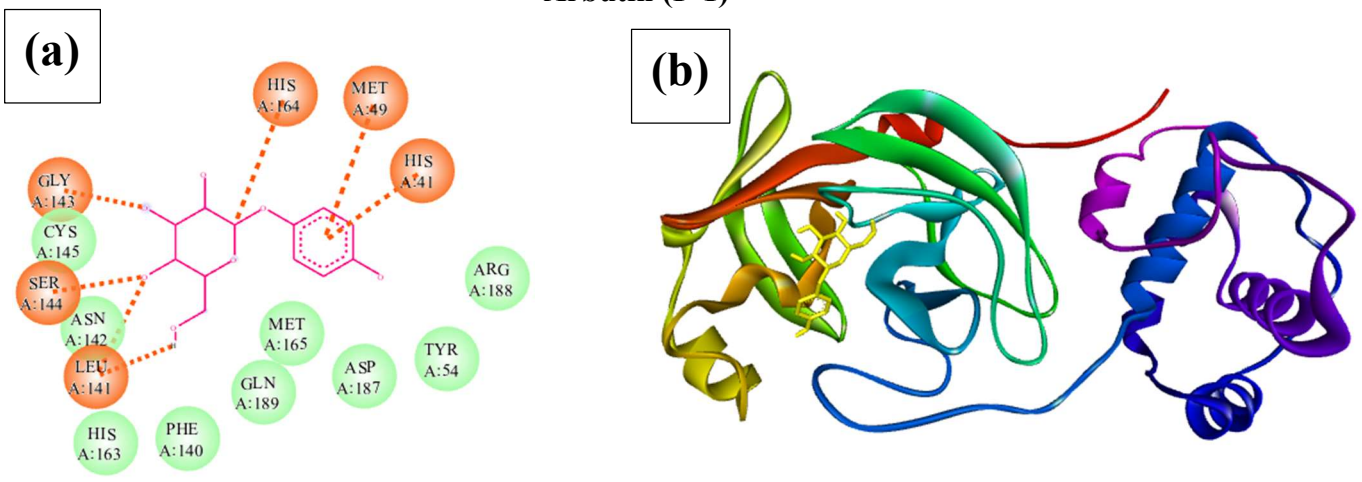
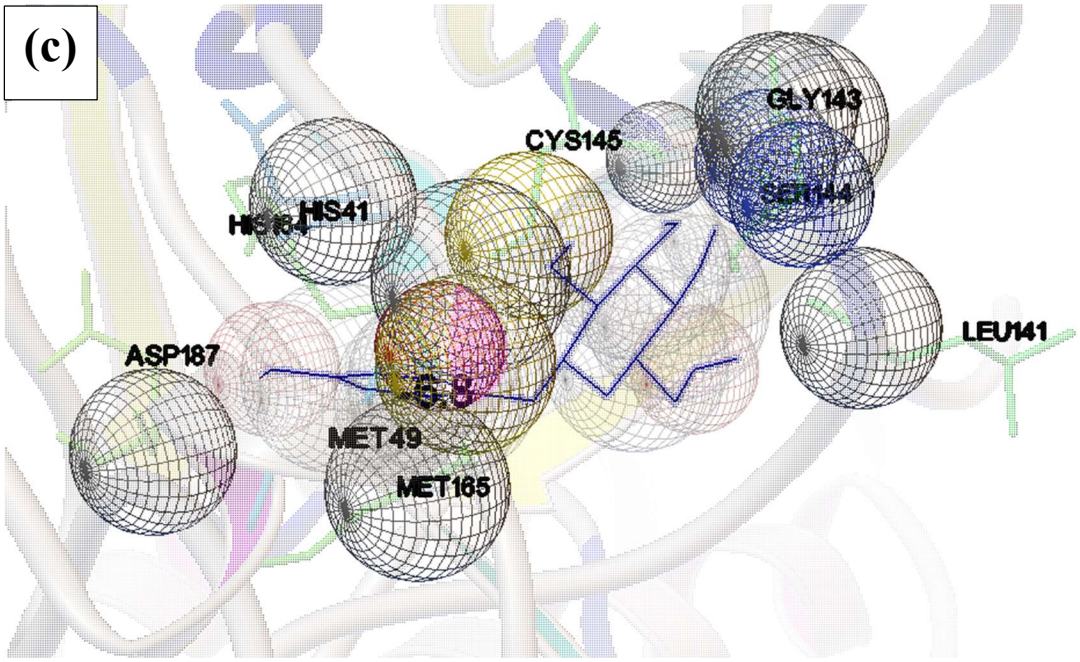
Supporting information

