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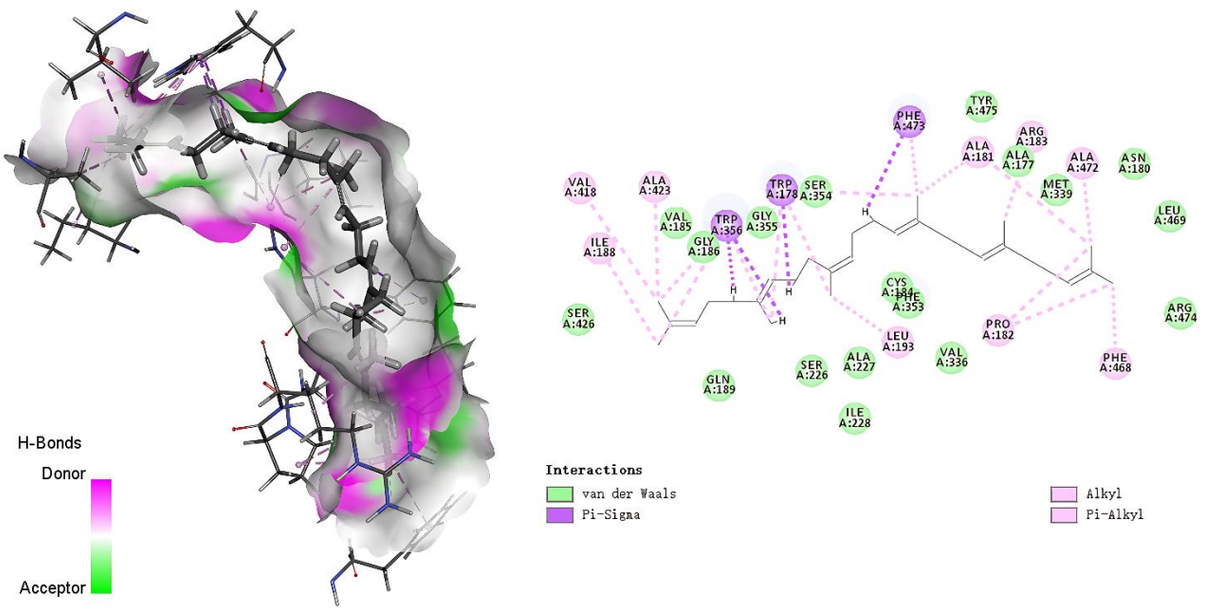
H-Bonds
Donor
Acceptor
PHE A:473
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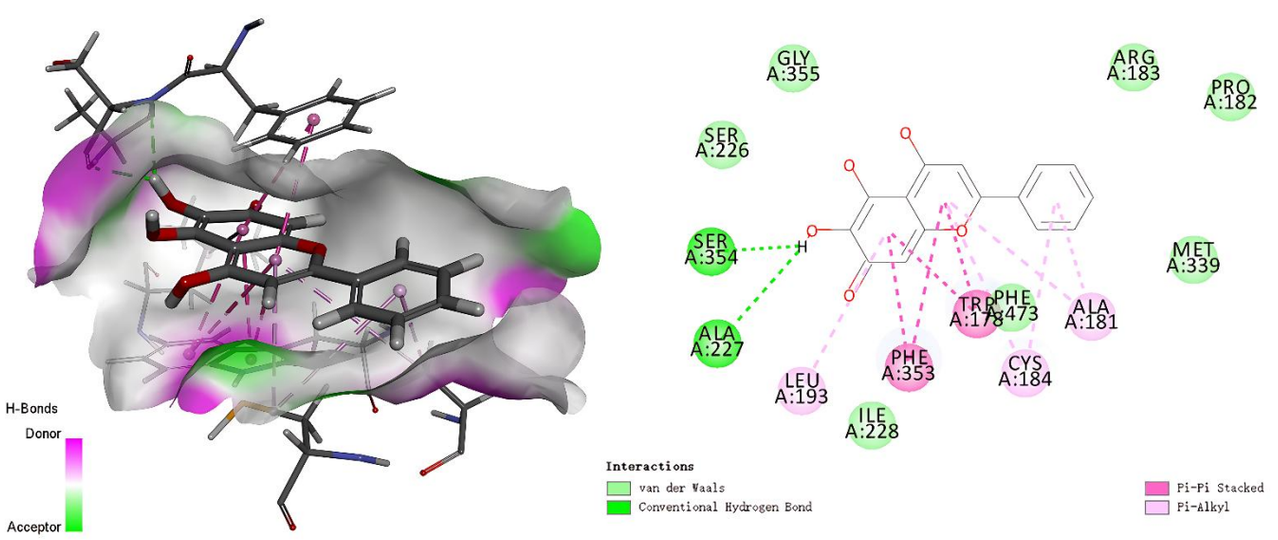
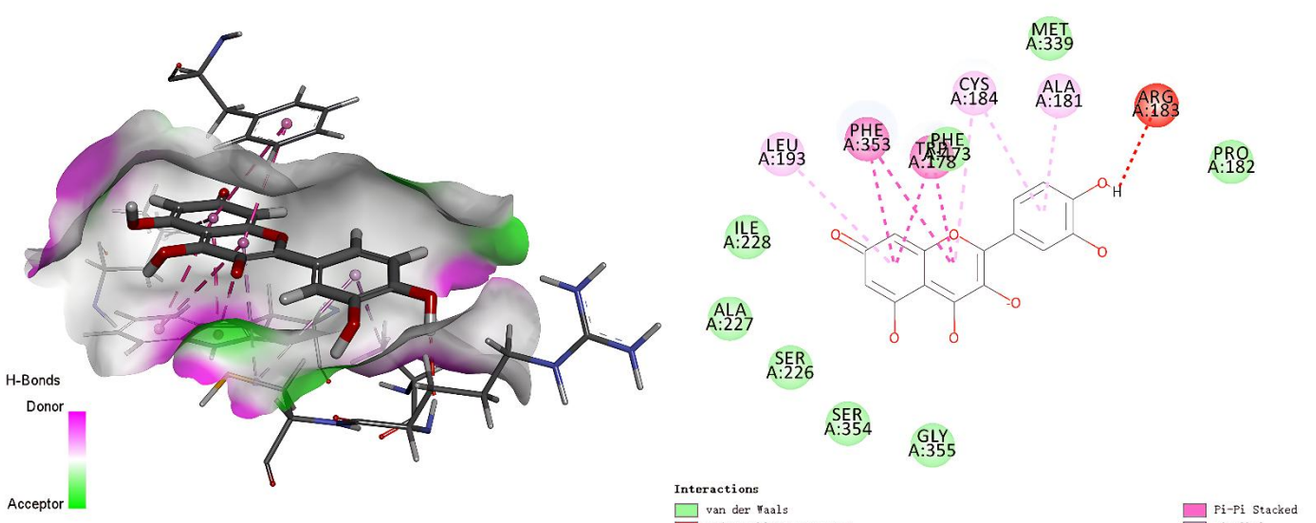
ARG A:183
ALA A:181
ALA A:177
ALA A:472
ASN A:180
MET A:339
LEU A:469
VAL A:418
ALA A:423
TRP A:178
SER A:354
VAL A:185
TRP A:356
GLY A:355
ILE A:188
GLY A:186
CYS A:184
PHE A:353
ARG A:474
SER A:426
PRO A:182
LEU A:193
VAL A:336
PHE A:468
SER A:226
ALA A:227
GLN A:189
ILE A:228
Interactions
van der Waals
Pi-Sigma
Alkyl
Pi-Alkyl

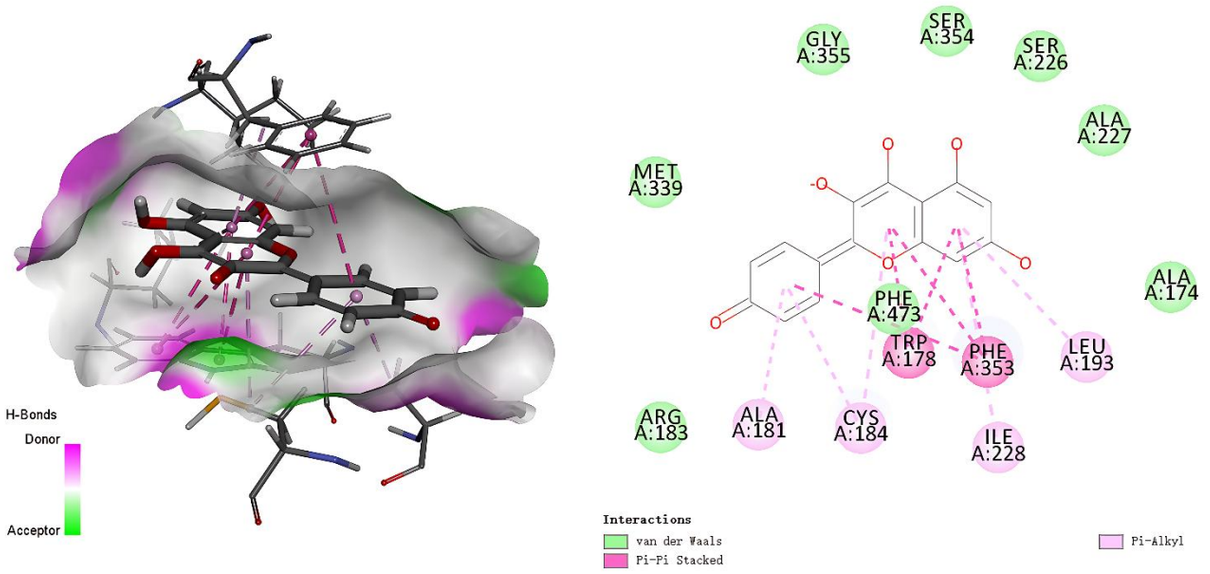
B


H-Bonds
Donor
Acceptor
GLY A:355
ARG A:183
PRO A:182
SER A:226
SER A:354
MET A:339
TRP A:178
PHE A:473
ALA A:181
ALA A:227
PHE A:353
CYS A:184
LEU A:193
ILE A:228
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Pi Stacked
Pi-Alkyl

C


H-Bonds
Donor
Acceptor
MET A:339
CYS A:184
ALA A:181
ARG A:183
PHE A:353
LEU A:193
PHE A:473
TRP A:178
PRO A:182
ILE A:228
ALA A:227
SER A:226
SER A:354
GLY A:355
Interactions
van der Waals
Unfavorable Donor-Donor
Pi-Pi Stacked
Pi-Alkyl

