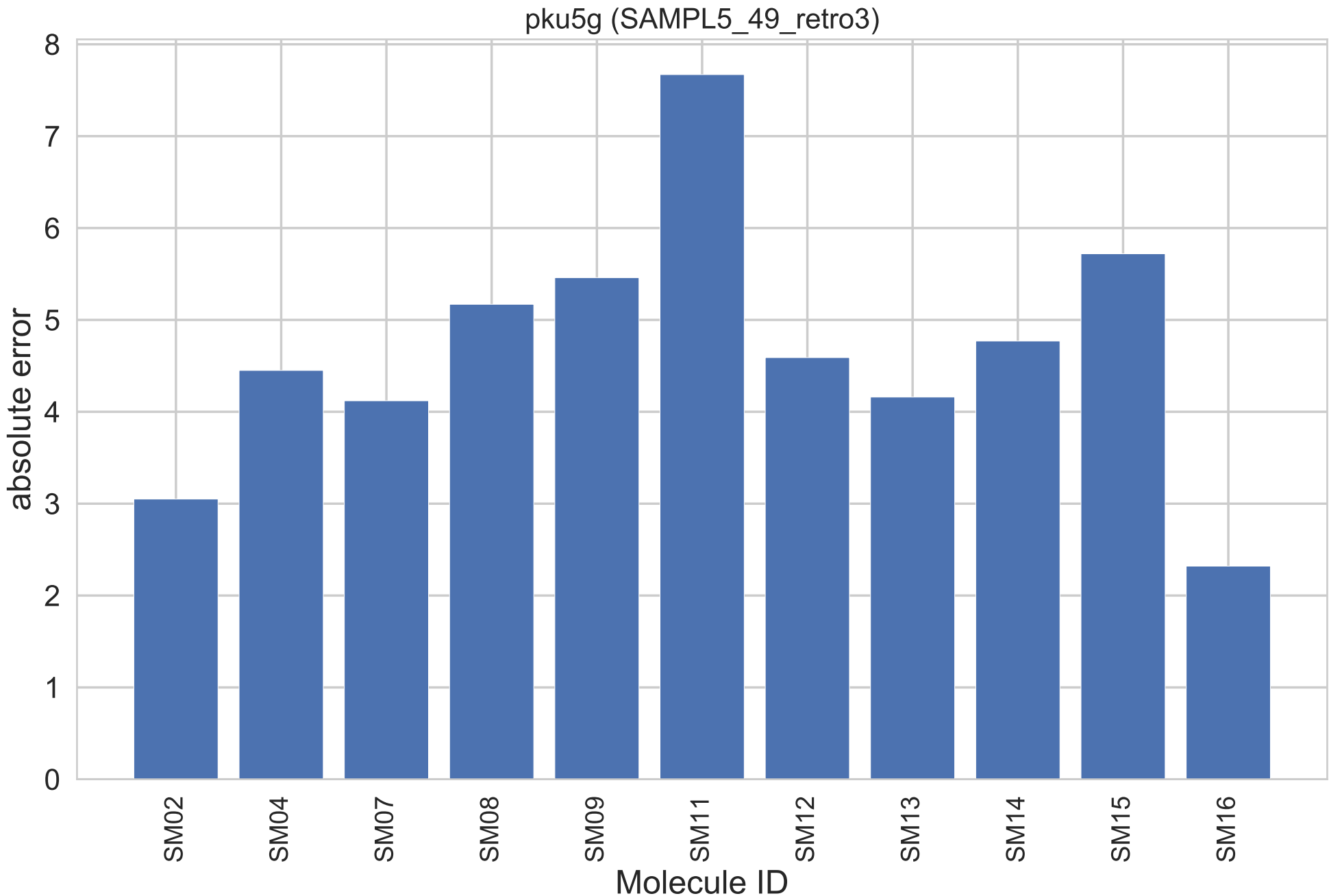
pku5g (SAMPL5_49_retro3)
absolute error
0
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SM02
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Molecule ID