for

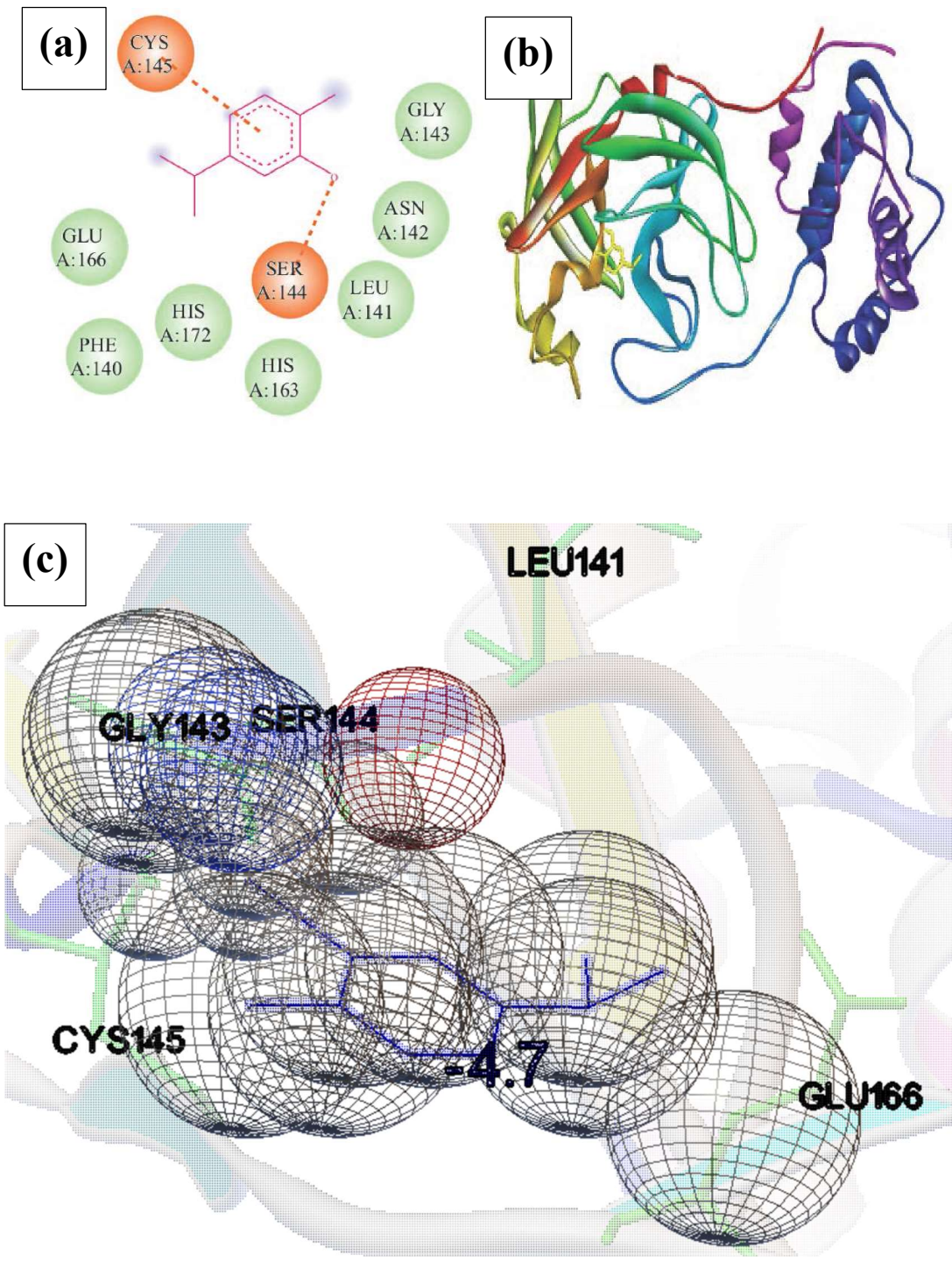
SAR, Molecular Docking and Molecular Dynamic Simulation of Natural inhibitors against SARS-CoV-19 Mpro spike protein

Arbutin (P-1)