D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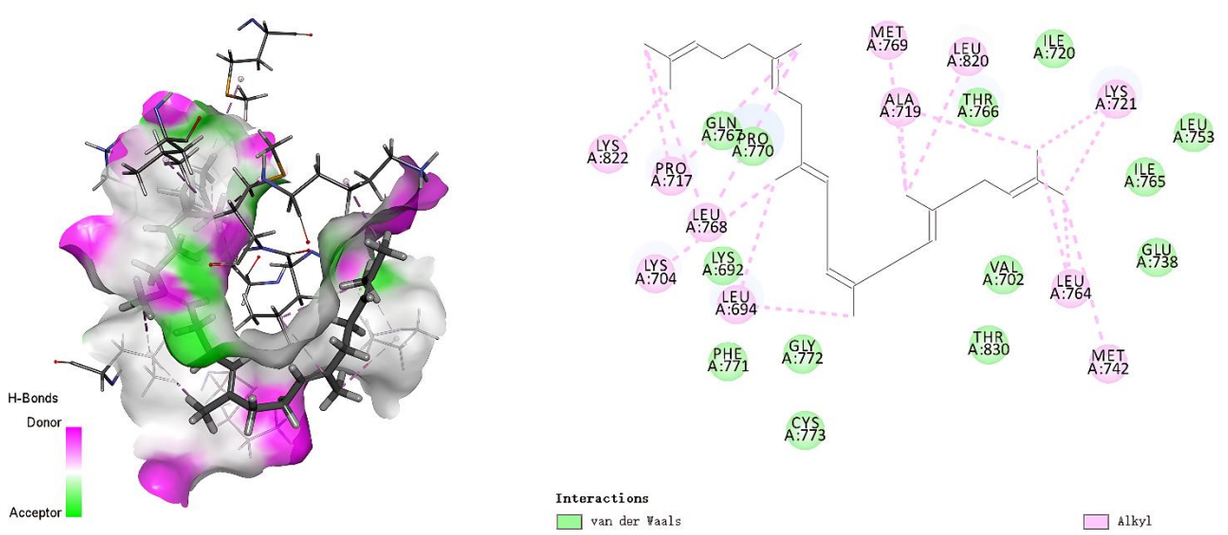
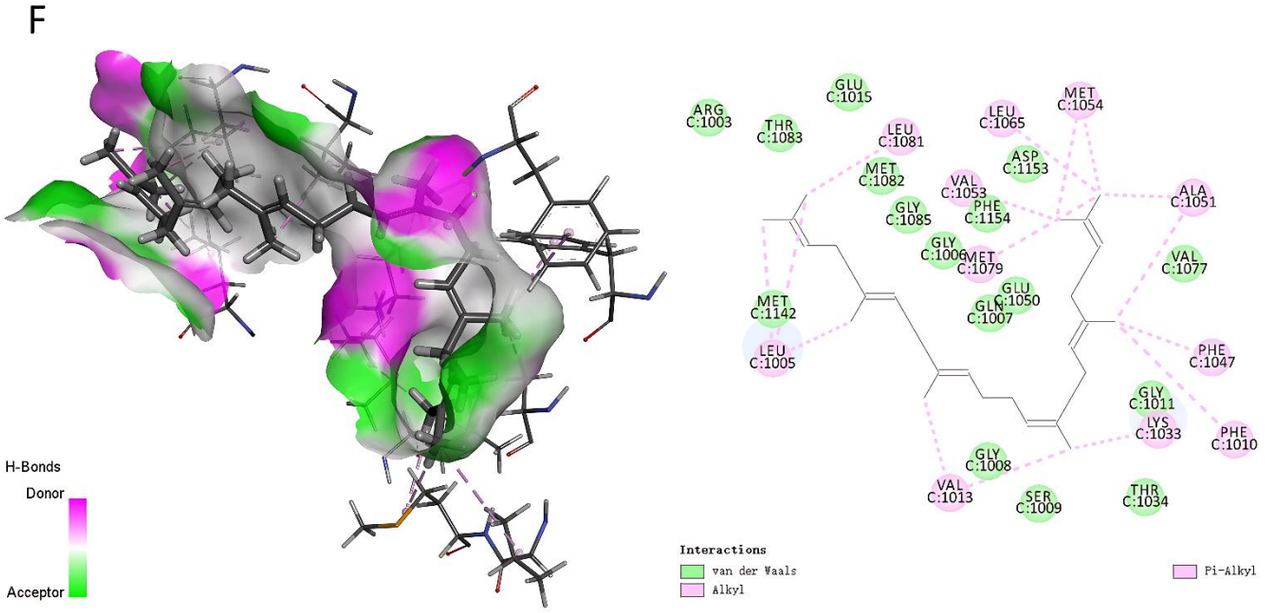
Donor
Acceptor
GLY A:355
SER A:354
SER A:226
ALA A:227
MET A:339
ALA A:174
PHE A:473
TRP A:178
PHE A:353
LEU A:193
ARG A:183
ALA A:181
CYS A:184
ILE A:228
Interactions
van der Waals
Pi-Pi Stacked
Pi-Alkyl

E


H-Bonds
Donor
Acceptor
MET A:769
LEU A:820
ILE A:720
ALA A:719
THR A:766
LYS A:721
LEU A:753
GLN A:767
PRO A:770
LYS A:822
PRO A:717
ILE A:765
LEU A:768
GLU A:738
LYS A:704
LYS A:692
VAL A:702
LEU A:764
LEU A:694
THR A:830
PHE A:771
GLY A:772
MET A:742
CYS A:773
Interactions
van der Waals
Alkyl

F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Donor
Acceptor
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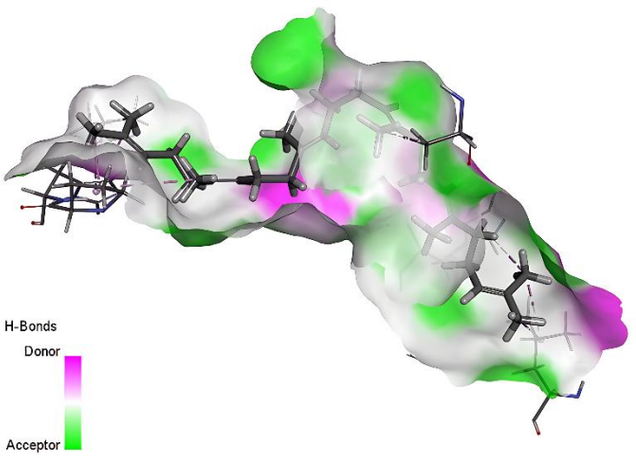
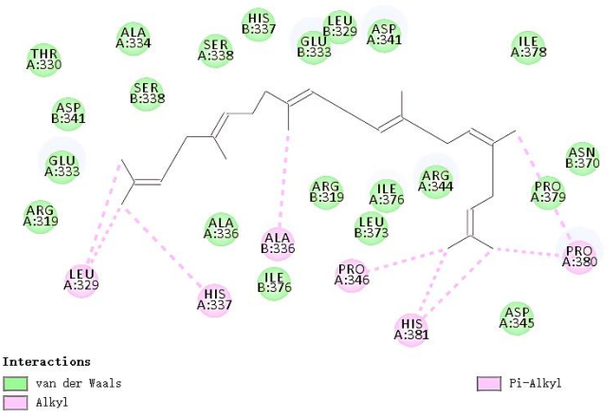
GLU C:1015
THR C:1083
LEU C:1081
MET C:1054
LEU C:1065
ASP C:1153
MET C:1082
VAL C:1053
ALA C:1051
GLY C:1085
PHE C:1154
GLY C:1006
MET C:1079
VAL C:1077
GLU C:1050
MET C:1142
GLN C:1007
PHE C:1047
LEU C:1005
GLY C:1011
LYS C:1033
PHE C:1010
GLY C:1008
VAL C:1013
SER C:1009
THR C:1034
Interactions
van der Waals
Alkyl
Pi-Alkyl

G


H-Bonds
Donor
Acceptor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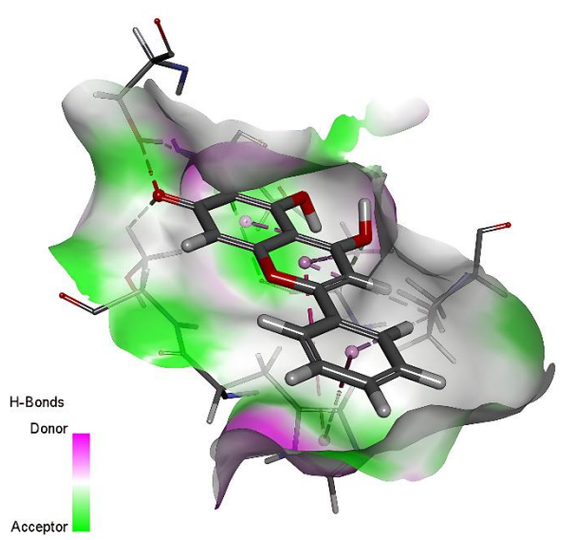
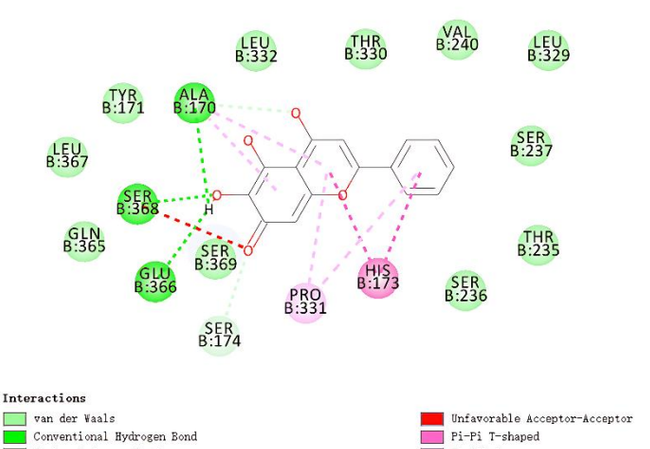
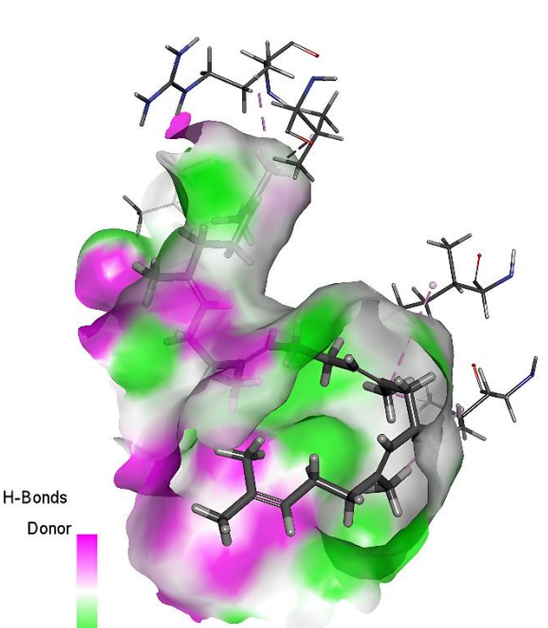
ALA A:334
HIS B:337
SER A:338
LEU B:329
GLU B:333
ASP A:341
ILE A:378
SER B:338
ASP B:341
GLU A:333
ASN B:370
ARG A:344
ARG B:319
ILE A:376
PRO A:379
ARG A:319
LEU B:373
ALA A:336
ALA B:336
PRO A:380
LEU A:329
PRO A:346
ILE B:376
HIS A:337
ASP A:345
HIS A:381
Interactions
van der Waals
Alkyl
Pi-Alkyl

