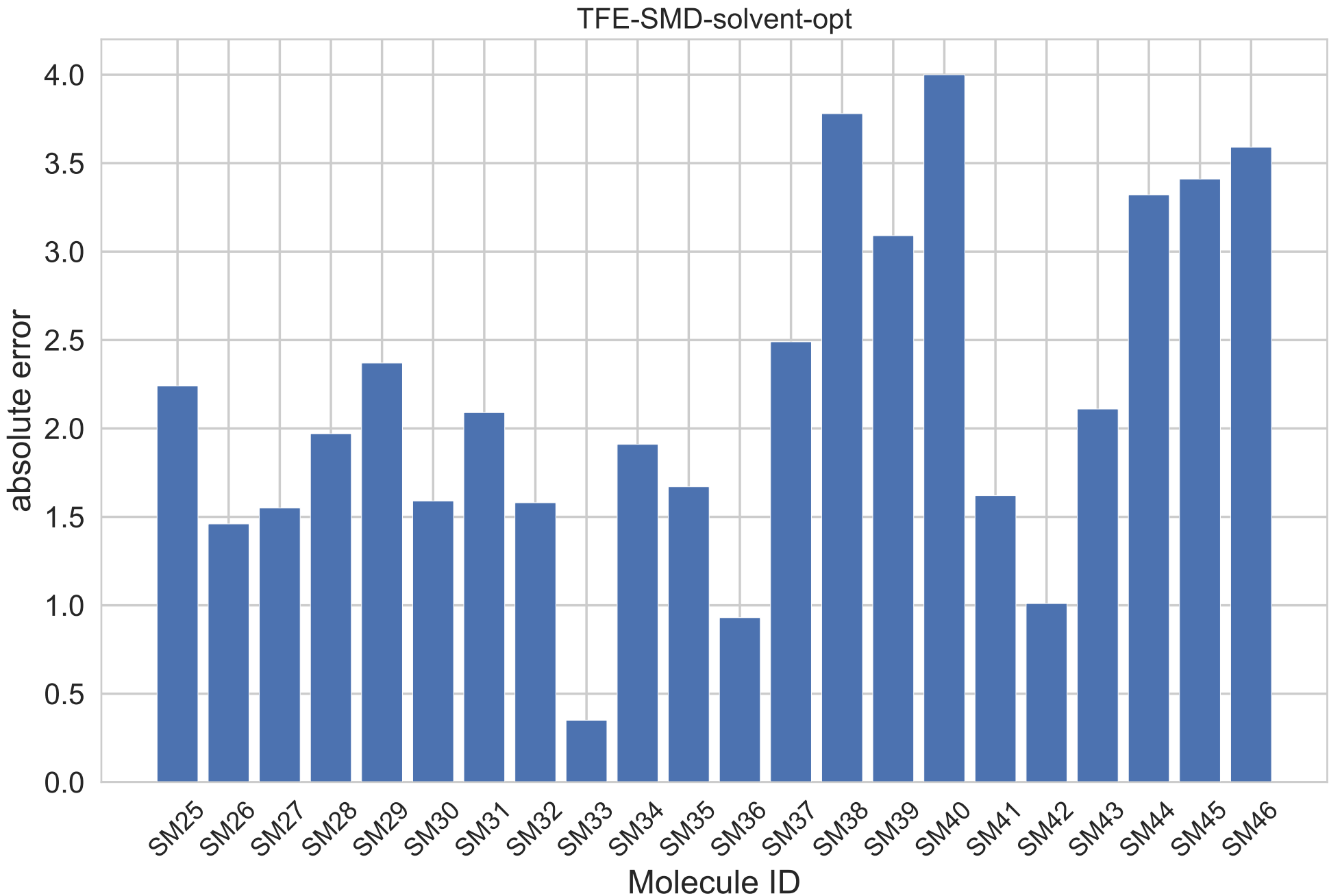
TFE-SMD-solvent-opt
absolute error
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
SM25
SM26
SM27
SM28
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Molecule ID