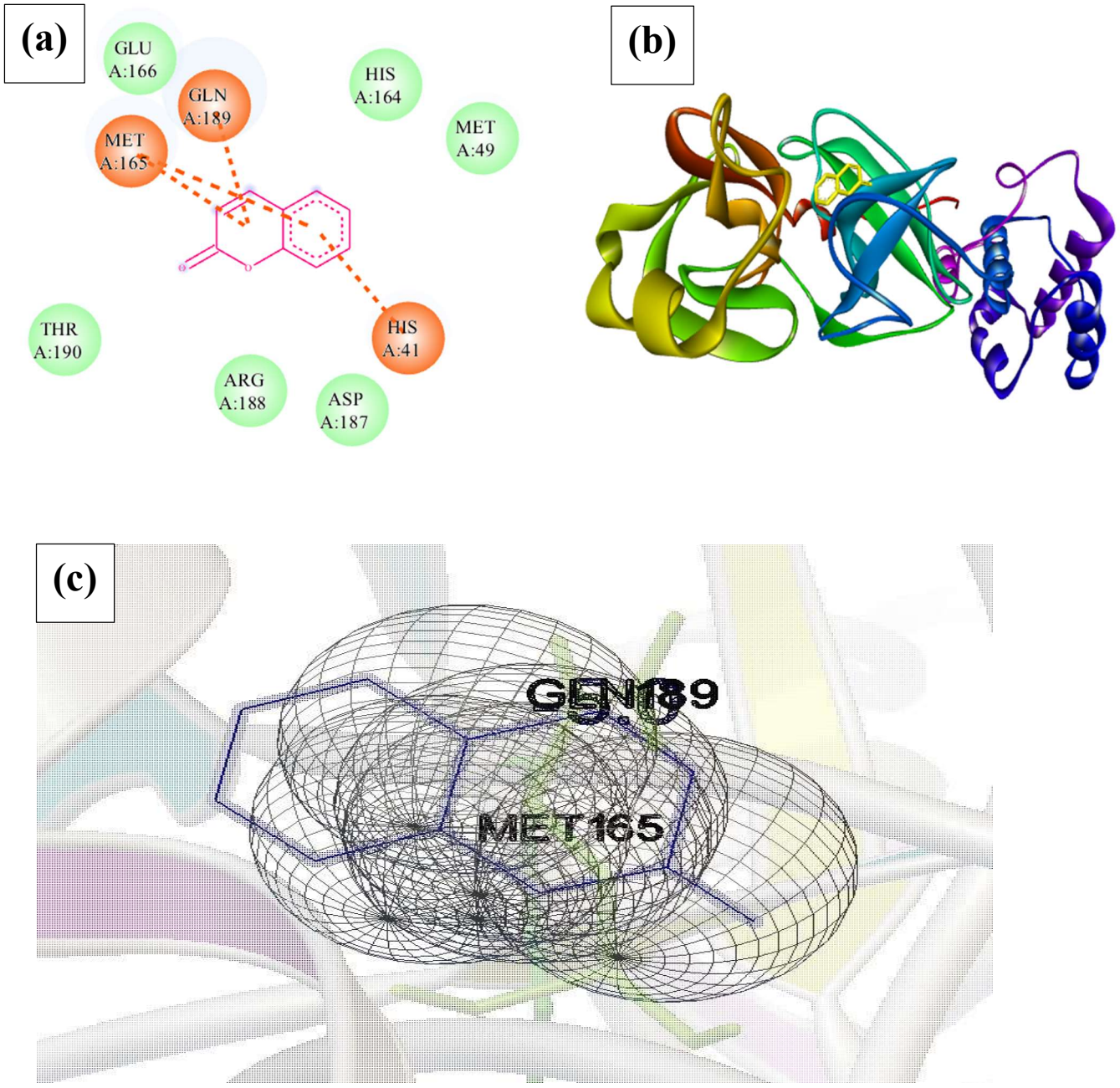




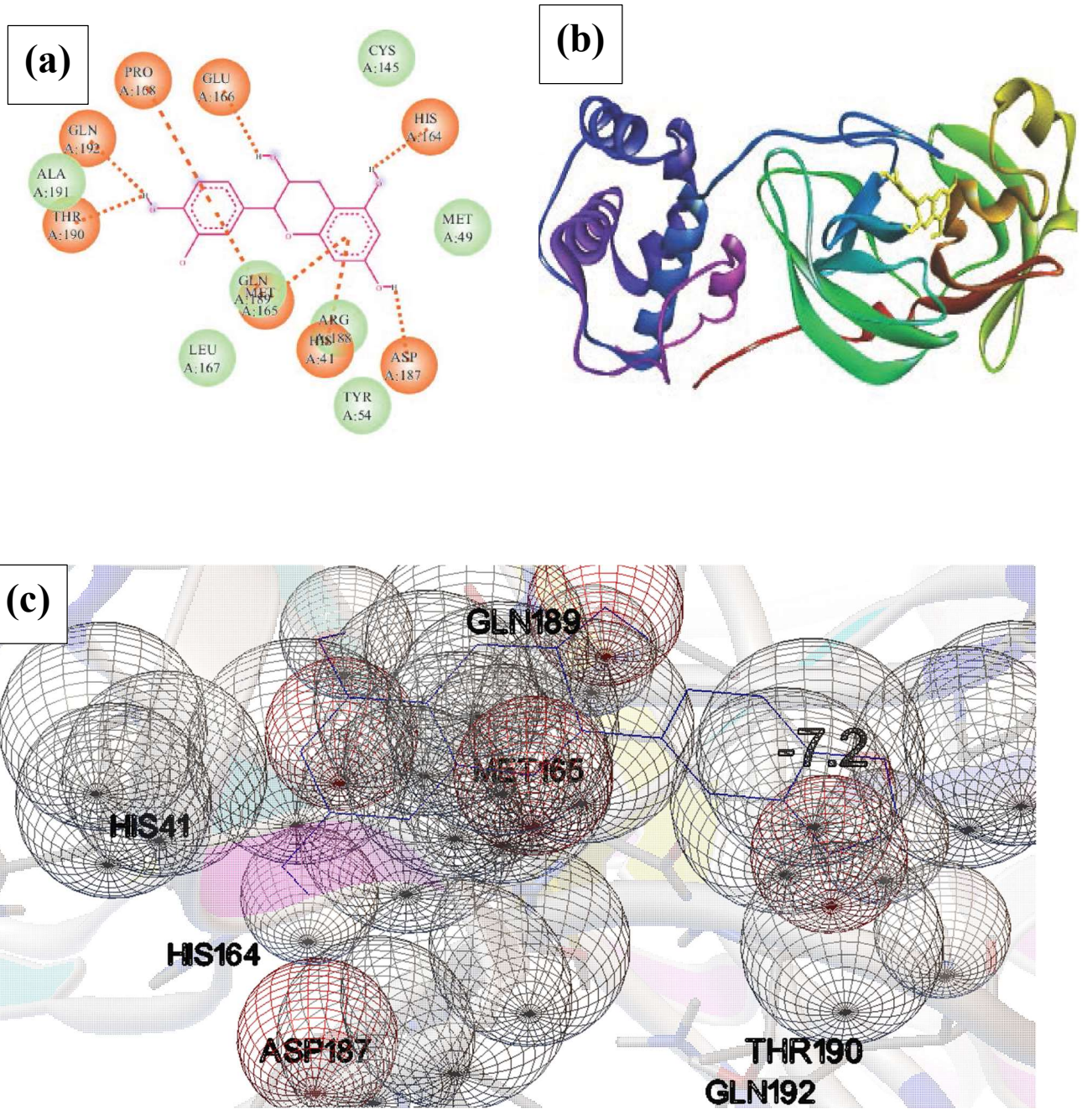
Carvacrol P-2



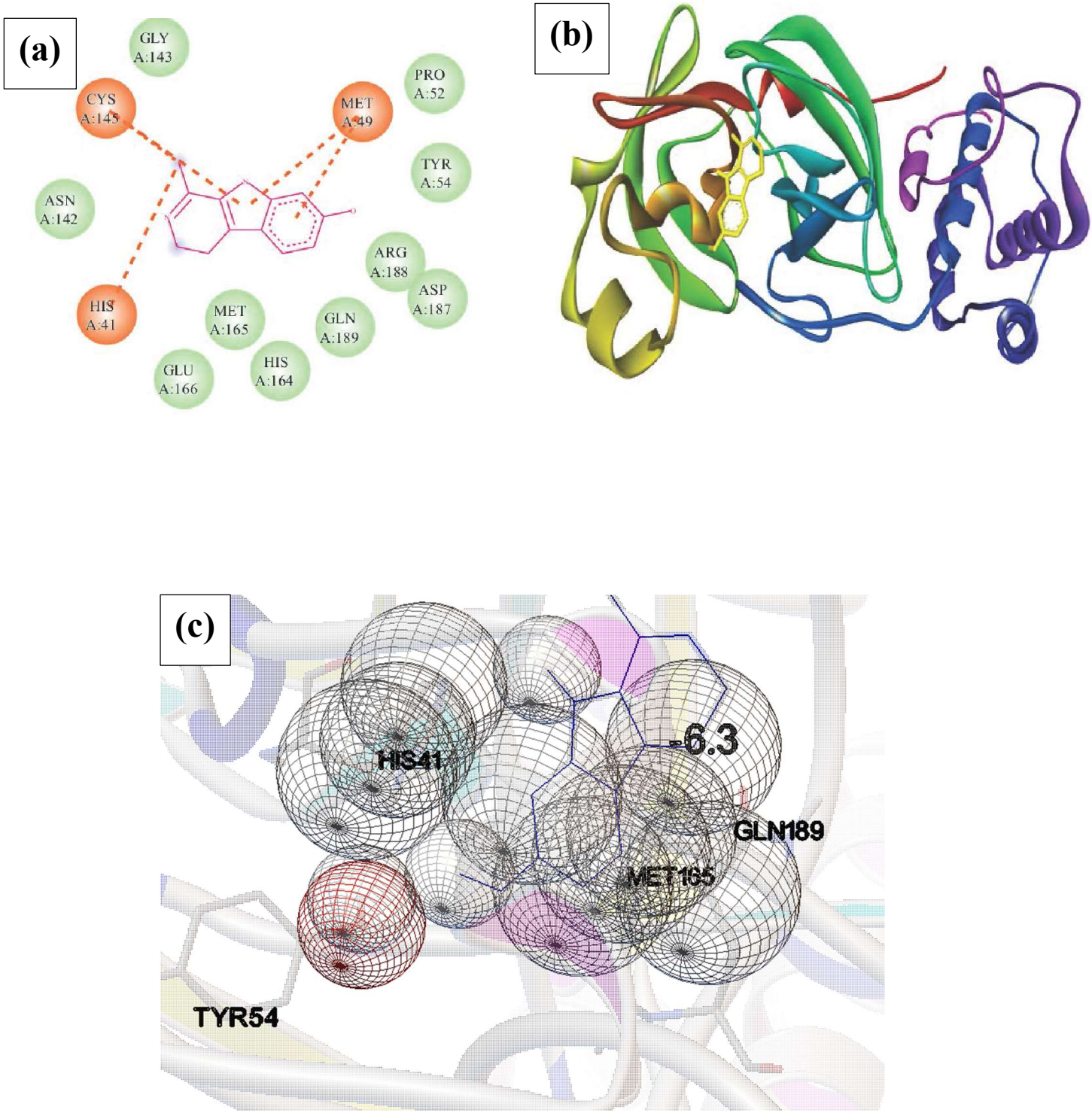
Coumarin P-3


(a)
GLU A:166
GLN A:189
