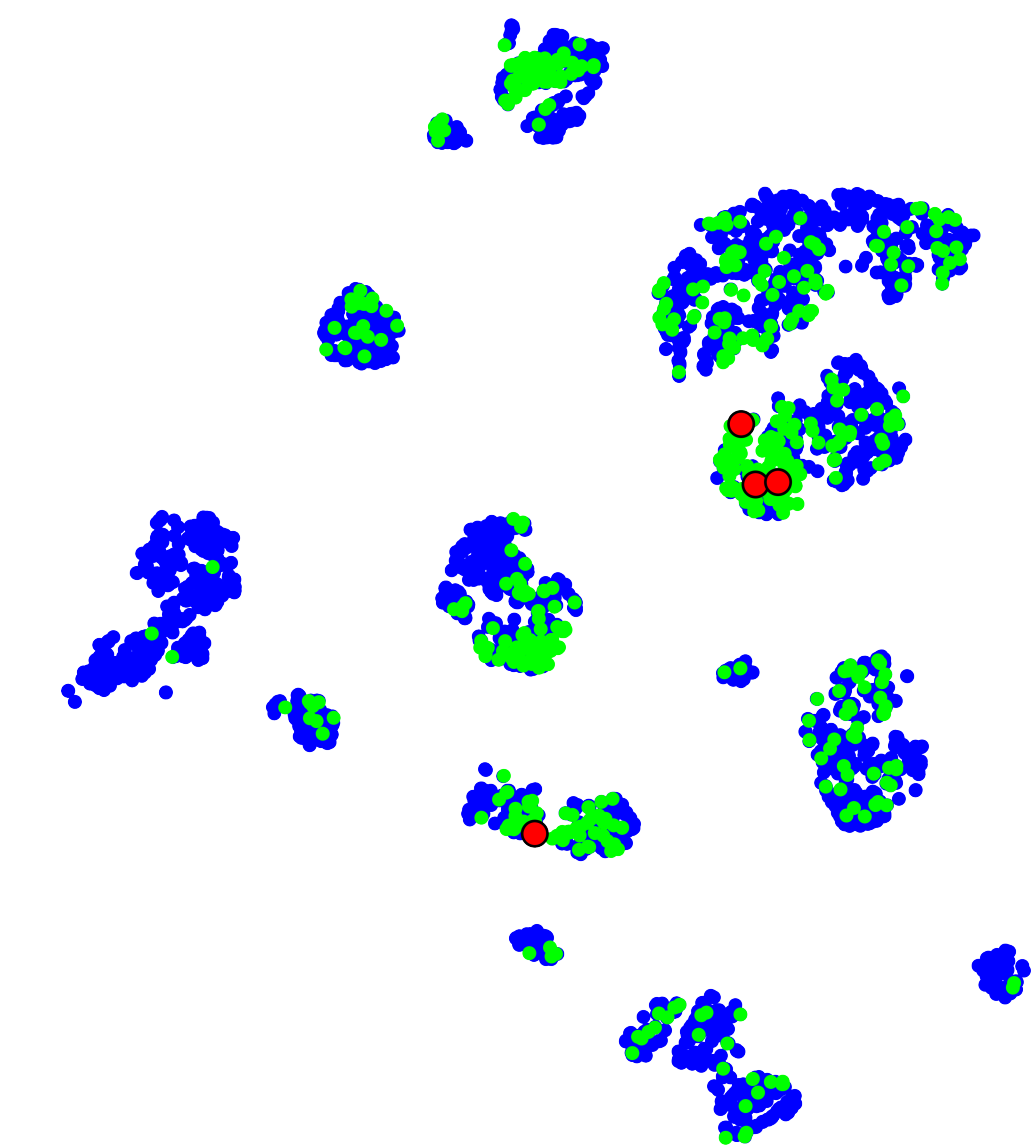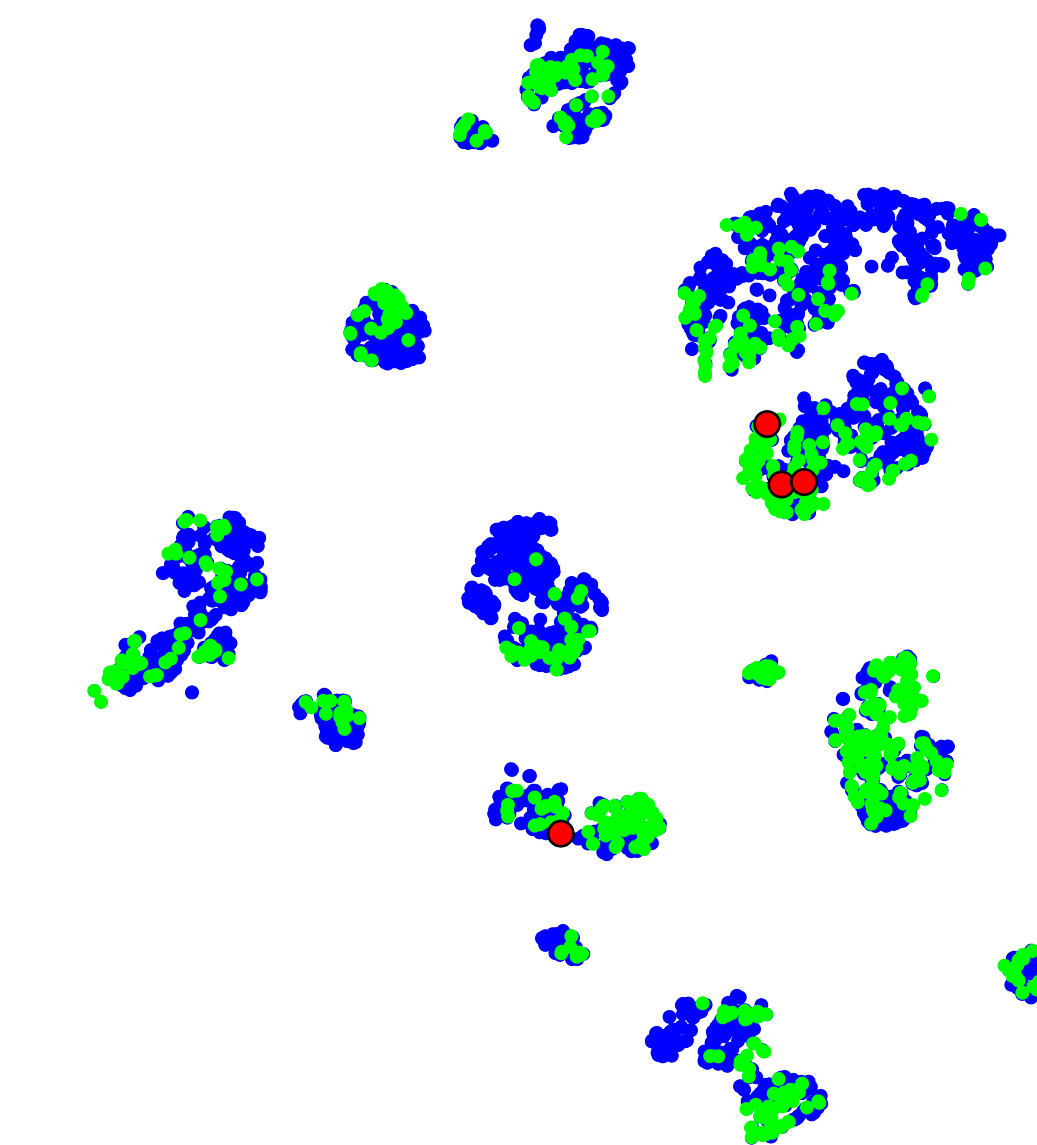