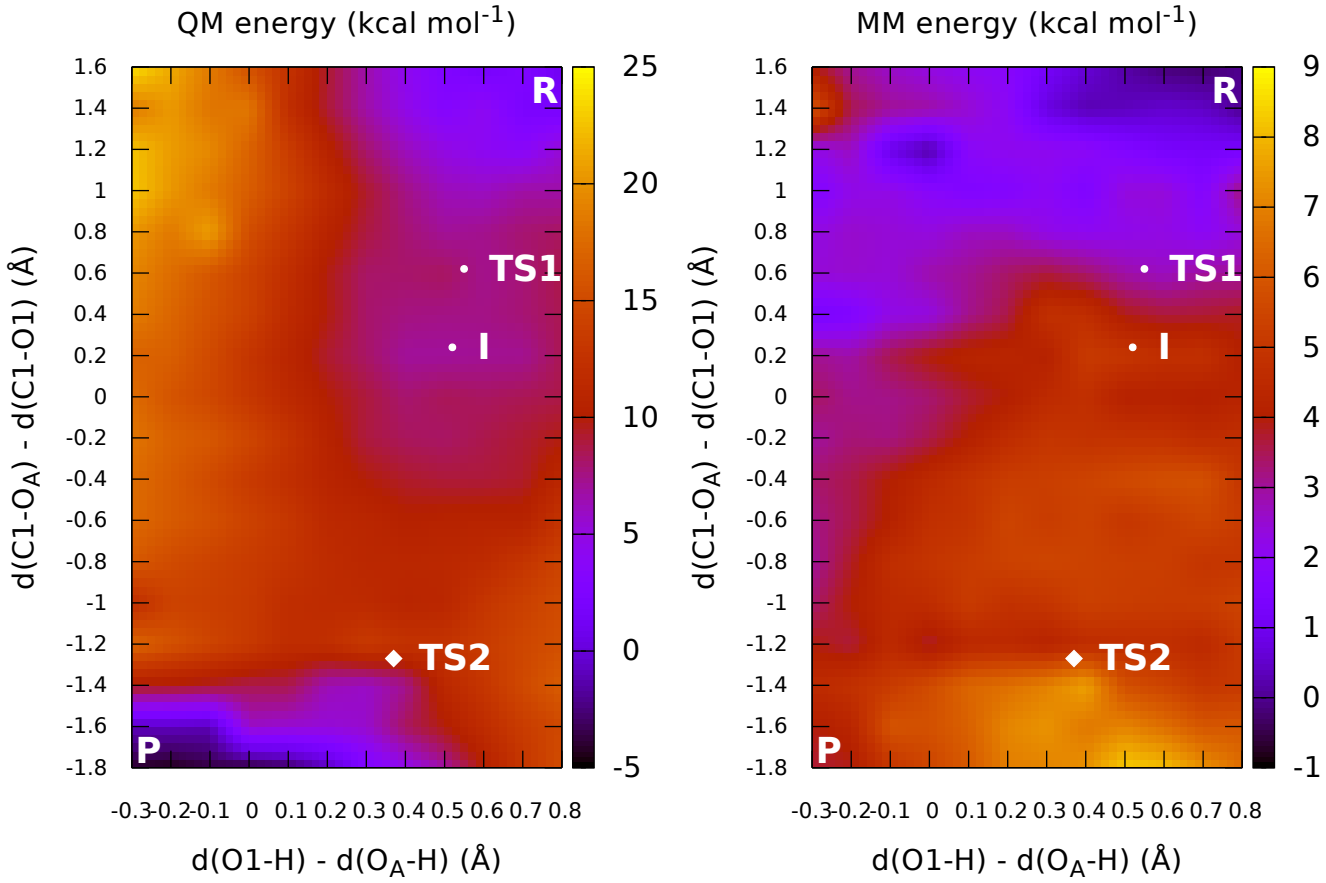
QM energy (kcal mol-1)
MM energy (kcal mol-1)
R
TS1
I
TS2
P
d(C1-OA) - d(C1-O1) (Å)
d(O1-H) - d(OA-H) (Å)
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-1.2
-1.4
-1.6
-1.8
-0.3 -0.2 -0.1 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8
25
20
15
10
5
0
-5
9
8
7
6
5
4
3
2
1
0
-1