HIS A:164
MET A:165
MET A:49
THR A:190
HIS A:41
ARG A:188
ASP A:187
(b)
(c)
GLN189
MET165

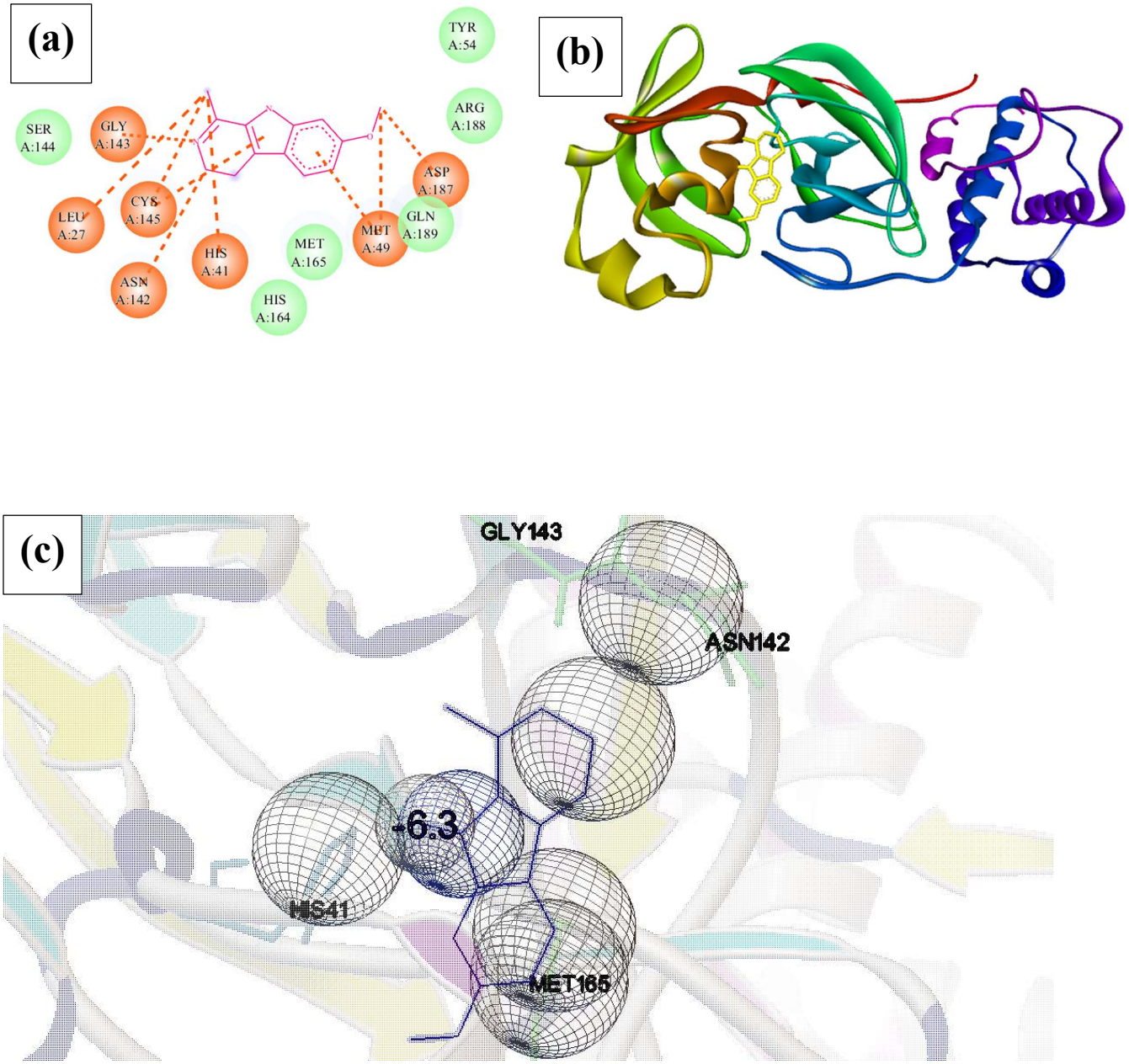
Catechin P-4


(a)
PRO A:168
GLU A:166
CYS A:145
HIS A:164
GLN A:192
ALA A:191
THR A:190
MET A:49
GLN A:189
MET A:165
ARG A:188
HIS A:41
ASP A:187
LEU A:167
TYR A:54
(b)
(c)
GLN189
MET165
-7.2
HIS41
HIS164
ASP187
THR190
GLN192

