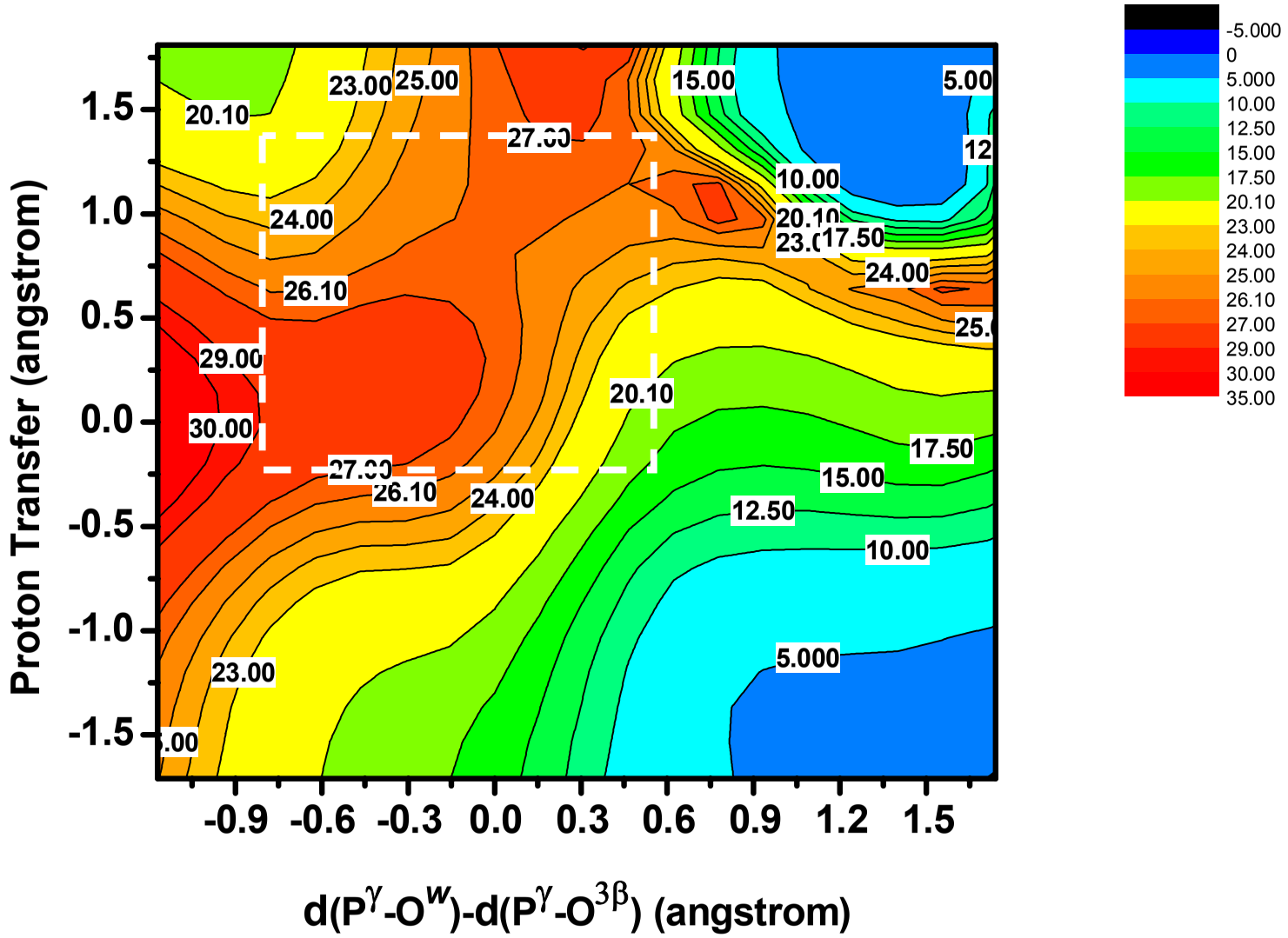
Supporting Information: comparison between SCC-DFTBPR/MM and B3LYP/MM adiabatic maps

We note that the two-dimensional adiabatic map at the SCC-DFTBPR/MM level (Figure S1) has qualitatively the same feature as the B3LYP/MM result (Figure 4 in main text). The position for the saddle point is slightly different from that at the B3LYP/MM level. For example, on the SCC-DFTBPR/MM surface, the saddle point is at (0.0, 0.7), while at the B3LYP/MM level, the saddle point is at (-0.15, 0.4). However, the flat nature of the potential energy near the saddle point is observed at both levels. For example, on the SCC-DFTBPR/MM surface, the energy difference between the saddle point and the B3LYP/MM saddle point, (-0.15, 0.4), is less than 1 kcal/mol. Similarly, on the B3LYP/MM surface, the energy difference between the saddle point and the SCC-DFTBPR/MM saddle point, (0.0, 0.7), is also smaller than 1 kcal/mol. Therefore, SCC-DFTBPR/MM is very consistent with the B3LYP/MM result, which justifies the use of SCC-DFTBPR/MM in potential mean force calculations[16].

Figure S1

Same as Figure 4 in the main text, but at the SCC-DFTBPR/MM level.

Figure S1


Proton Transfer (angstrom)
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-0.9 -0.6 -0.3 0.0 0.3 0.6 0.9 1.2 1.5
d(P^γ-O^w)-d(P^γ-O^3β) (angstrom)
-5.000
0
5.000
10.00
12.50
15.00
17.50
20.10
23.00
24.00
25.00
26.10
27.00
29.00
30.00
35.00