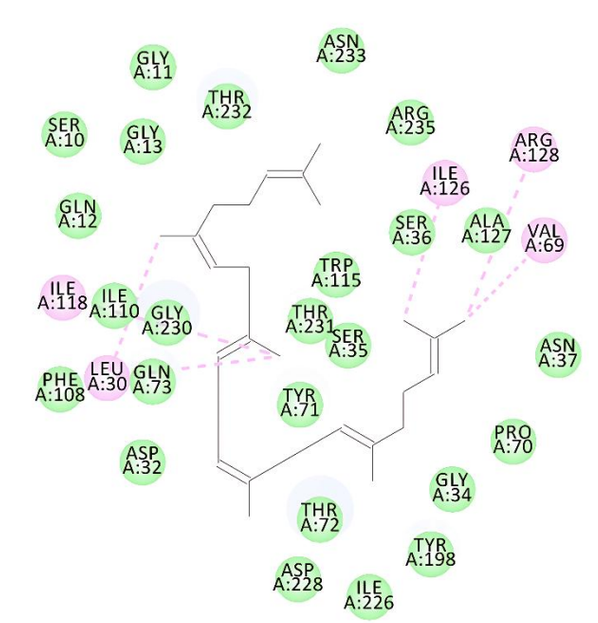
H


H-Bonds
Donor
Acceptor


LEU B:332
THR B:330
VAL B:240
LEU B:329
TYR B:171
ALA B:170
LEU B:367
SER B:237
SER B:368
H
GLN B:365
SER B:369
THR B:235
GLU B:366
HIS B:173
SER B:236
PRO B:331
SER B:174
Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Acceptor-Acceptor
Pi-Pi T-shaped
Pi-Alkyl

I


H-Bonds
Donor
Acceptor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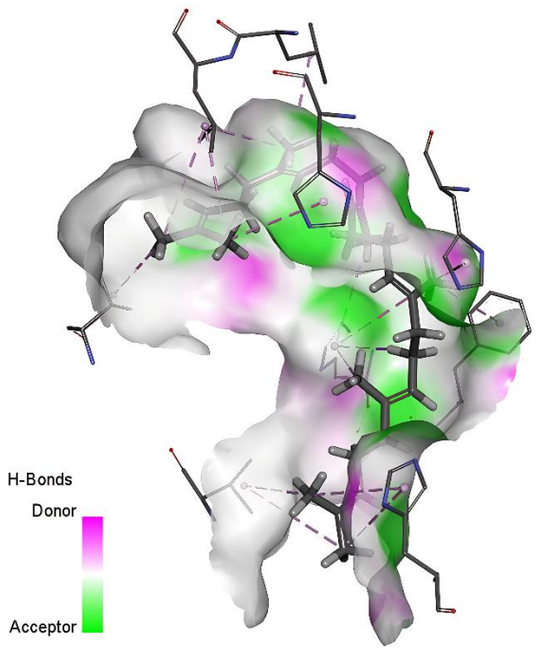
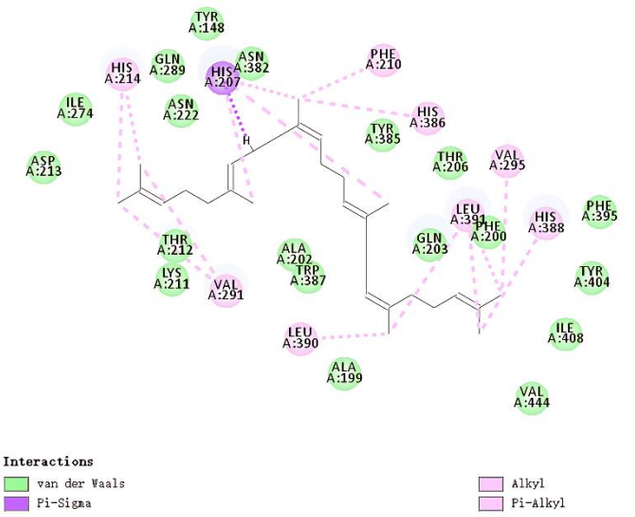
GLY A:11
THR A:232
ARG A:235
SER A:10
GLY A:13
ARG A:128
ILE A:126
GLN A:12
SER A:36
ALA A:127
VAL A:69
TRP A:115
ILE A:118
ILE A:110
GLY A:230
THR A:231
SER A:35
ASN A:37
PHE A:108
LEU A:30
GLN A:73
TYR A:71
PRO A:70
ASP A:32
GLY A:34
THR A:72
TYR A:198
ASP A:228
ILE A:226
Interactions
van der Waals
Alkyl

J


H-Bonds
Donor
Acceptor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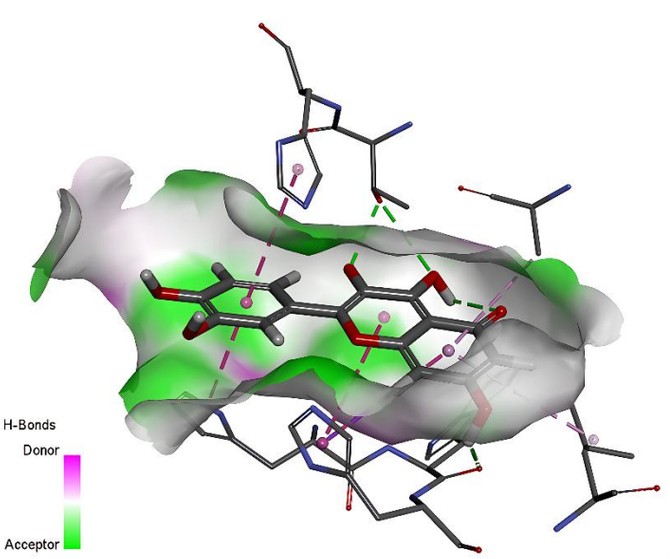
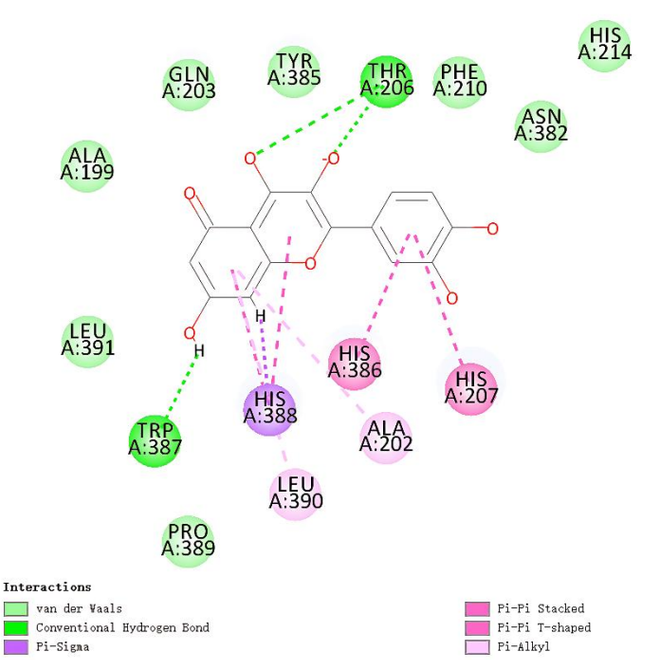
HIS A:214
GLN A:289
HIS A:207
ASN A:382
PHE A:210
ILE A:274
ASN A:222
HIS A:386
TYR A:385
ASP A:213
THR A:206
VAL A:295
LEU A:391
PHE A:395
HIS A:388
PHE A:200
GLN A:203
THR A:212
ALA A:202
TRP A:387
TYR A:404
LYS A:211
VAL A:291
LEU A:390
ILE A:408
ALA A:199
VAL A:444
Interactions
van der Waals
Pi-Sigma
Alkyl
Pi-Alkyl

K


H-Bonds
Donor
Acceptor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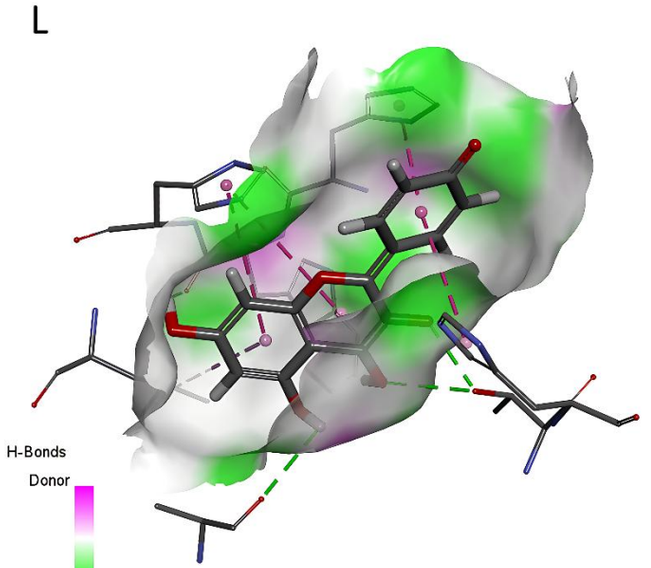
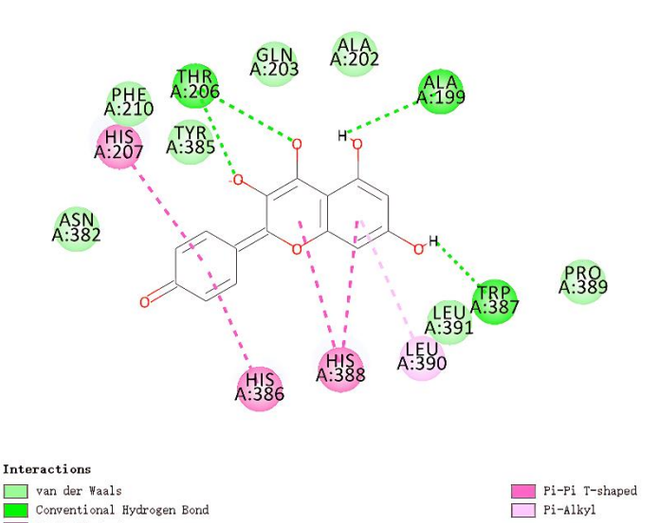
GLN A:203
TYR A:385
THR A:206
PHE A:210
ASN A:382
ALA A:199
LEU A:391
HIS A:386
HIS A:207
HIS A:388
TRP A:387
ALA A:202
LEU A:390
PRO A:389
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Sigma
Pi-Pi Stacked
Pi-Pi T-shaped
Pi-Alkyl