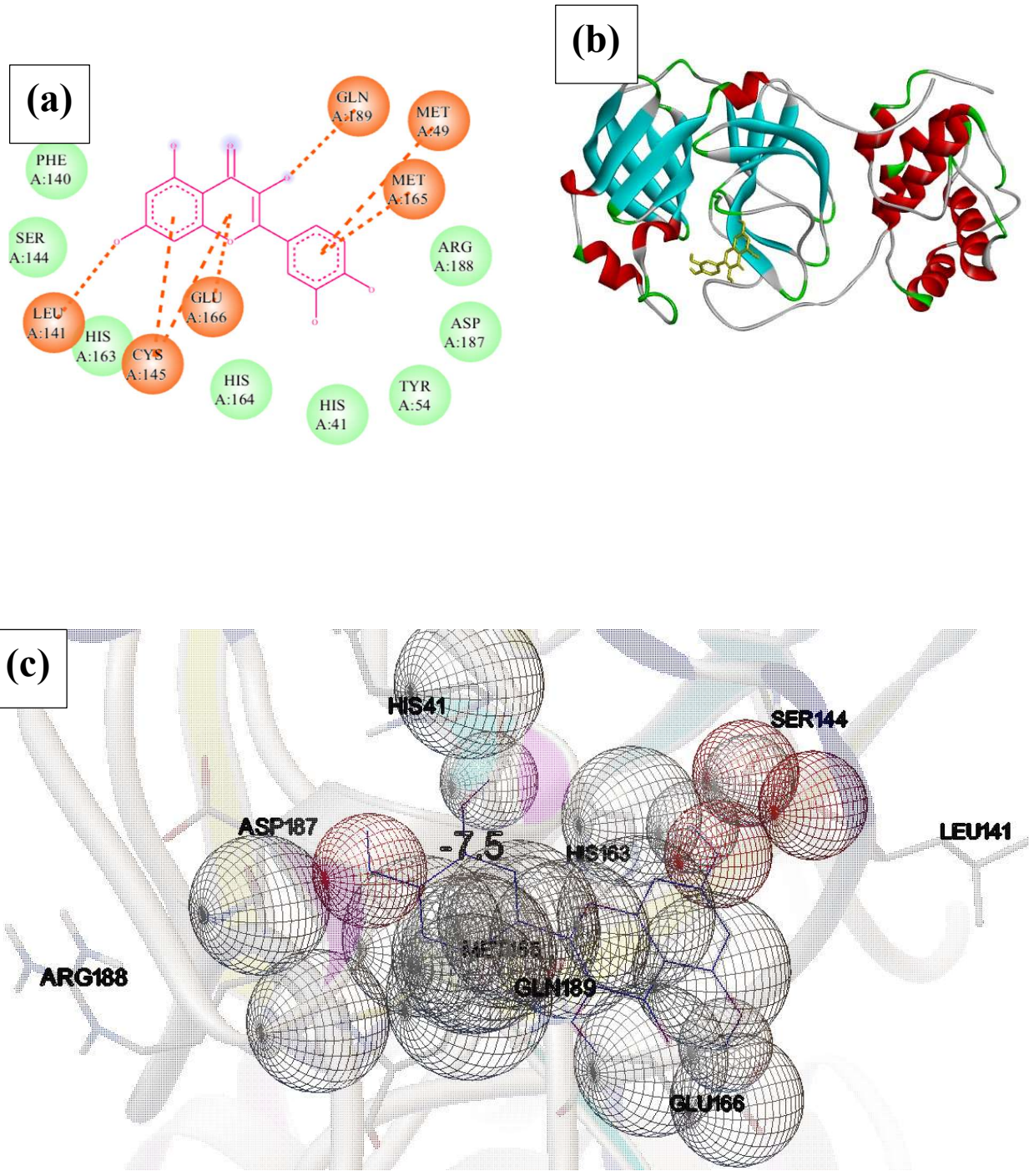
Harmalol P-5


(a)
GLY A:143
PRO A:52
CYS A:145
MET A:49
TYR A:54
ASN A:142
ARG A:188
ASP A:187
HIS A:41
MET A:165
GLN A:189
GLU A:166
HIS A:164
(b)
(c)
HIS41
-6.3
GLN189
MET165
TYR54

