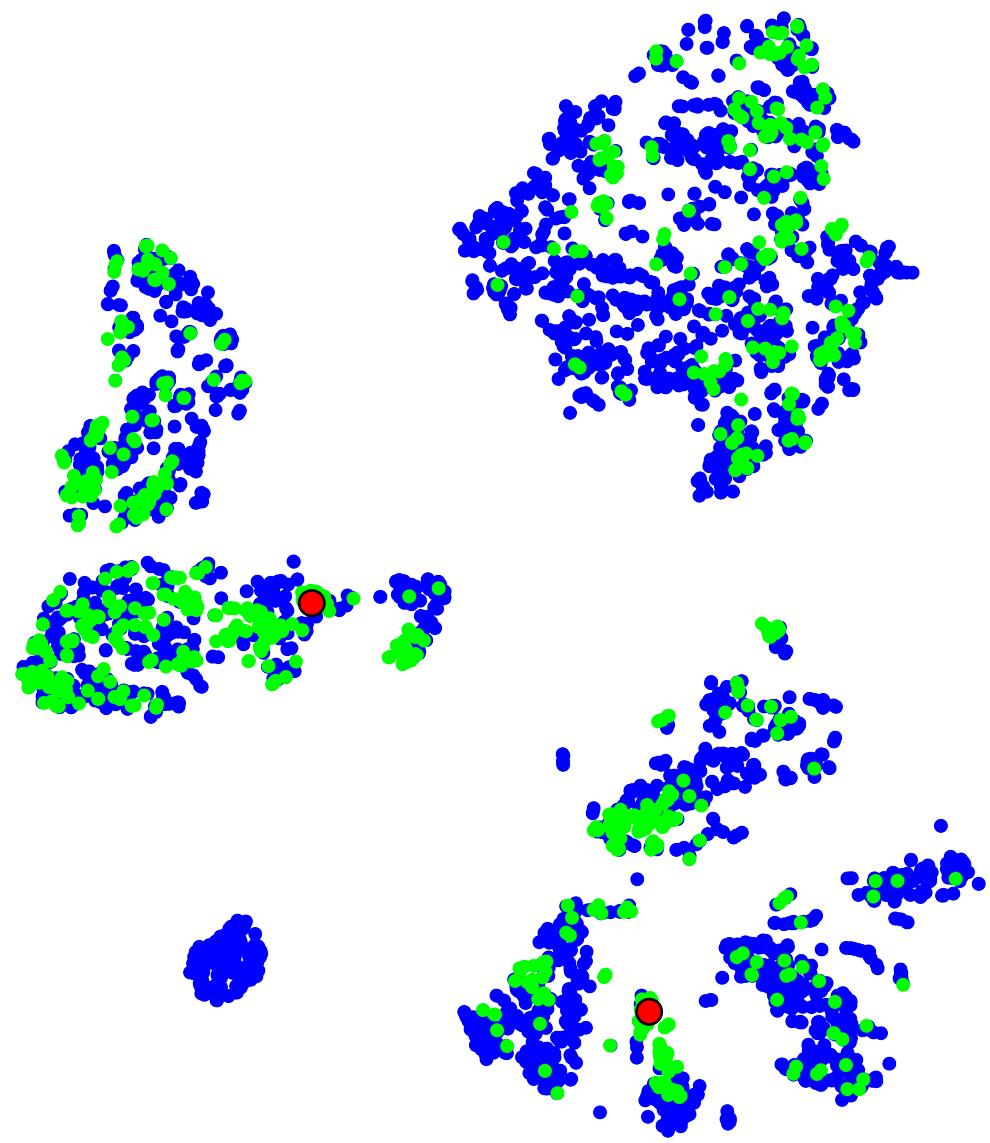
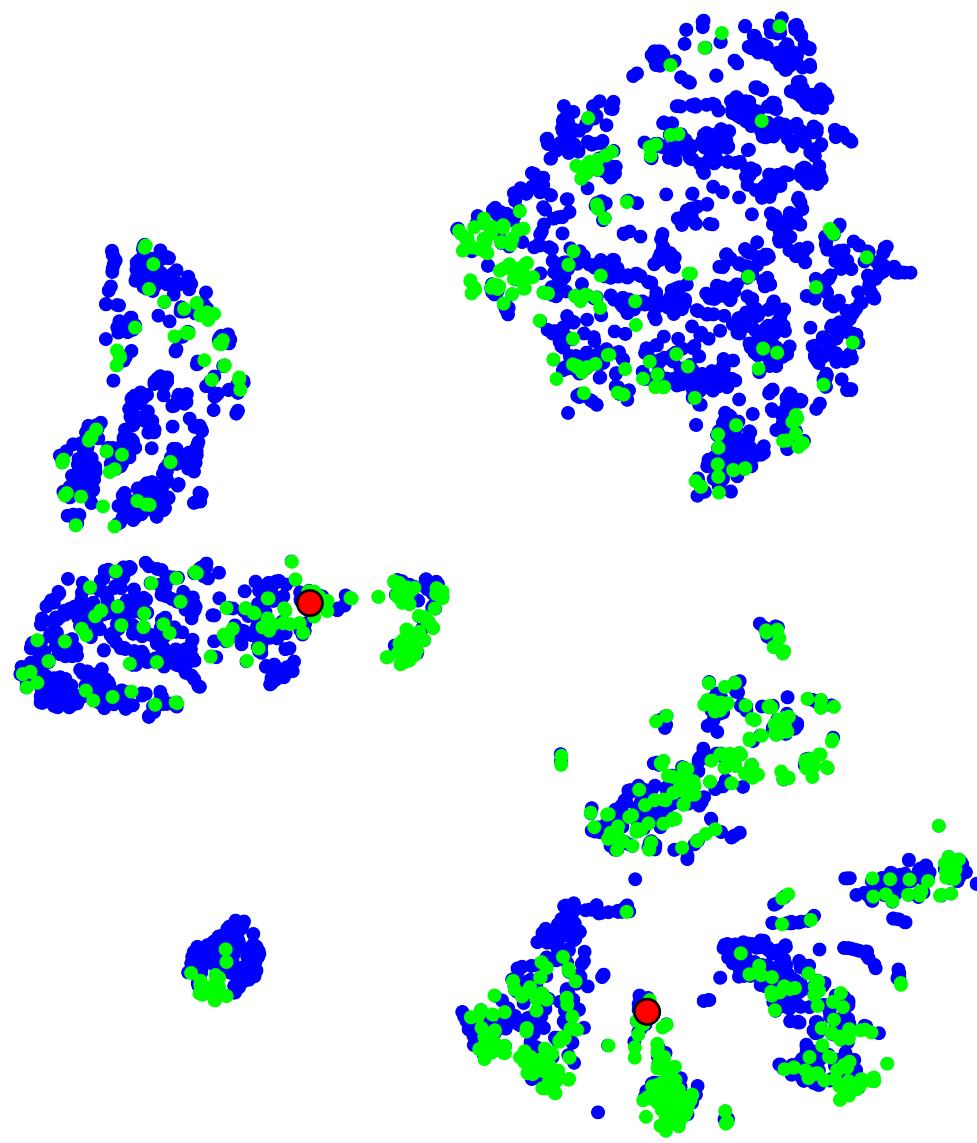


