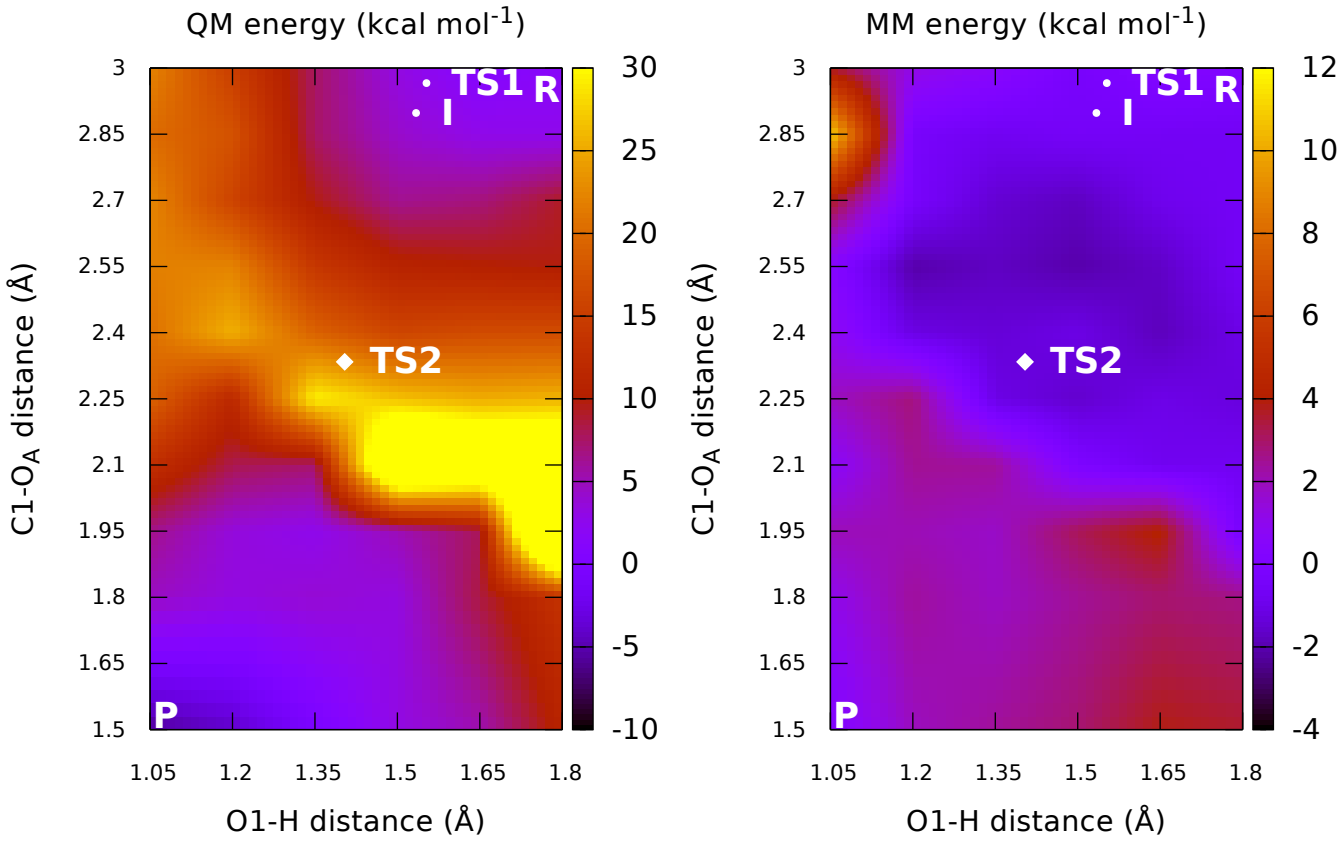
QM energy (kcal mol-1)
MM energy (kcal mol-1)
C1-OA distance (Å)
O1-H distance (Å)
TS1
R
I
TS2
P
3
2.85
2.7
2.55
2.4
2.25
2.1
1.95
1.8
1.65
1.5
1.05
1.2
1.35
1.5
1.65
1.8
30
25
20
15
10
5
0
-5
-10
12
10
8
6
4
2
0
-2
-4