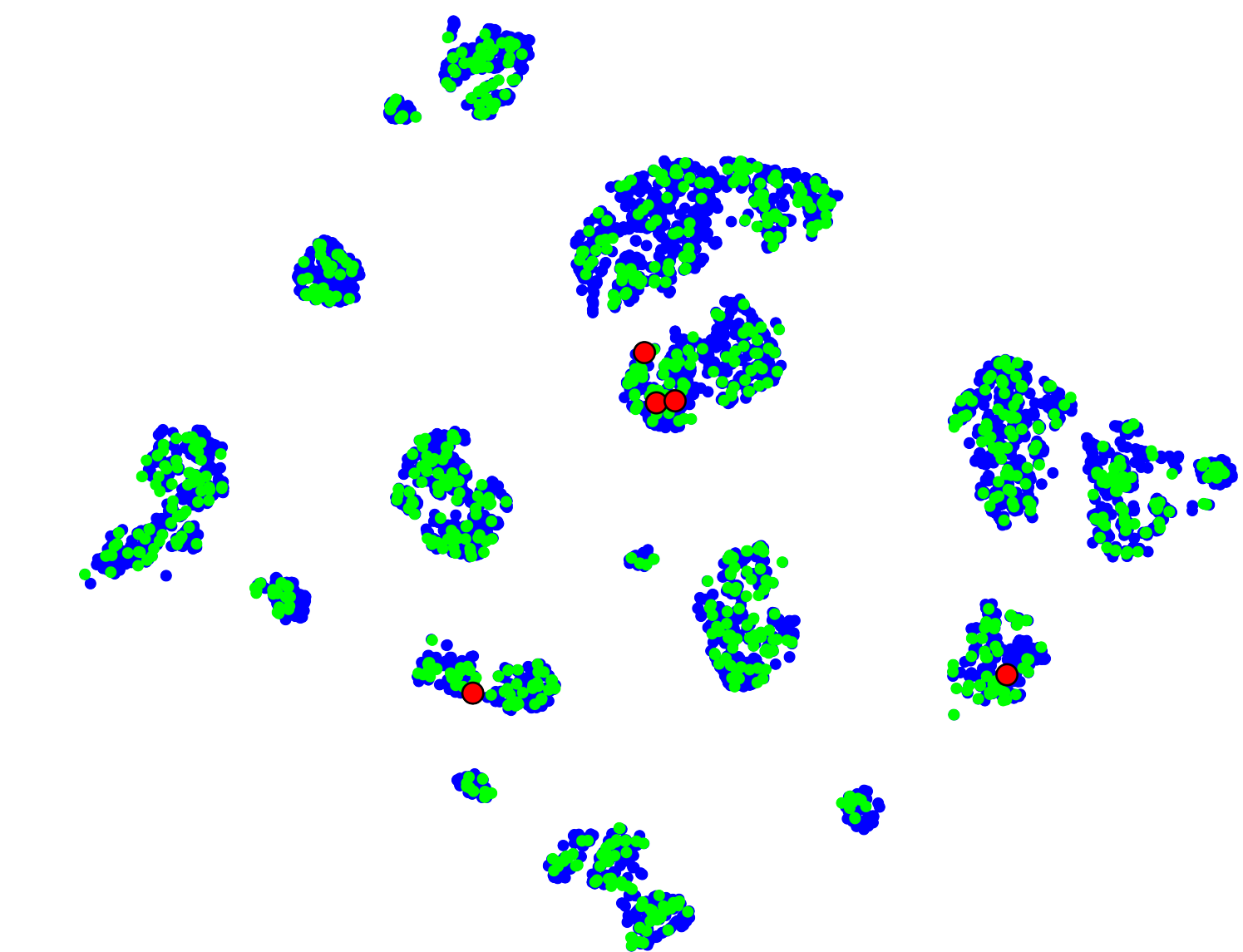