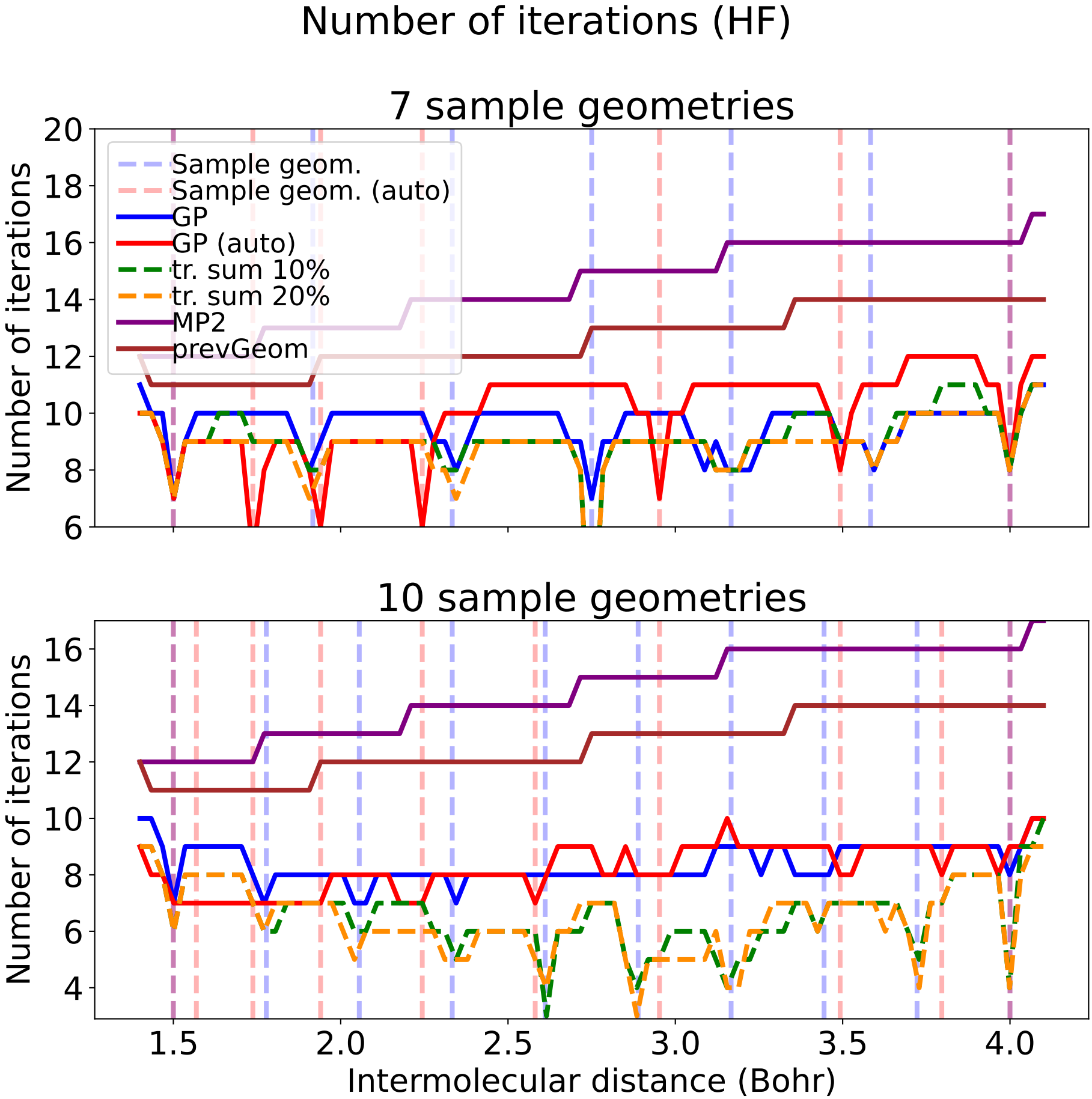
Number of iterations (HF)
7 sample geometries
10 sample geometries
Number of iterations
Intermolecular distance (Bohr)
Sample geom.
Sample geom. (auto)
GP
GP (auto)
tr. sum 10%
tr. sum 20%
MP2
prevGeom
20
18
16
14
12
10
8
6
4
1.5
2.0
2.5
3.0
3.5
4.0