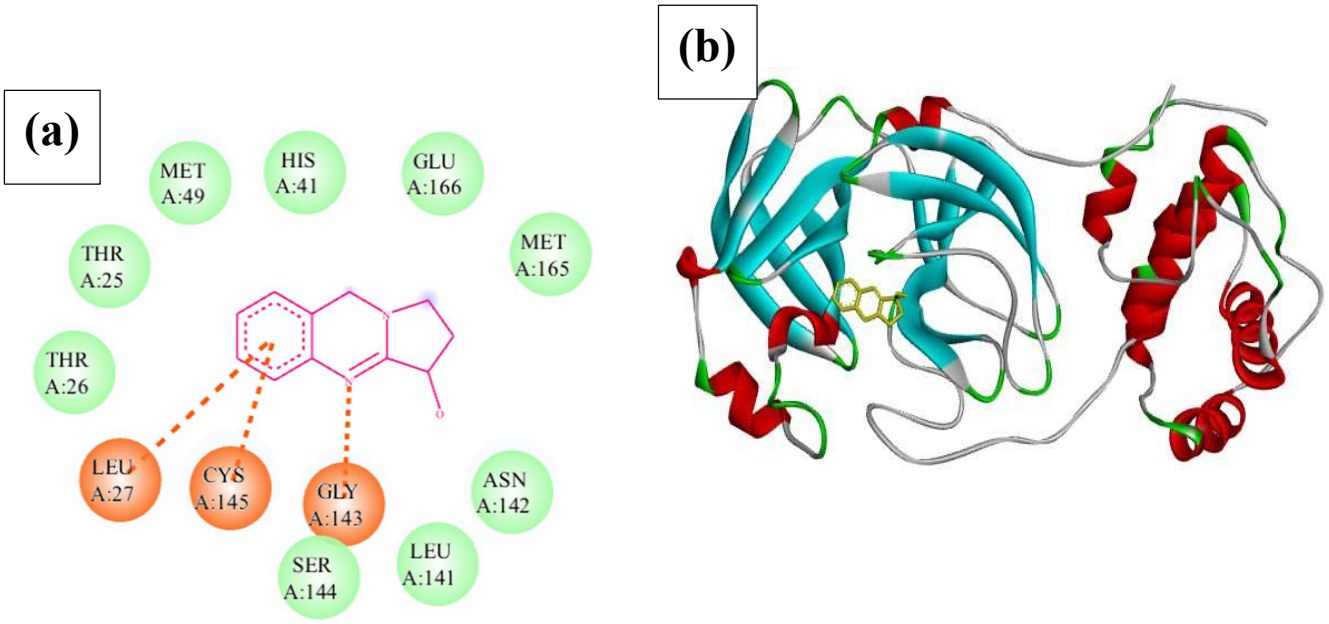
Harmaline P-6

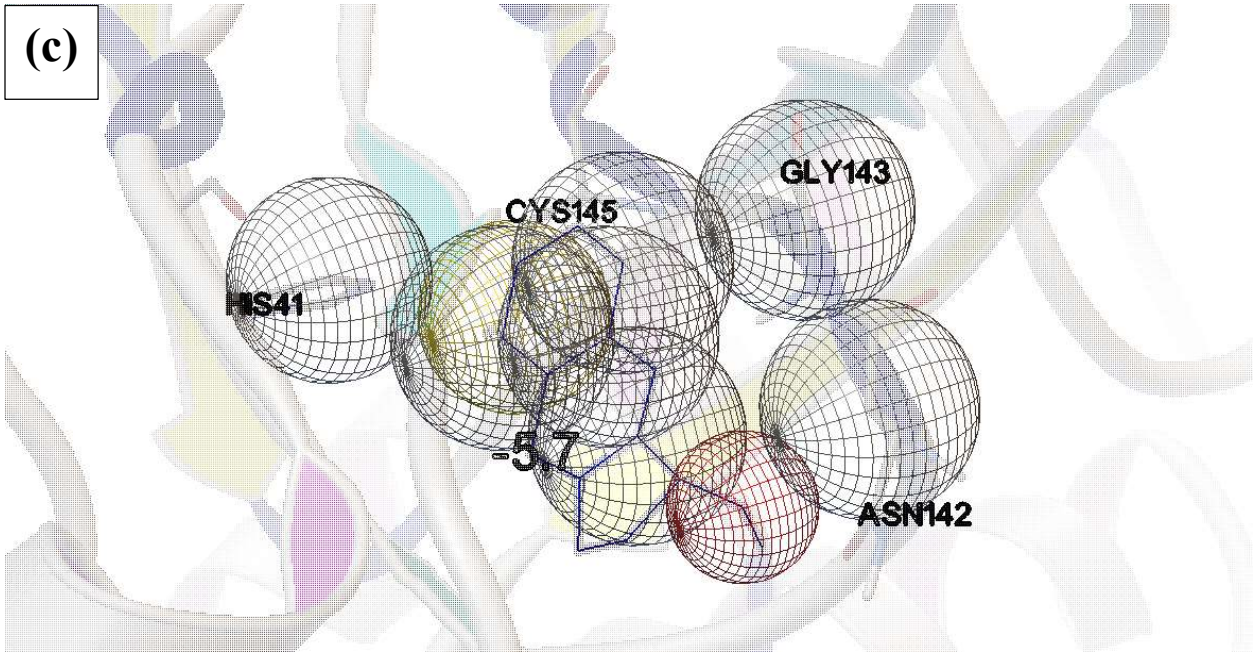


Quercetin P-8



Vasicine P-9


(a)
MET A:49
HIS A:41
GLU A:166
MET A:165
THR A:25
THR A:26
LEU A:27
CYS A:145
GLY A:143
ASN A:142
SER A:144
LEU A:141
(b)