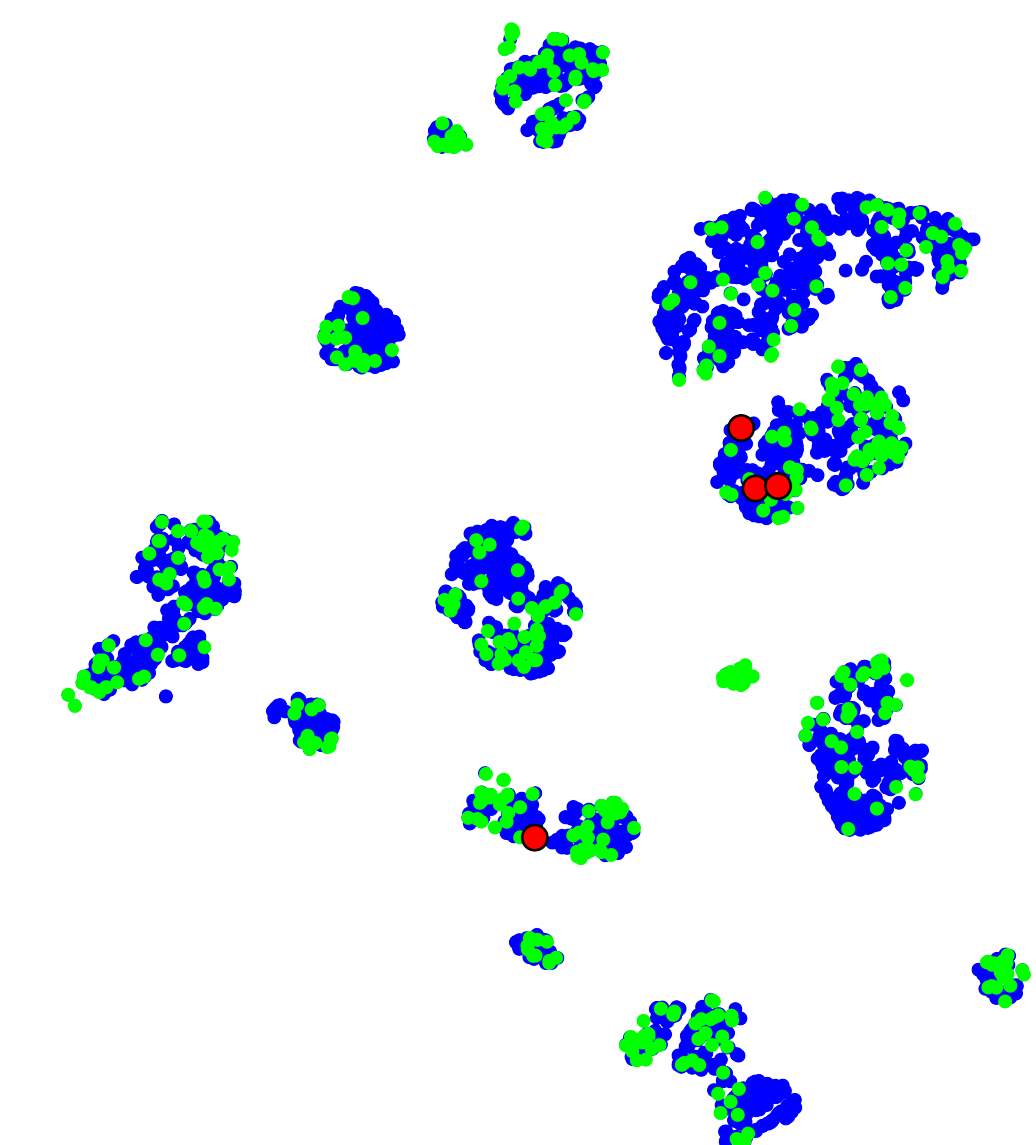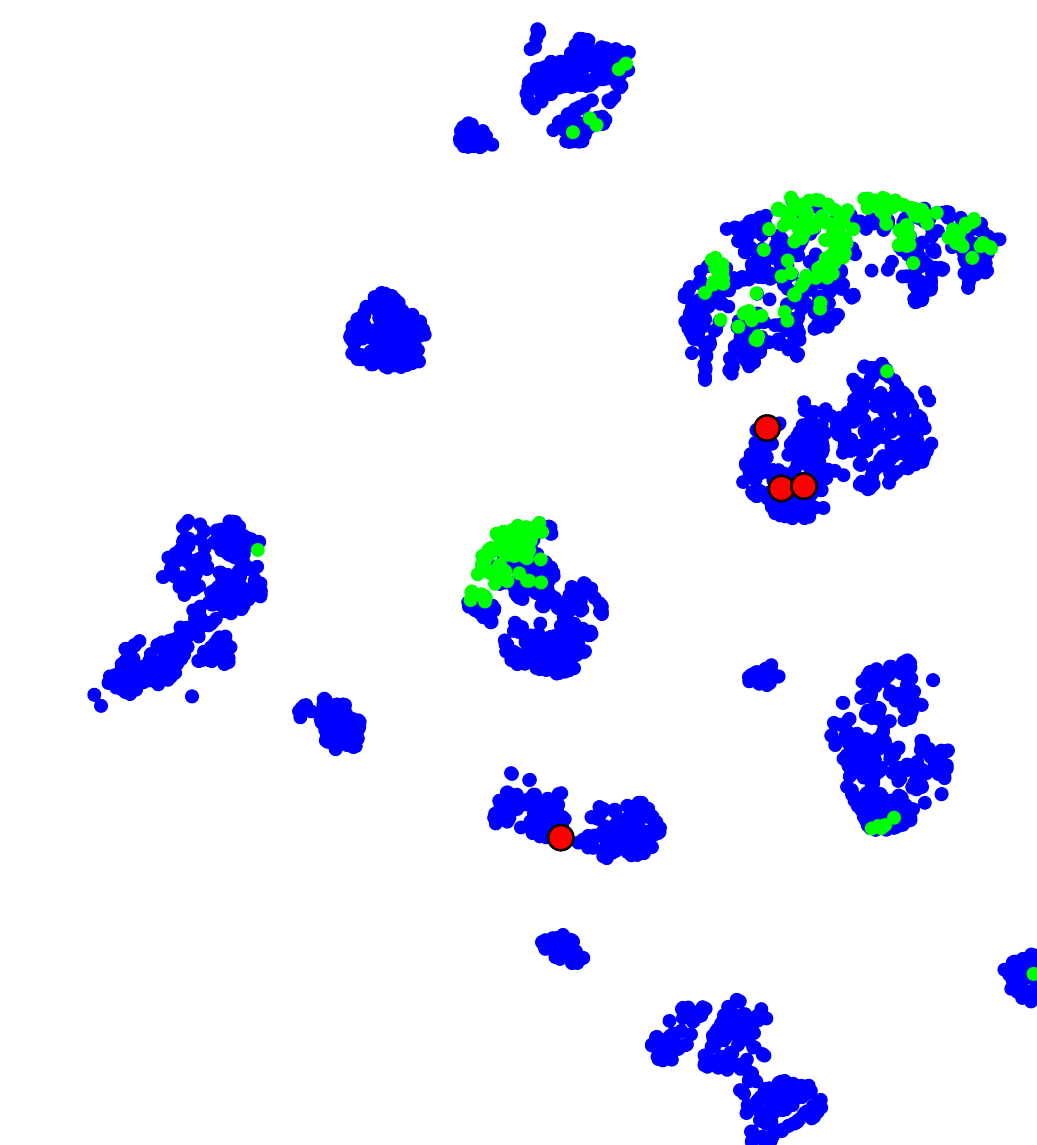