pregabalin (O)

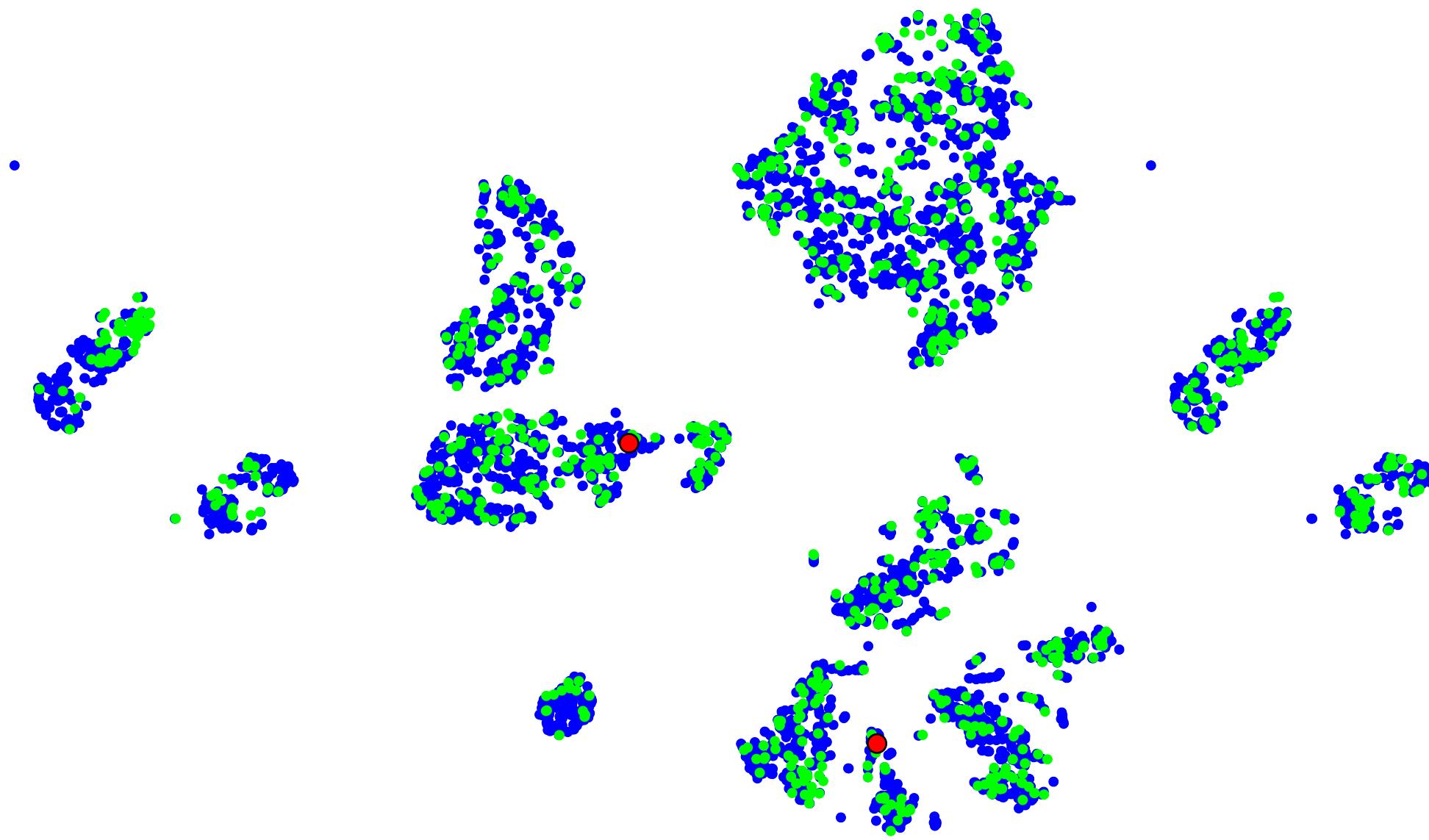
(a) ILP($p=0$)



