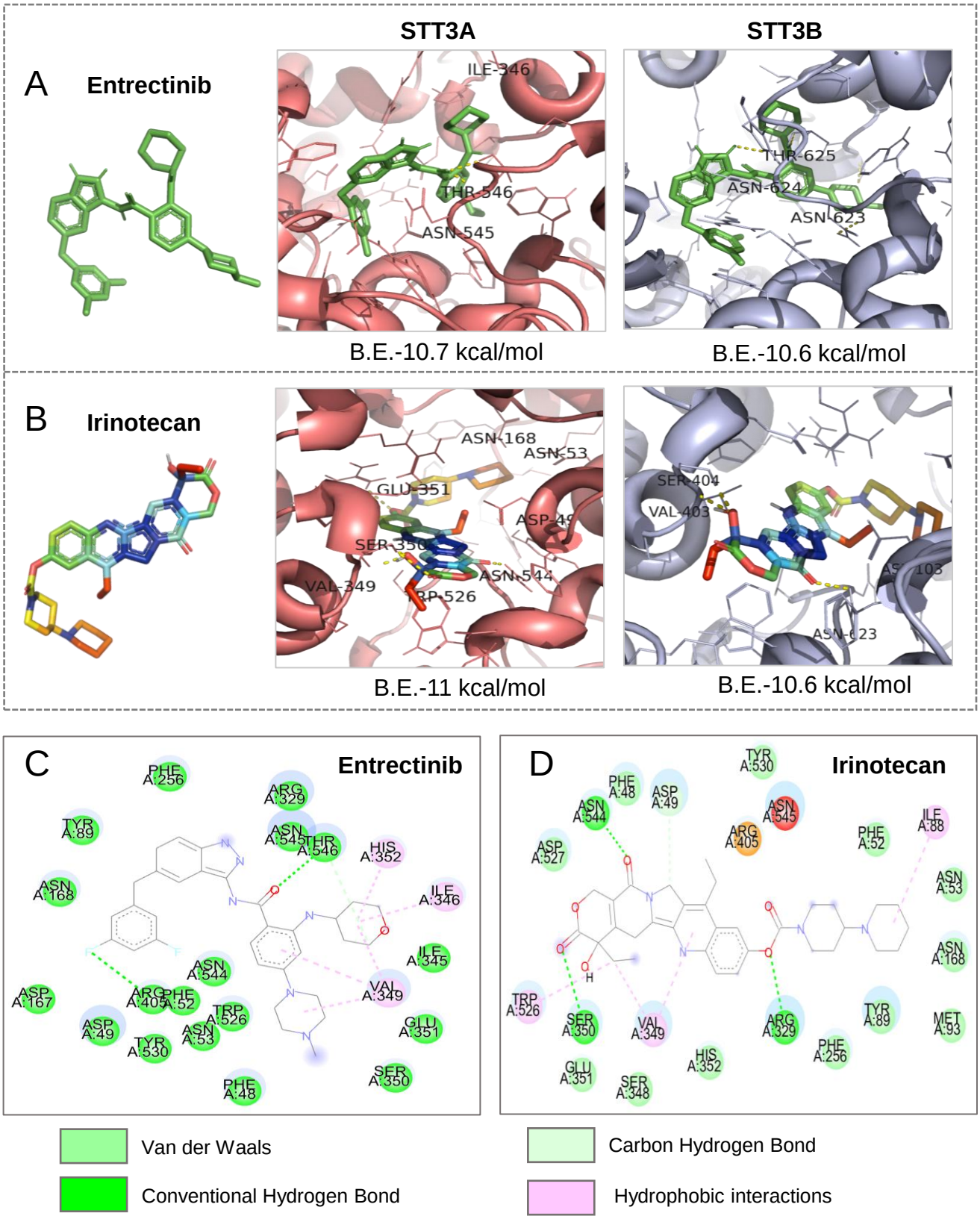
STT3A
STT3B
A
Entrectinib
ILE-346
THR-546
ASN-545
THR-625
ASN-624
ASN-623
B.E.-10.7 kcal/mol
B.E.-10.6 kcal/mol
B
Irinotecan
ASN-168
ASN-53
GLU-351
SER-350
ASN-544
VAL-349
TRP-526
SER-404
VAL-403
ASN-623
B.E.-11 kcal/mol
B.E.-10.6 kcal/mol
C
Entrectinib
PHE A:256
ARG A:329
TYR A:89
ASN A:545
THR A:546
HIS A:352
ASN A:168
ILE A:346
ILE A:345
ASN A:544
ASP A:167
ARG A:405
PHE A:52
VAL A:349
TRP A:526
ASP A:49
ASN A:53
GLU A:351
TYR A:530
SER A:350
PHE A:48
D
Irinotecan
TYR A:530
PHE A:48
ASP A:49
ASN A:544
ASN A:545
ILE A:88
ARG A:405
PHE A:52
ASP A:527
ASN A:53
ASN A:168
TRP A:526
SER A:350
VAL A:349
ARG A:329
TYR A:89
MET A:93
PHE A:256
HIS A:352
GLU A:351
SER A:348
Van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Hydrophobic interactions

Figure 5