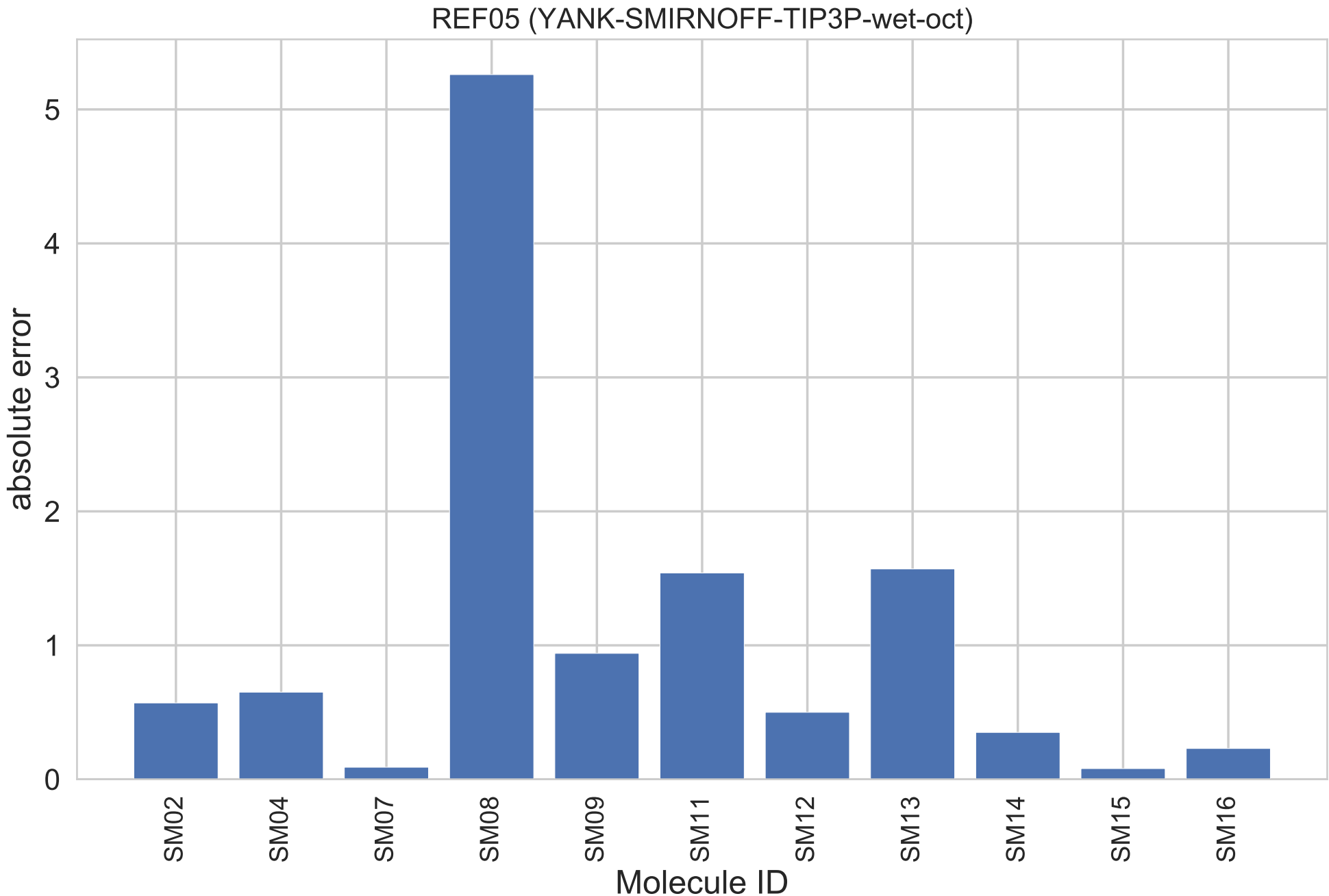
REF05 (YANK-SMIRNOFF-TIP3P-wet-oct)
absolute error
0
1
2
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SM02
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Molecule ID