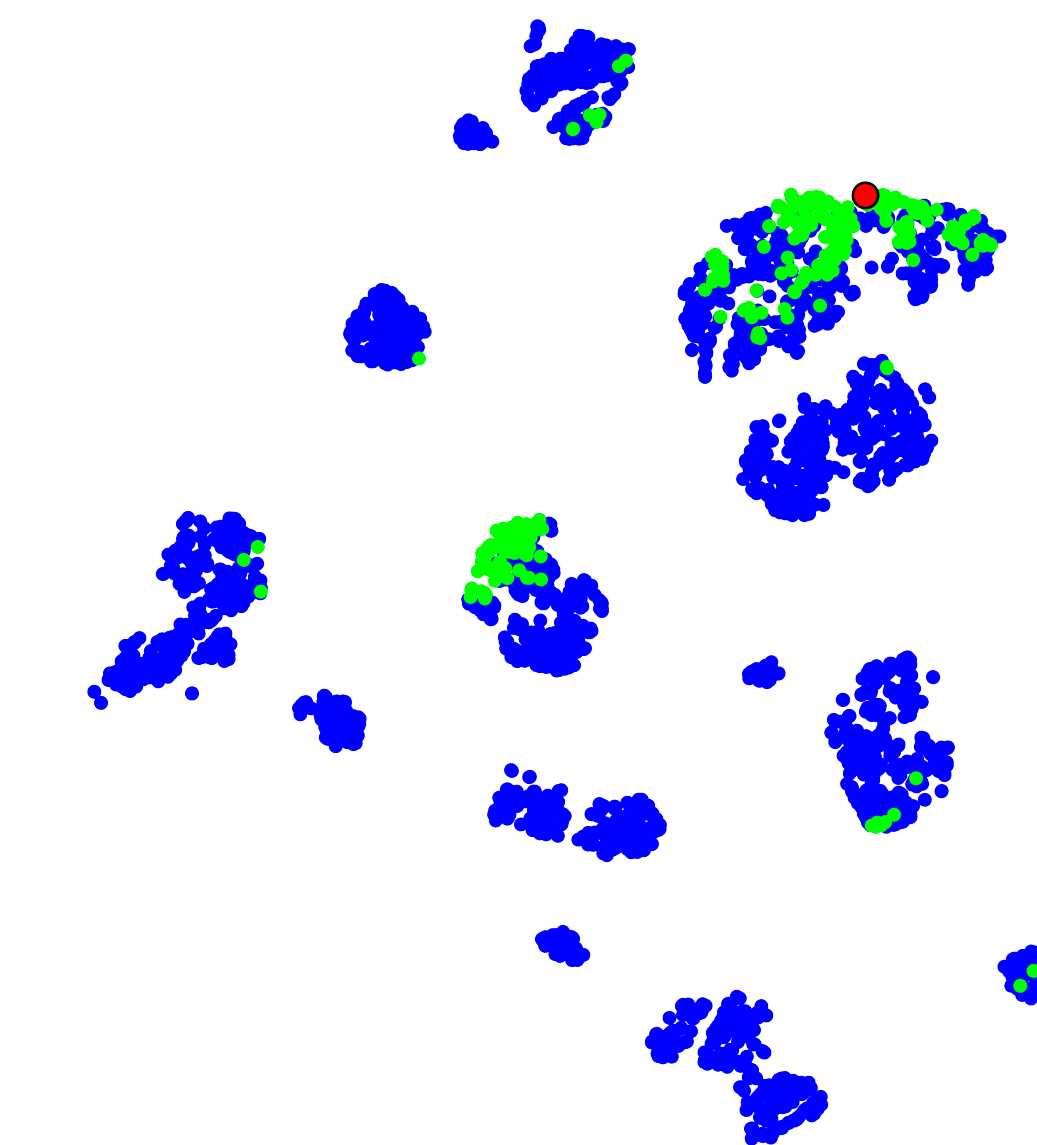
(c) FPS



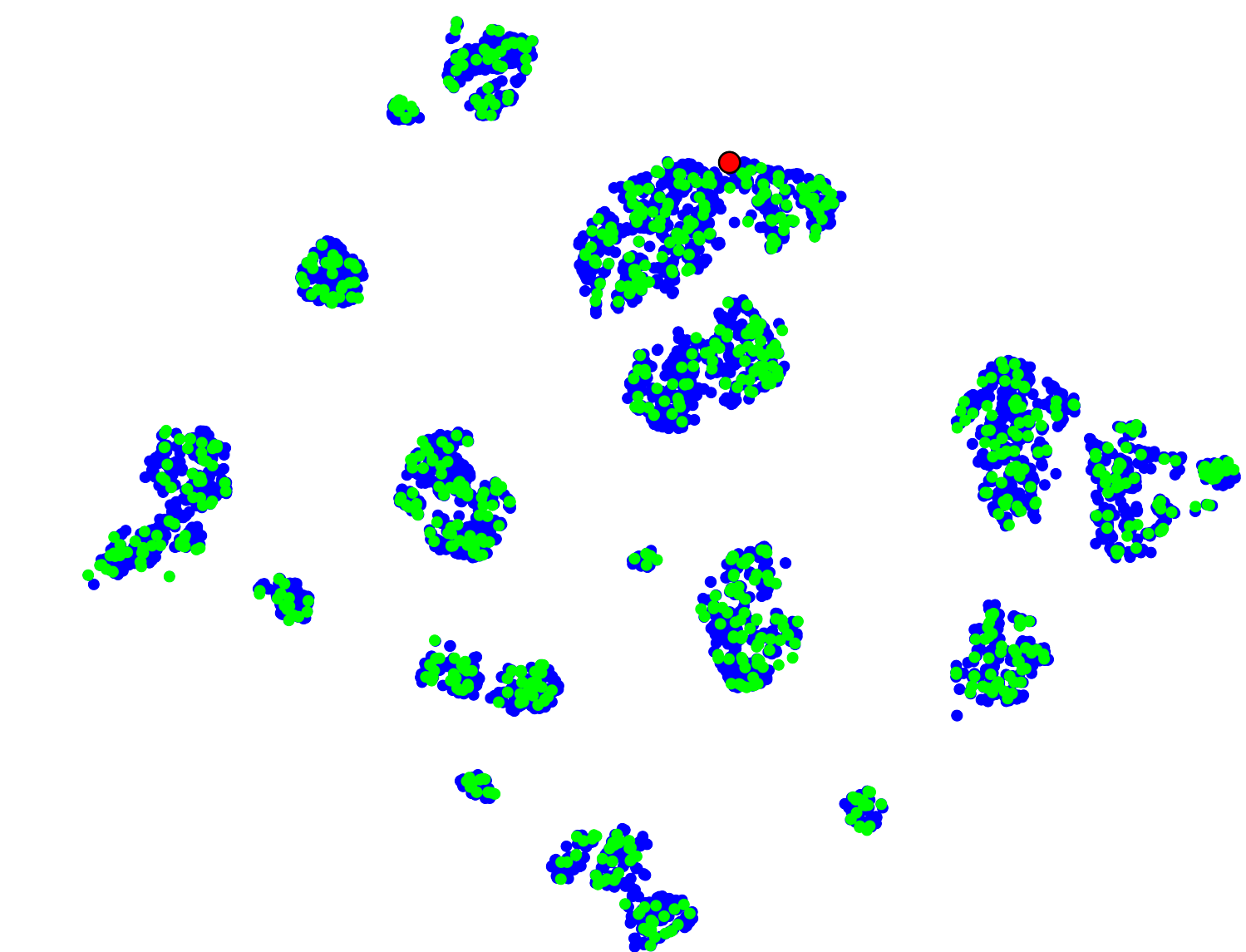
(d) CUR



(e) SML



(f) random



■ target ■ selected from QM7 ■ other in QM7