L


H-Bonds
Donor
Acceptor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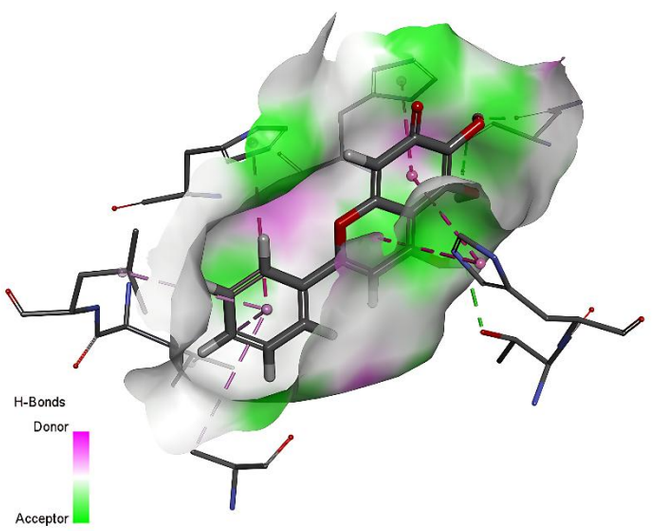
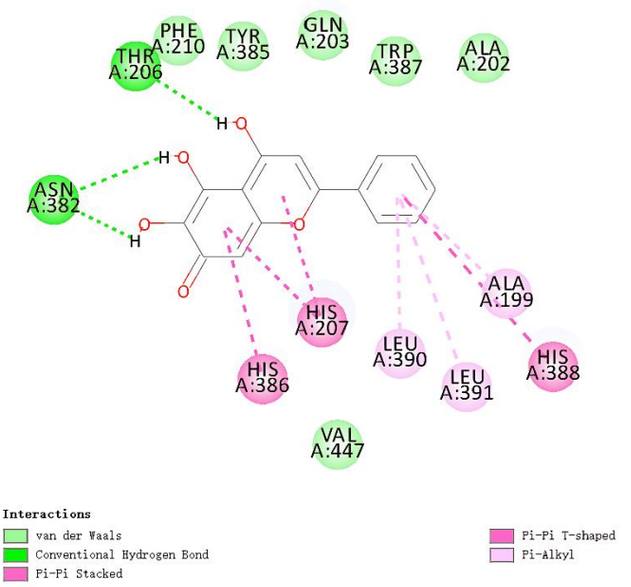
ALA A:202
THR A:206
ALA A:199
PHE A:210
HIS A:207
TYR A:385
ASN A:382
PRO A:389
TRP A:387
LEU A:391
LEU A:390
HIS A:388
HIS A:386
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Pi Stacked
Pi-Pi T-shaped
Pi-Alkyl

M


H-Bonds
Donor
Acceptor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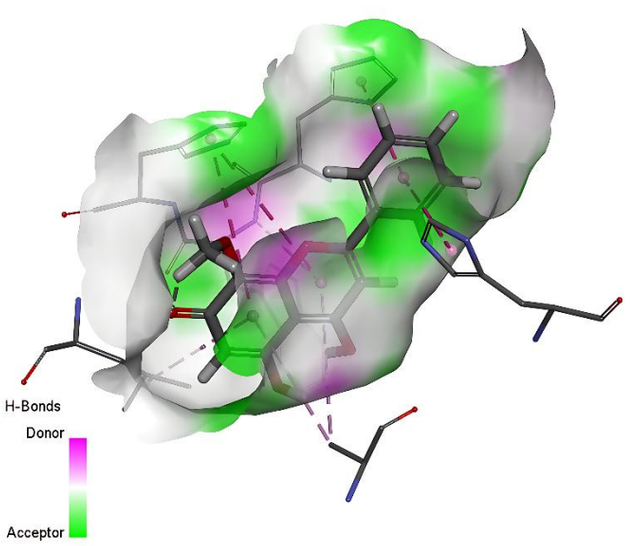
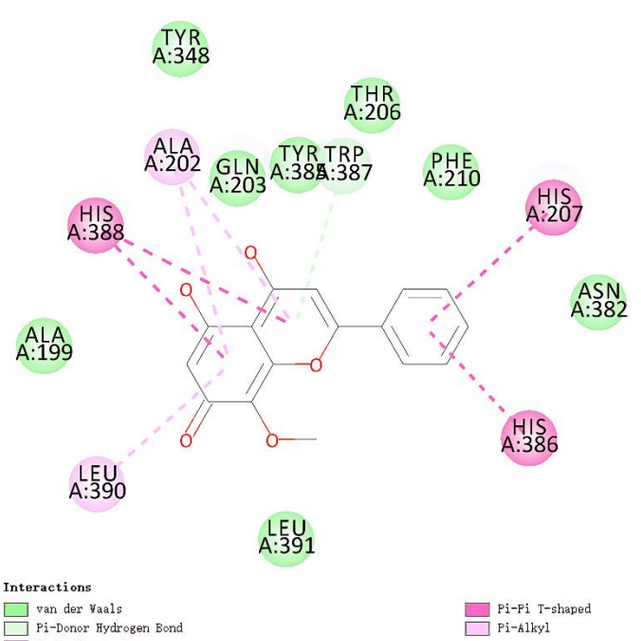
GLN A:203
TRP A:387
ALA A:202
THR A:206
ASN A:382
ALA A:199
HIS A:207
LEU A:390
HIS A:388
HIS A:386
LEU A:391
VAL A:447
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Pi Stacked
Pi-Pi T-shaped
Pi-Alkyl

N


H-Bonds
Donor
Acceptor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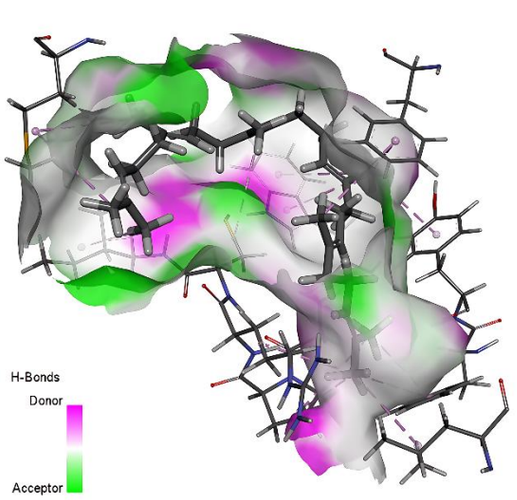
GLN A:203
TYR A:385
TRP A:387
PHE A:210
HIS A:388
HIS A:207
ASN A:382
ALA A:199
HIS A:386
LEU A:390
LEU A:391
Interactions
van der Waals
Pi-Donor Hydrogen Bond
Pi-Pi Stacked
Pi-Pi T-shaped
Pi-Alkyl

O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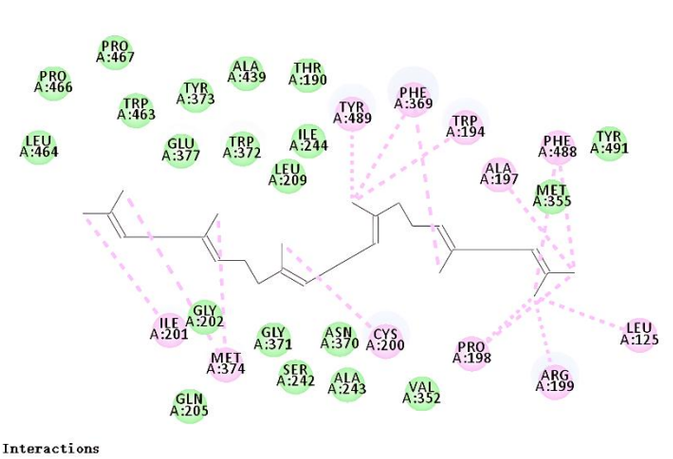
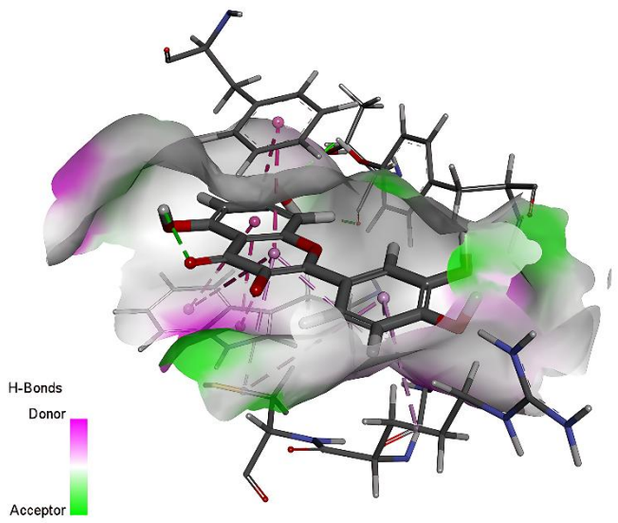
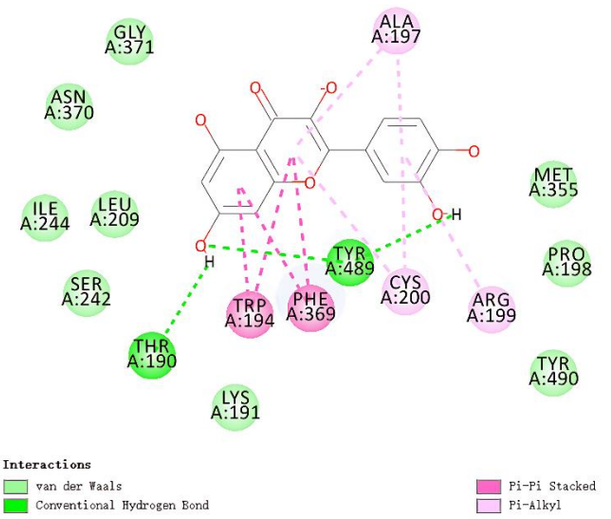
Donor
Acceptor


PRO A:467
PRO A:466
ALA A:439
THR A:190
TYR A:373
TRP A:463
TYR A:489
PHE A:369
TRP A:194
LEU A:464
GLU A:377
TRP A:372
ILE A:244
PHE A:488
TYR A:491
LEU A:209
ALA A:197
MET A:355
ILE A:201
GLY A:202
GLY A:371
ASN A:370
CYS A:200
LEU A:125
PRO A:198
MET A:374
SER A:242
ALA A:243
VAL A:352
ARG A:199
GLN A:205
Interactions
van der Waals
Alkyl
Pi-Alkyl

