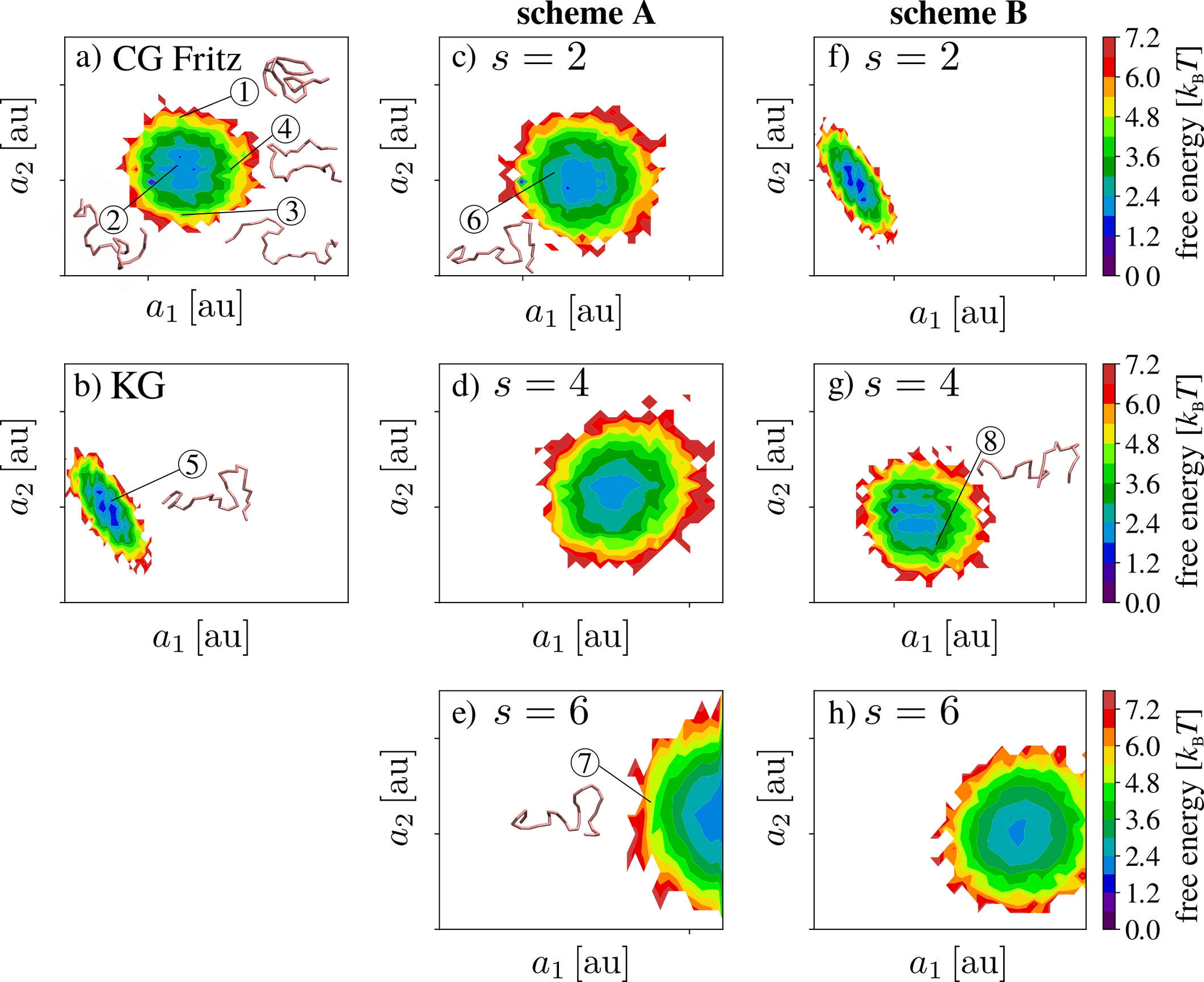
scheme A
scheme B
a) CG Fritz
b) KG
c) $s = 2$
d) $s = 4$
e) $s = 6$
f) $s = 2$
g) $s = 4$
h) $s = 6$
1
2
3
4
5
6
7
8
a_1 [au]
a_2 [au]
free energy [$k_B T$]
7.2
6.0
4.8
3.6
2.4
1.2
0 0
0.0