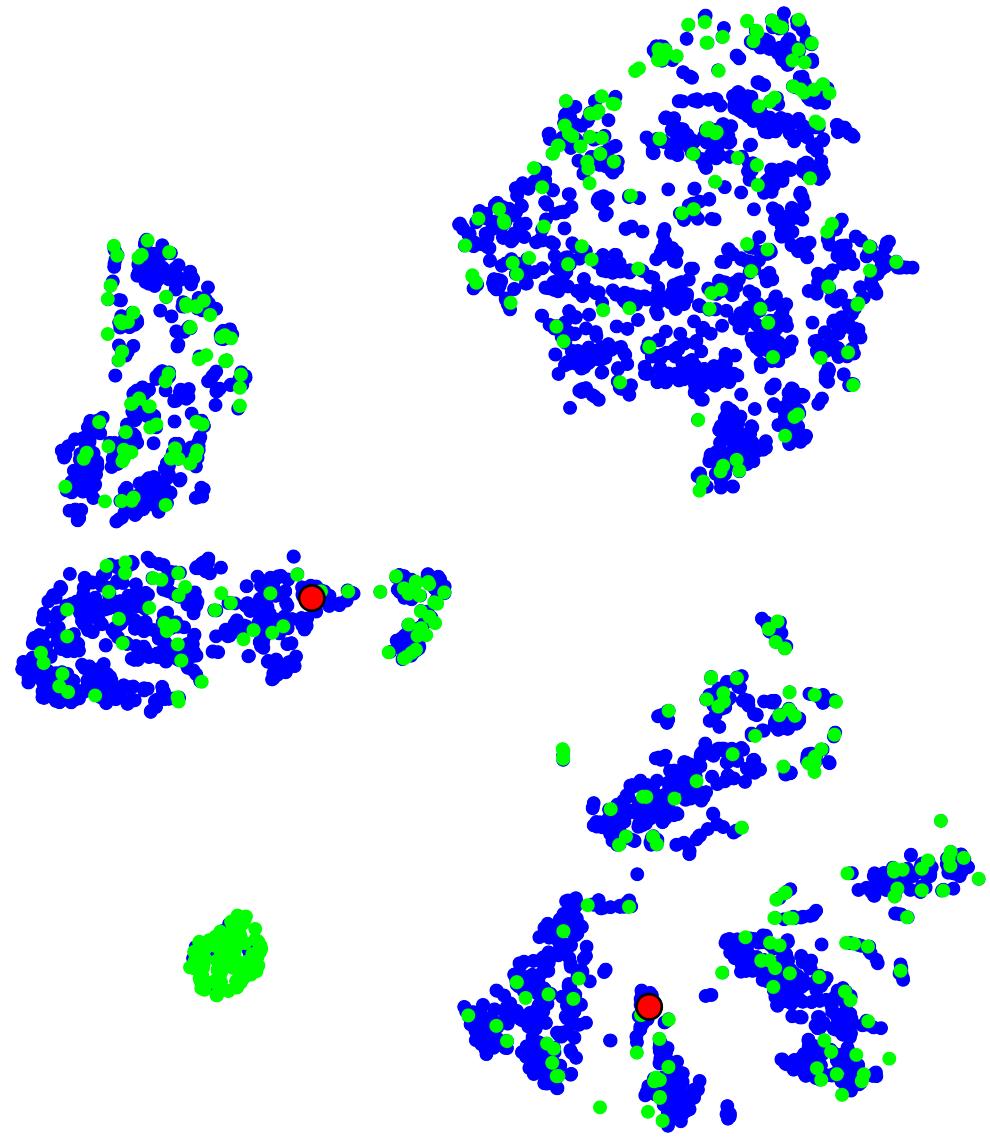
(b) ILP($p=1$)