P


H-Bonds
Donor
Acceptor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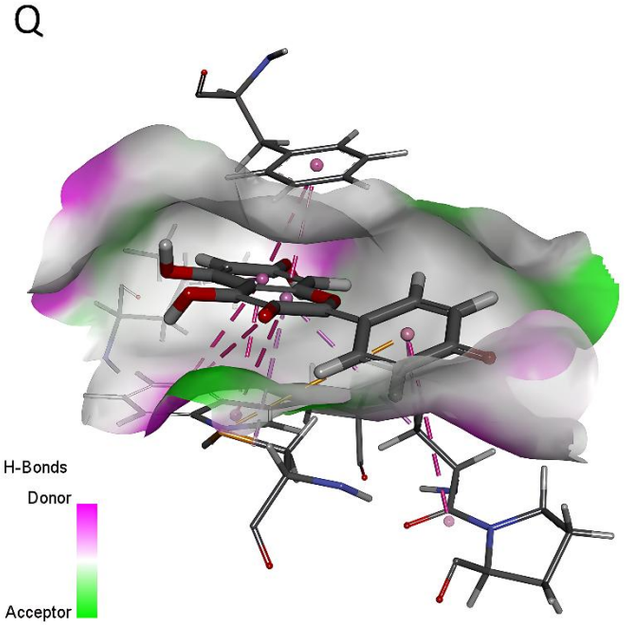
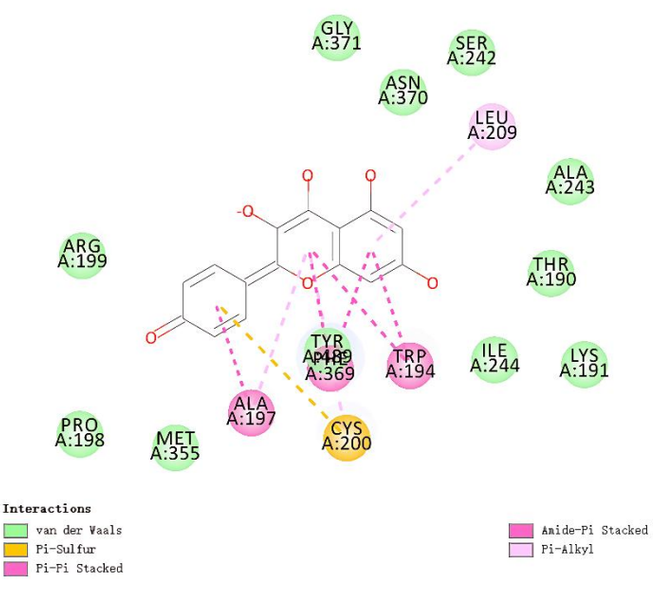
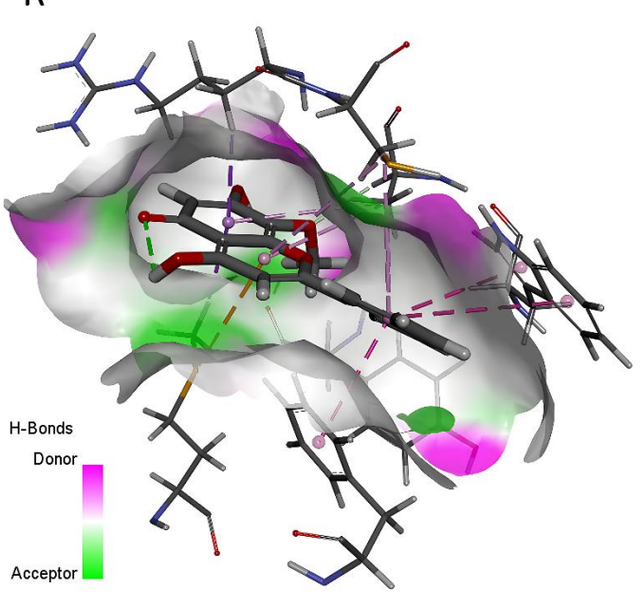
ALA A:197
ASN A:370
MET A:355
ILE A:244
LEU A:209
PRO A:198
SER A:242
TYR A:489
CYS A:200
TRP A:194
PHE A:369
ARG A:199
THR A:190
TYR A:490
LYS A:191
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Pi Stacked
Pi-Alkyl

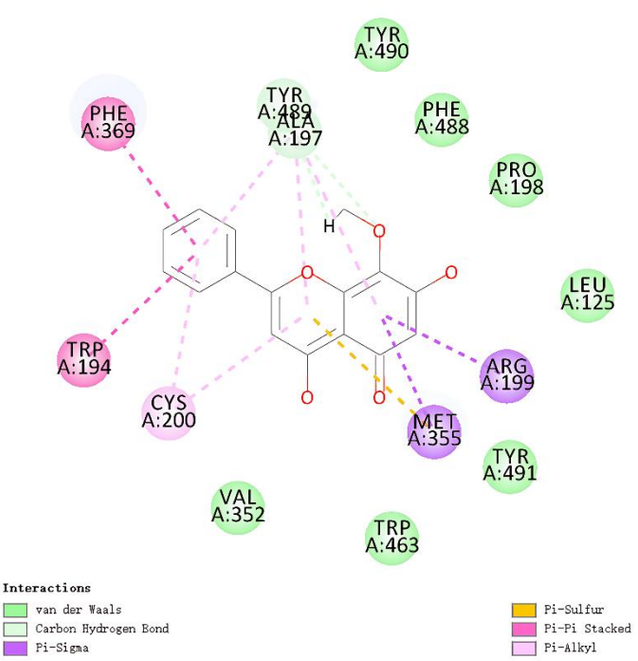
Q


H-Bonds
Donor
Acceptor


GLY A:371
SER A:242
ASN A:370
LEU A:209
ALA A:243
ARG A:199
THR A:190
TYR A:489
PHE A:369
TRP A:194
ILE A:244
LYS A:191
ALA A:197
PRO A:198
MET A:355
CYS A:200
Interactions
van der Waals
Pi-Sulfur
Pi-Pi Stacked
Amide-Pi Stacked
Pi-Alkyl

R


H-Bonds
Donor
Acceptor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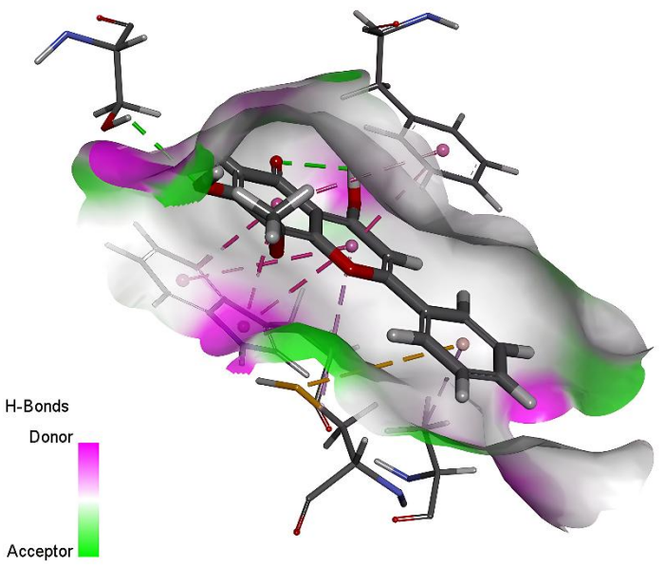
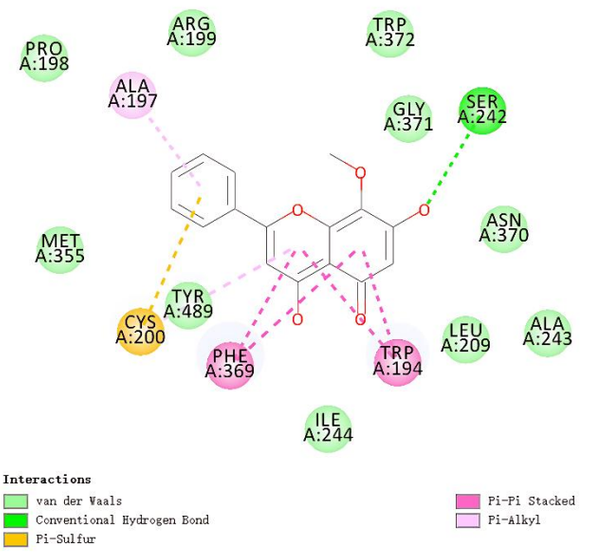
TYR A:489
ALA A:197
PHE A:488
PRO A:198
LEU A:125
TRP A:194
ARG A:199
CYS A:200
MET A:355
TYR A:491
VAL A:352
TRP A:463
Interactions
van der Waals
Carbon Hydrogen Bond
Pi-Sigma
Pi-Sulfur
Pi-Pi Stacked
Pi-Alkyl

S


H-Bonds
Donor
Acceptor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ARG A:199
TRP A:372
ALA A:197
GLY A:371
SER A:242
ASN A:370
MET A:355
TYR A:489
CYS A:200
PHE A:369
TRP A:194
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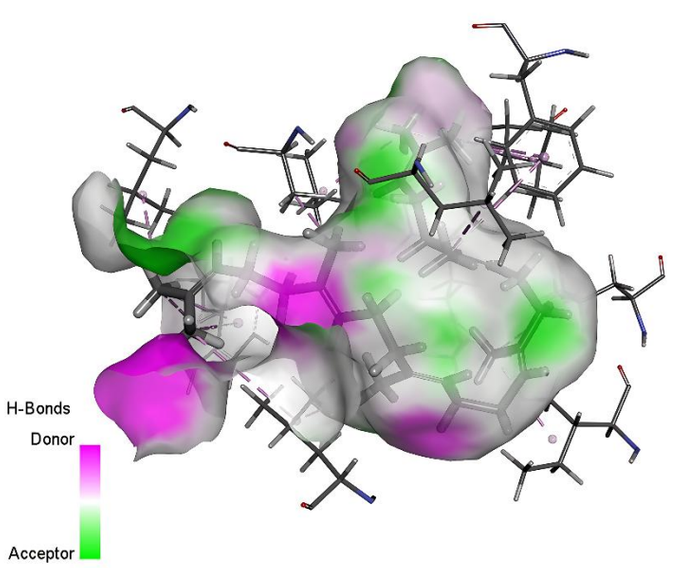
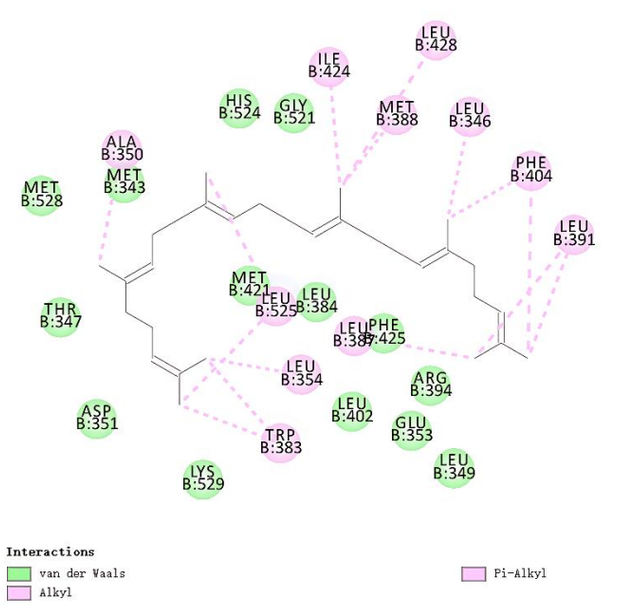
ILE A:244
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Sulfur
Pi-Pi Stacked
Pi-Alkyl

