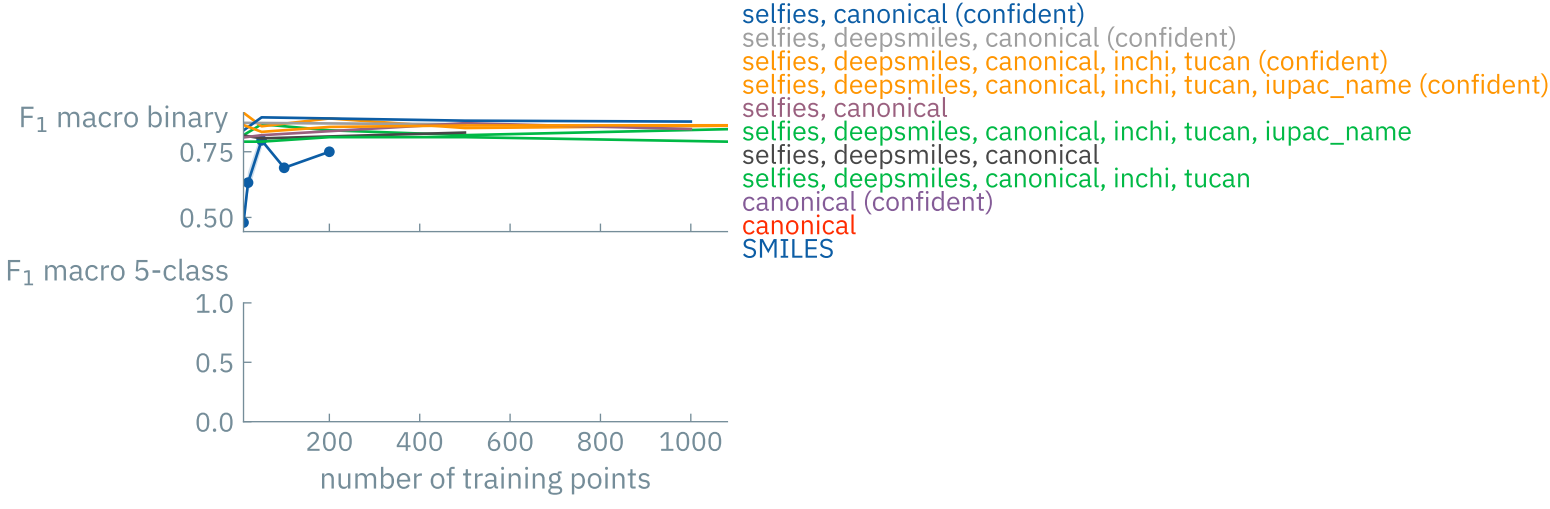
selfies, canonical (confident)
selfies, deepsmiles, canonical (confident)
selfies, deepsmiles, canonical, inchi, tucan (confident)
selfies, deepsmiles, canonical, inchi, tucan, iupac_name (confident)
selfies, canonical
selfies, deepsmiles, canonical, inchi, tucan, iupac_name
selfies, deepsmiles, canonical
selfies, deepsmiles, canonical, inchi, tucan
canonical (confident)
canonical
SMILES
F1 macro binary
0.75
0.50
F1 macro 5-class
1.0
0.5
0.0
200
400
600
800
1000
number of training points