(c)
GLY143
CYS145
HIS41
-5.7
ASN142

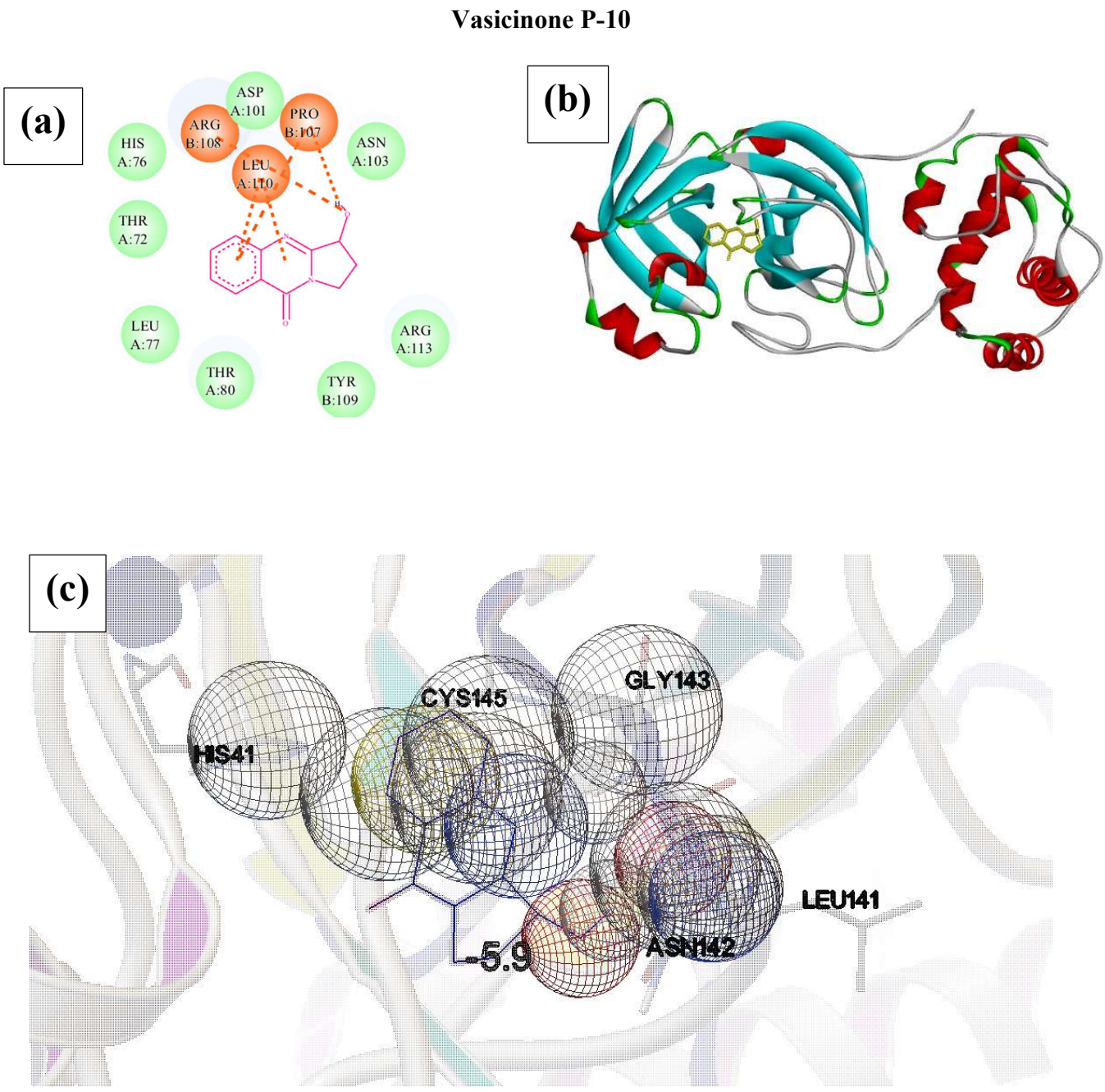


Fig. SI. 1: Two-dimensional (a), three-dimensional (b) and residue interactions analysis (c) based structures of **P-1** to **P-10** complexes except for **P7-6LU7** complex.