T


H-Bonds
Donor
Acceptor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GLY B:521
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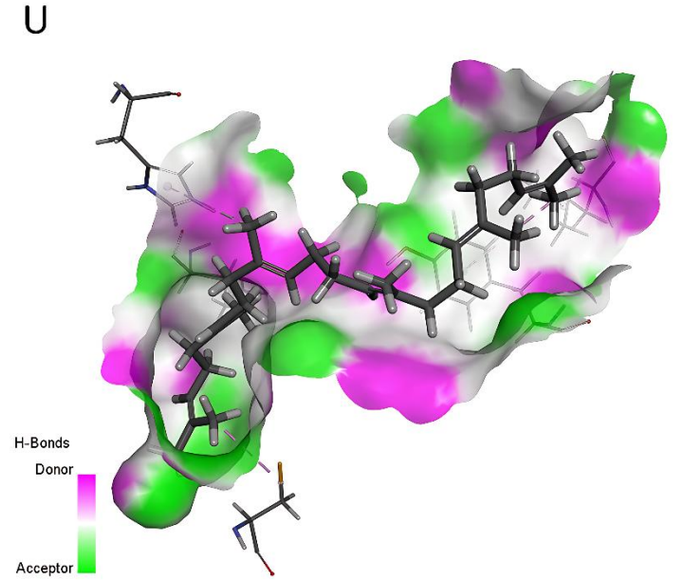
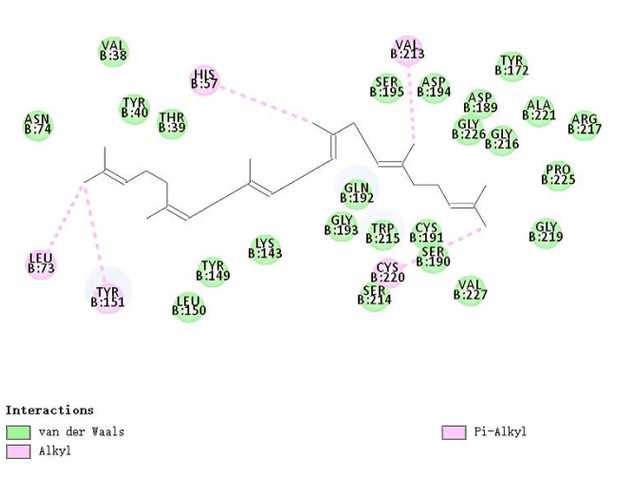
LEU B:346
ALA B:350
MET B:343
PHE B:404
MET B:528
LEU B:391
MET B:421
LEU B:525
LEU B:384
THR B:347
LEU B:387
PHE B:425
LEU B:354
ARG B:394
ASP B:351
LEU B:402
GLU B:353
TRP B:383
LEU B:349
LYS B:529
Interactions
van der Waals
Alkyl
Pi-Alkyl

U


H-Bonds
Donor
Acceptor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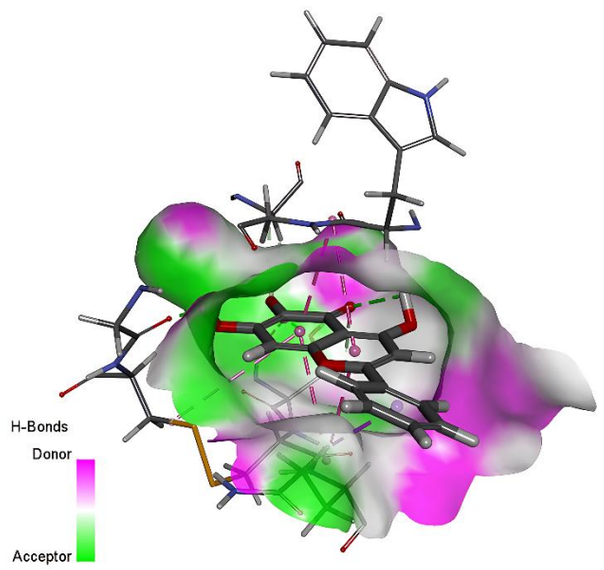
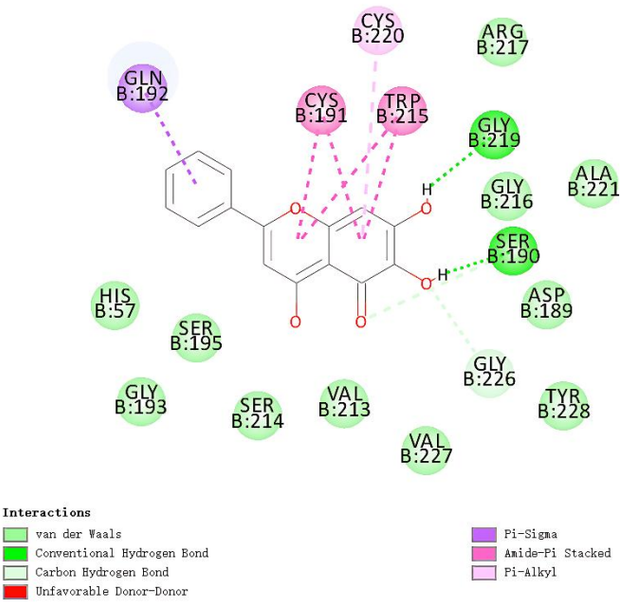
VAL B:213
TYR B:172
HIS B:57
SER B:195
ASP B:194
ASP B:189
TYR B:40
ALA B:221
ASN B:74
THR B:39
GLY B:226
GLY B:216
ARG B:217
PRO B:225
GLN B:192
GLY B:193
TRP B:215
CYS B:191
GLY B:219
LYS B:143
SER B:190
LEU B:73
TYR B:149
CYS B:220
TYR B:151
LEU B:150
SER B:214
VAL B:227
Interactions
van der Waals
Alkyl
Pi-Alkyl

V


H-Bonds
Donor
Acceptor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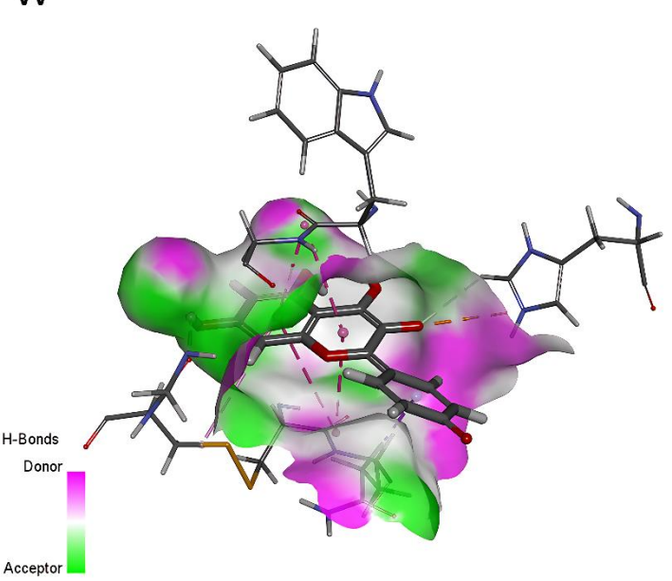
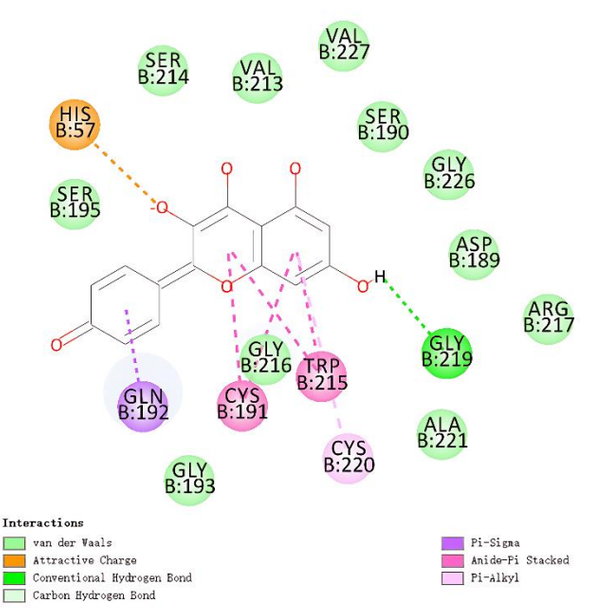
GLN B:192
CYS B:191
TRP B:215
GLY B:219
ALA B:221
GLY B:216
SER B:190
HIS B:57
ASP B:189
SER B:195
GLY B:226
GLY B:193
SER B:214
VAL B:213
TYR B:228
VAL B:227
Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Donor-Donor
Pi-Sigma
Amide-Pi Stacked
Pi-Alkyl

W


H-Bonds
Donor
Acceptor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VAL B:213
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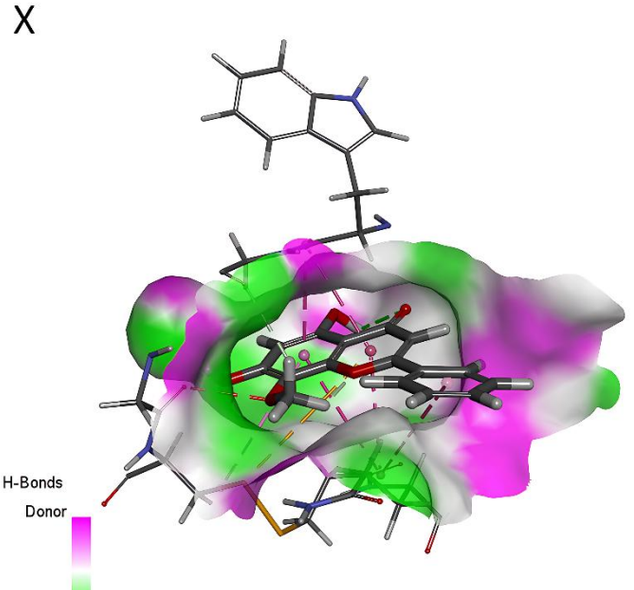
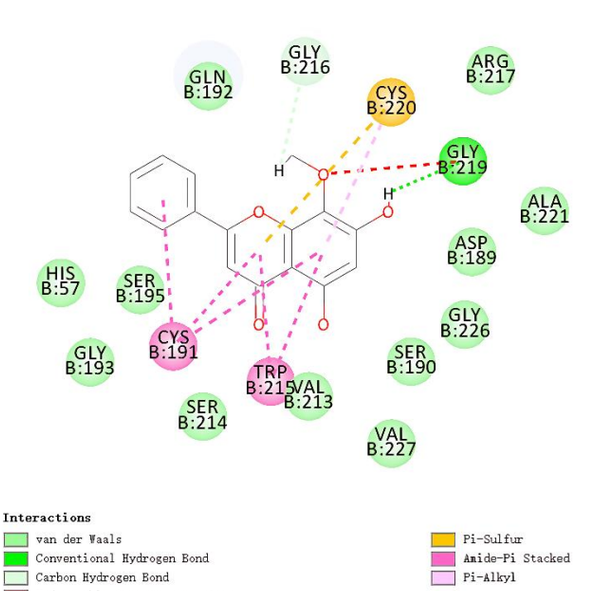
SER B:190
GLY B:226
SER B:195
ASP B:189
ARG B:217
GLY B:219
GLY B:216
TRP B:215
GLN B:192
CYS B:191
ALA B:221
CYS B:220
GLY B:193
Interactions
van der Waals
Attractive Charge
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Sigma
Amide-Pi Stacked
Pi-Alkyl