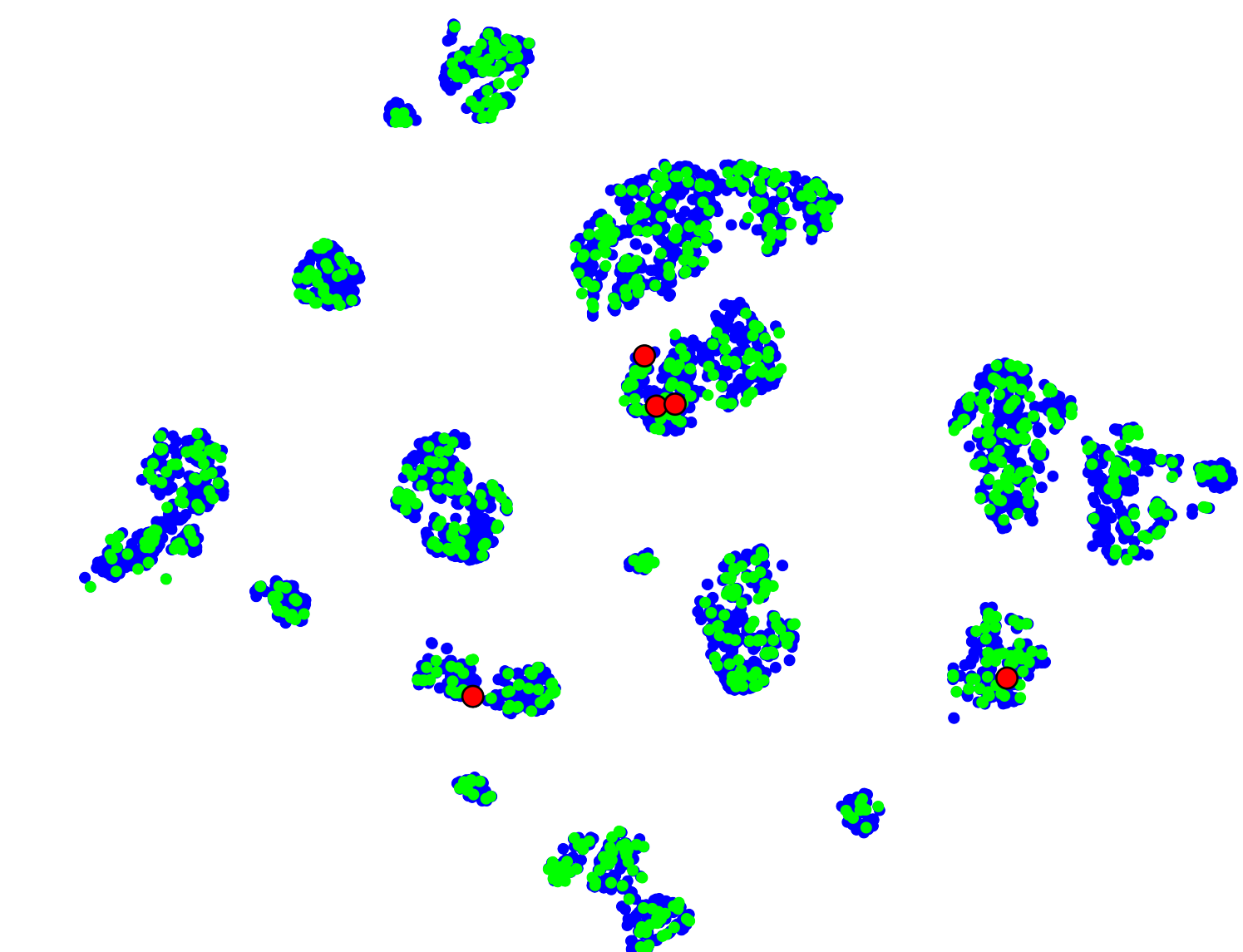pemetrexed (N)

(a) ILP(p=0)   (b) ILP(p=1)   (c) FPS

(d) CUR   (e) SML   (f) random

■ target   ■ selected from QM7   ■ other in QM7