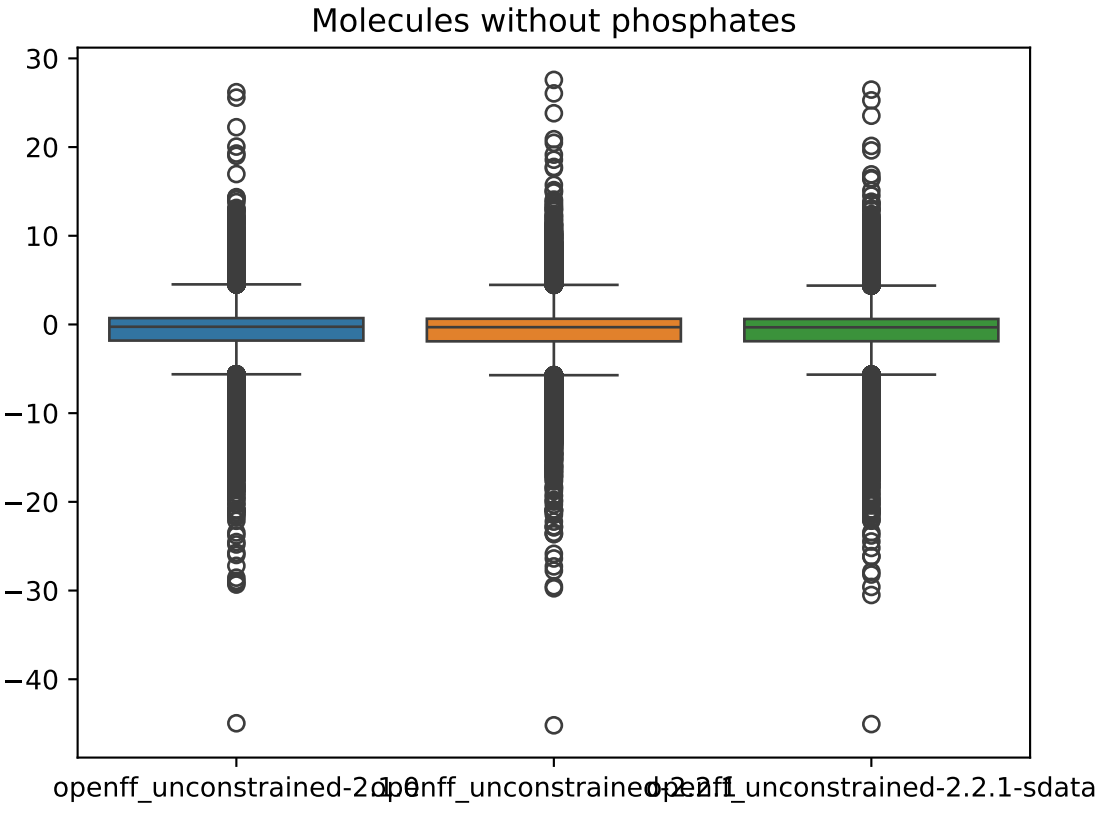
Molecules without phosphates
30
20
10
0
−10
−20
−30
−40
openff_unconstrained-2.2.0
openff_unconstrained-2.2.1
openff_unconstrained-2.2.1-sdata