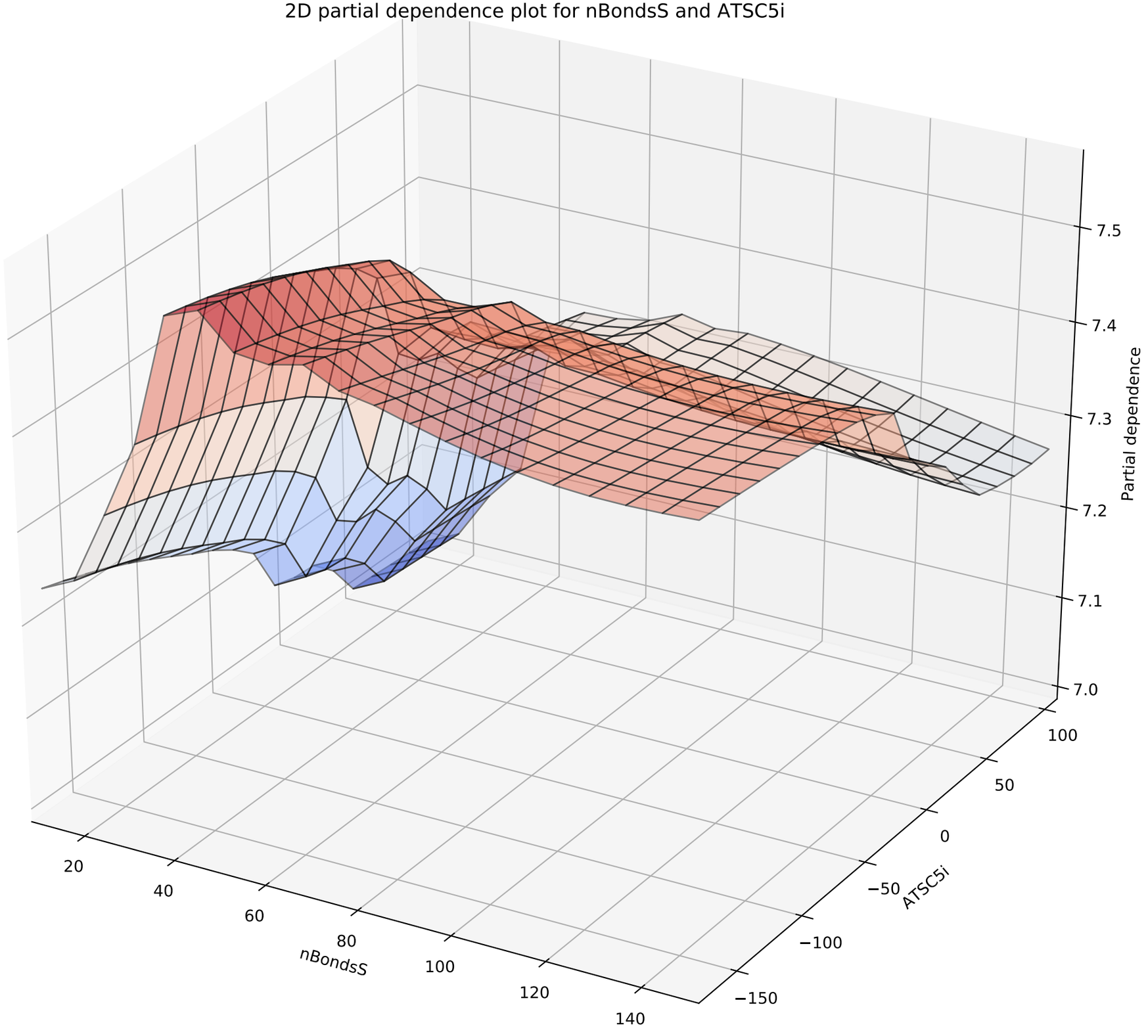

2D partial dependence plot for nBondsS and ATSC5i
Partial dependence
7.5
7.4
7.3
7.2
7.1
7.0
nBondsS
20
40
60
80
100
120
140
ATSC5i
100
50
0
−50
−100
−150