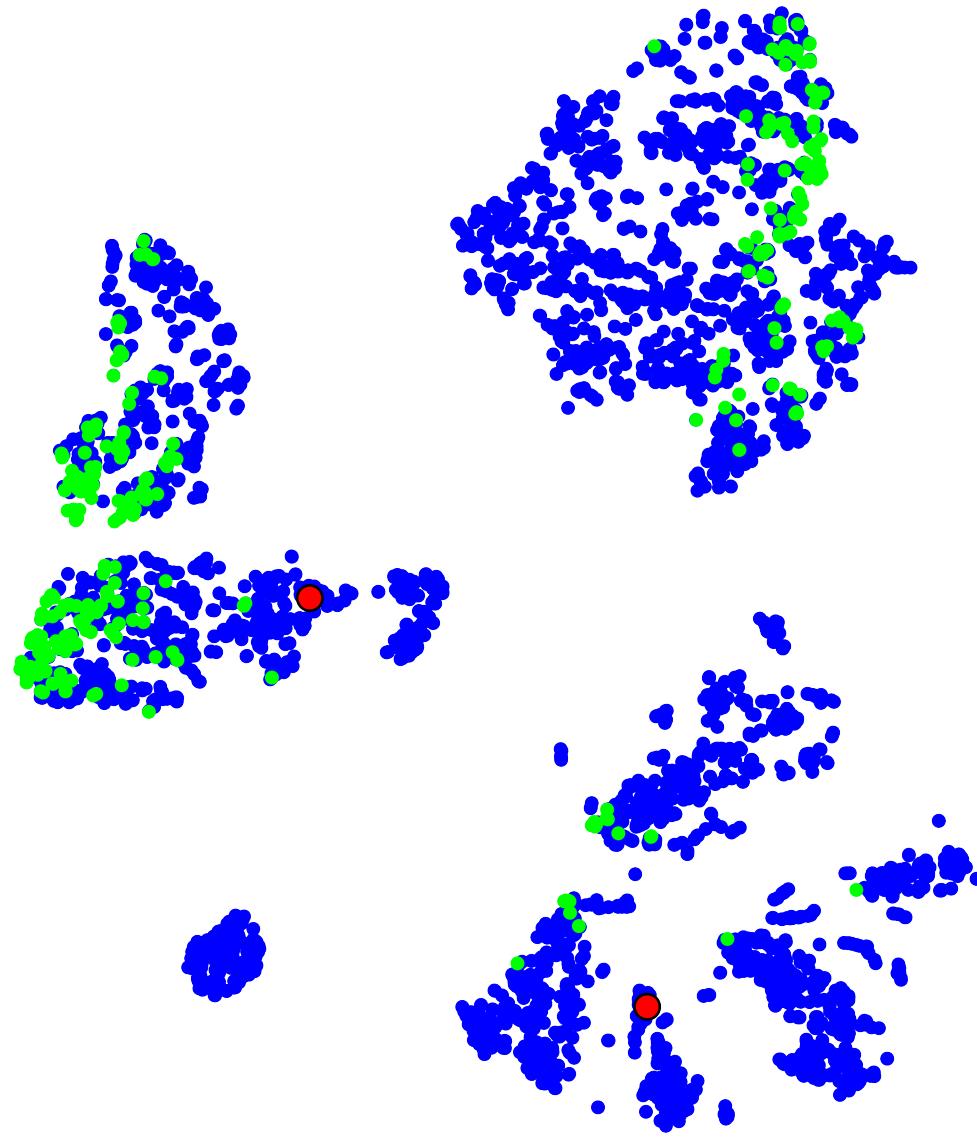
(c) FPS



(d) CUR



(e) SML



(f) random



■ target

■ selected from QM7

■ other in QM7