X


H-Bonds
Donor
Acceptor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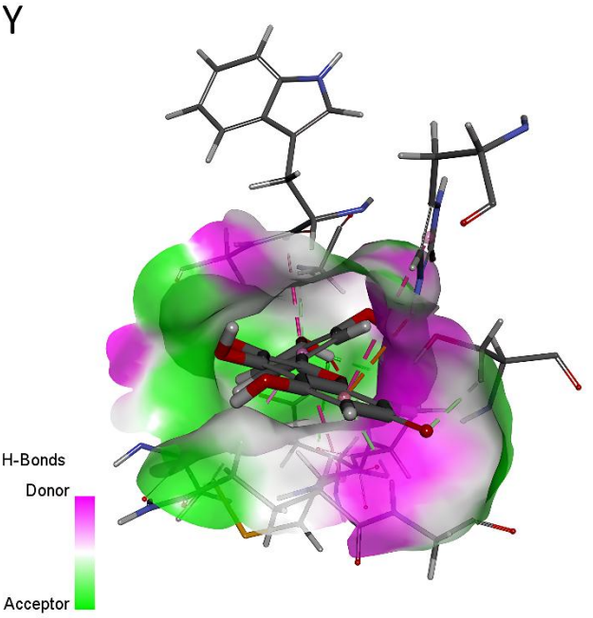
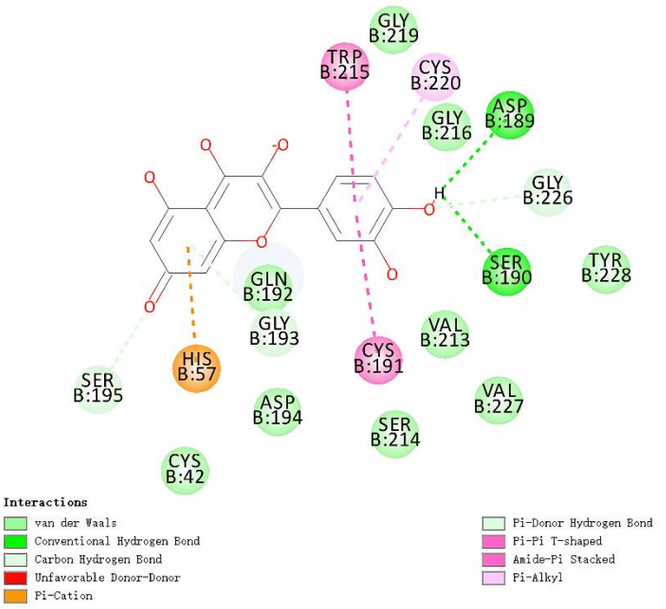
ARG B:217
CYS B:220
GLY B:219
ALA B:221
ASP B:189
HIS B:57
SER B:195
GLY B:226
CYS B:191
GLY B:193
SER B:190
TRP B:215
VAL B:213
SER B:214
VAL B:227
Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Acceptor-Acceptor
Pi-Sulfur
Amide-Pi Stacked
Pi-Alkyl

Y


H-Bonds
Donor
Acceptor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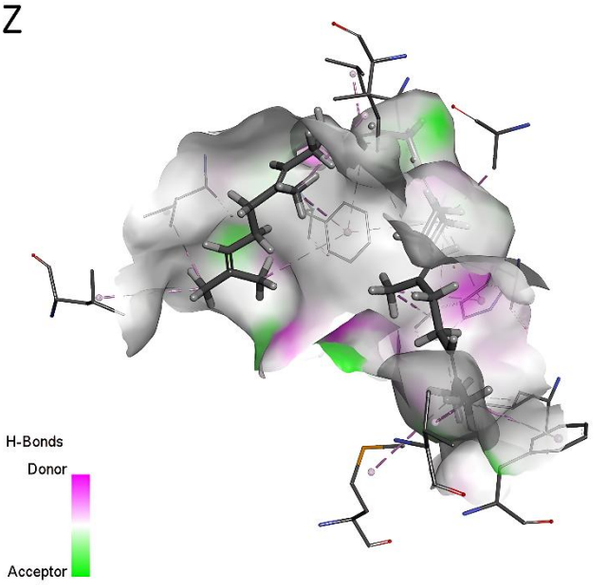
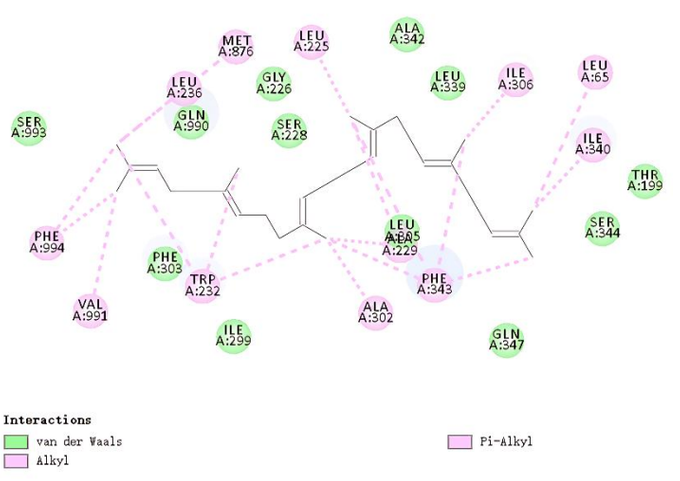
CYS B:220
GLY B:216
ASP B:189
GLY B:226
SER B:190
TYR B:228
GLN B:192
GLY B:193
VAL B:213
CYS B:191
HIS B:57
SER B:195
ASP B:194
VAL B:227
SER B:214
CYS B:42
Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Donor-Donor
Pi-Cation
Pi-Donor Hydrogen Bond
Pi-Pi T-shaped
Amide-Pi Stacked
Pi-Alkyl

Z


H-Bonds
Donor
Acceptor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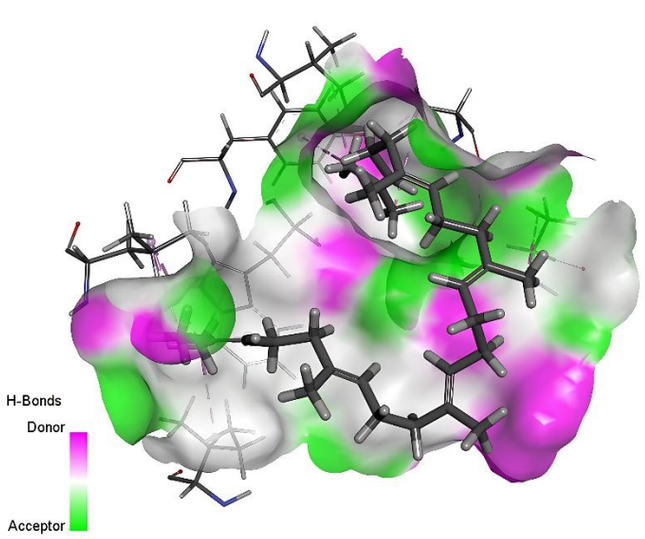
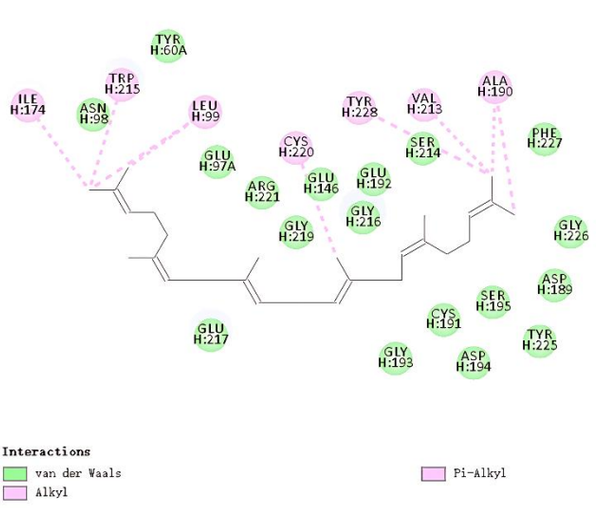
ALA A:342
LEU A:236
GLY A:226
LEU A:339
ILE A:306
LEU A:65
SER A:993
GLN A:990
SER A:228
ILE A:340
THR A:199
PHE A:994
LEU A:229
SER A:344
PHE A:303
TRP A:232
PHE A:343
VAL A:991
ALA A:302
ILE A:299
GLN A:347
Interactions
van der Waals
Alkyl
Pi-Alkyl

AA


H-Bonds
Donor
Acceptor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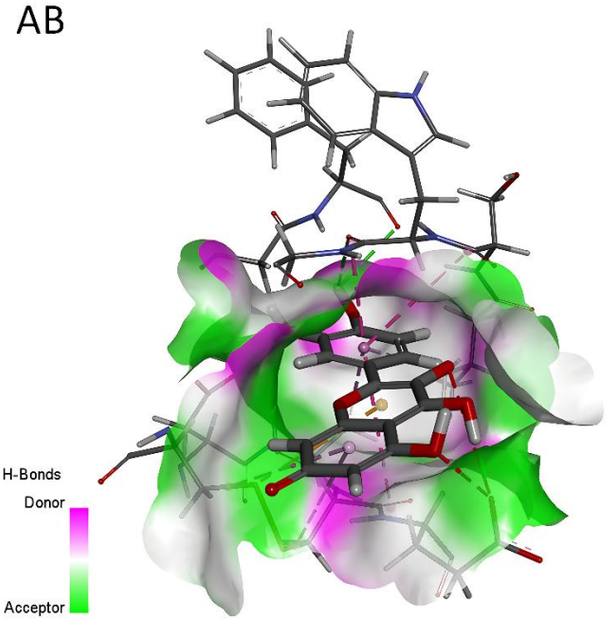
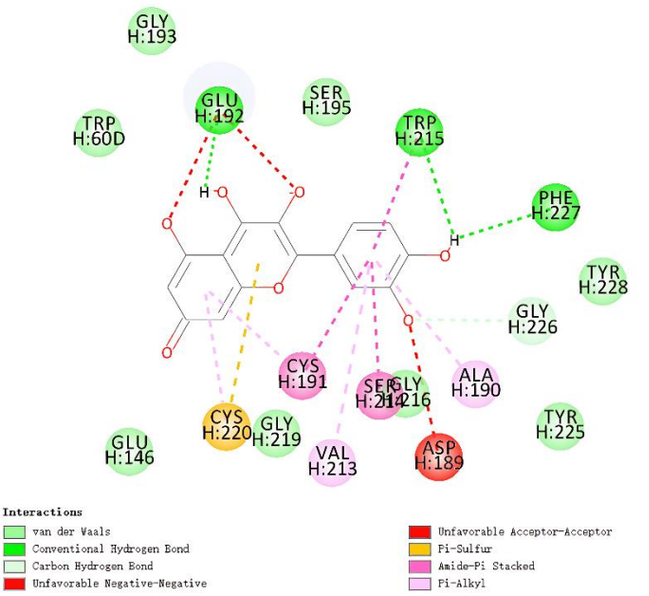
TRP H:215
ILE H:174
ASN H:98
LEU H:99
TYR H:228
VAL H:213
ALA H:190
PHE H:227
CYS H:220
SER H:214
GLU H:97A
ARG H:221
GLU H:146
GLU H:192
GLY H:216
GLY H:219
GLY H:226
ASP H:189
SER H:195
CYS H:191
TYR H:225
GLU H:217
GLY H:193
ASP H:194
Interactions
van der Waals
Alkyl
Pi-Alkyl

AB


H-Bonds
Donor
Acceptor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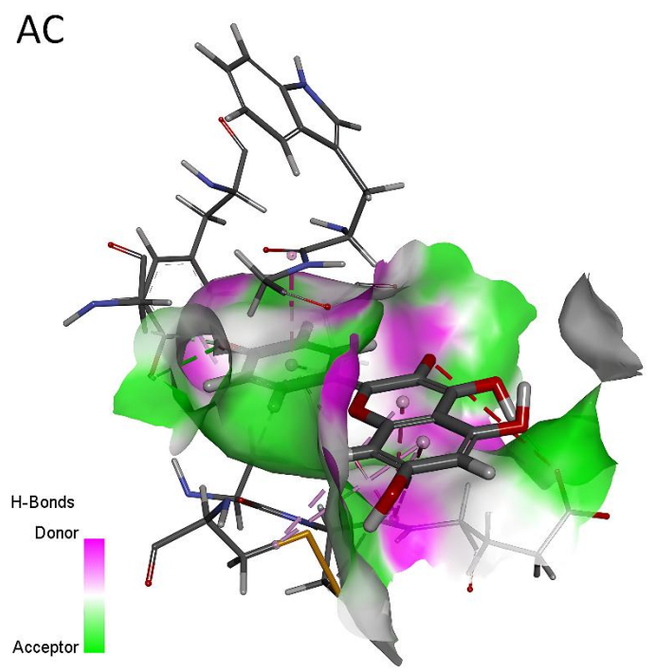
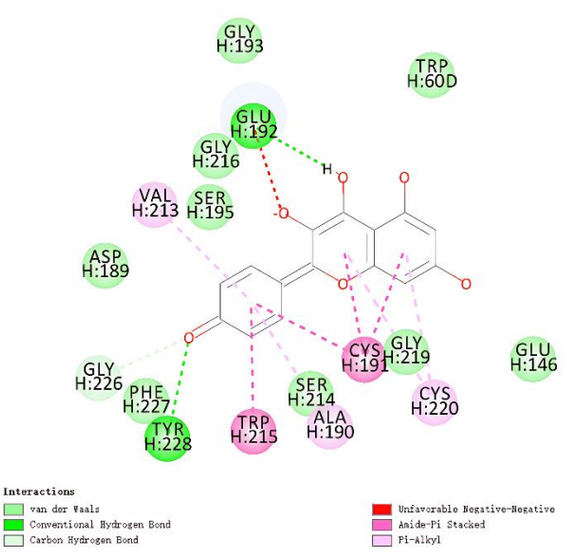
GLU H:192
SER H:195
TRP H:60D
TRP H:215
PHE H:227
TYR H:228
GLY H:226
CYS H:191
SER H:214
GLY H:216
ALA H:190
CYS H:220
GLY H:219
TYR H:225
GLU H:146
VAL H:213
ASP H:189
Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Negative-Negative
Unfavorable Acceptor-Acceptor
Pi-Sulfur
Amide-Pi Stacked
Pi-Alkyl

AC


H-Bonds
Donor
Acceptor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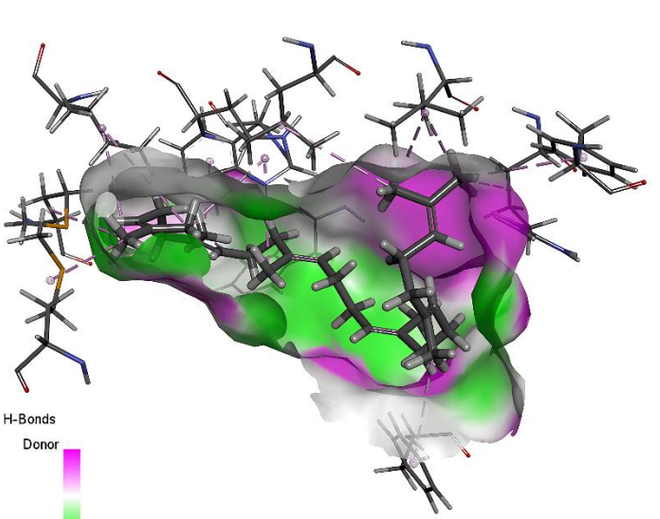
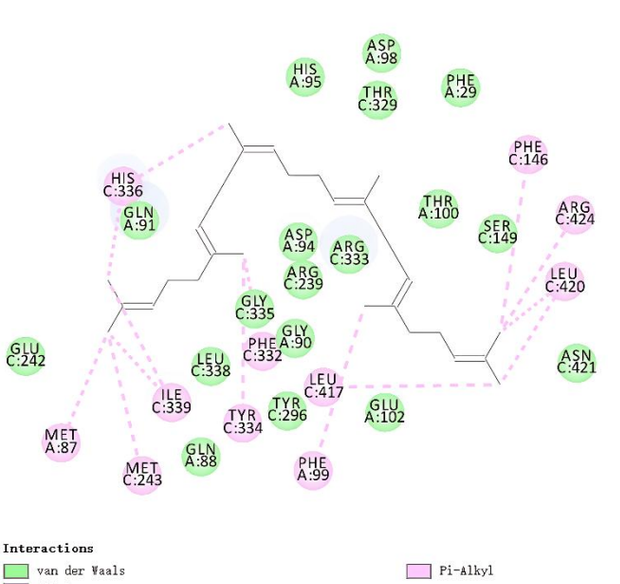
TRP H:60D
GLU H:192
GLY H:216
VAL H:213
SER H:195
ASP H:189
CYS H:191
GLY H:219
GLU H:146
GLY H:226
PHE H:227
SER H:214
CYS H:220
TYR H:228
TRP H:215
ALA H:190
Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Negative-Negative
Amide-Pi Stacked
Pi-Alkyl

AD


H-Bonds
Donor
Acceptor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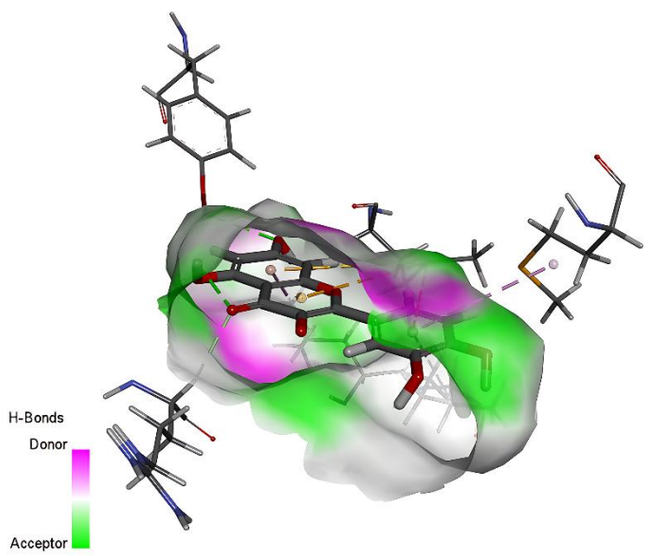
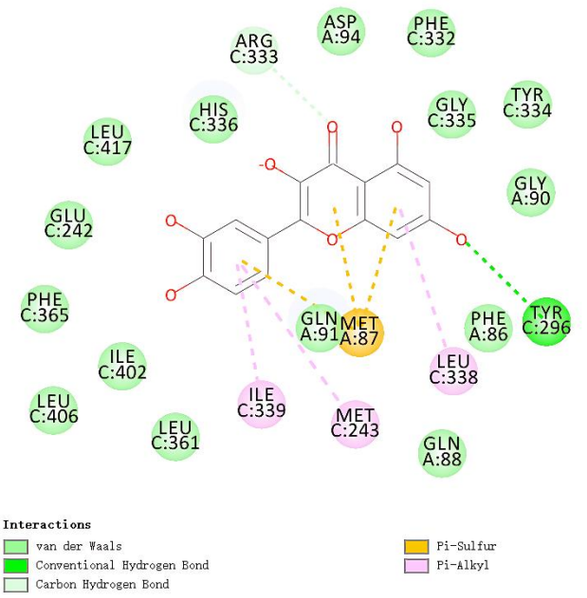
THR A:100
ARG C:424
SER C:149
ASP A:94
ARG C:333
ARG C:239
LEU C:420
GLY C:335
GLY A:90
PHE C:332
GLU C:242
LEU C:338
ASN C:421
LEU C:417
ILE C:339
TYR C:296
GLU A:102
TYR C:334
MET A:87
GLN A:88
MET C:243
PHE A:99
Interactions
van der Waals
Alkyl
Pi-Alkyl

AE


H-Bonds
Donor
Acceptor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ARG C:333
HIS C:336
GLY C:335
TYR C:334
LEU C:417
GLY A:90
GLU C:242
PHE C:365
GLN A:91
MET A:87
PHE A:86
TYR C:296
ILE C:402
LEU C:338
ILE C:339
LEU C:406
MET C:243
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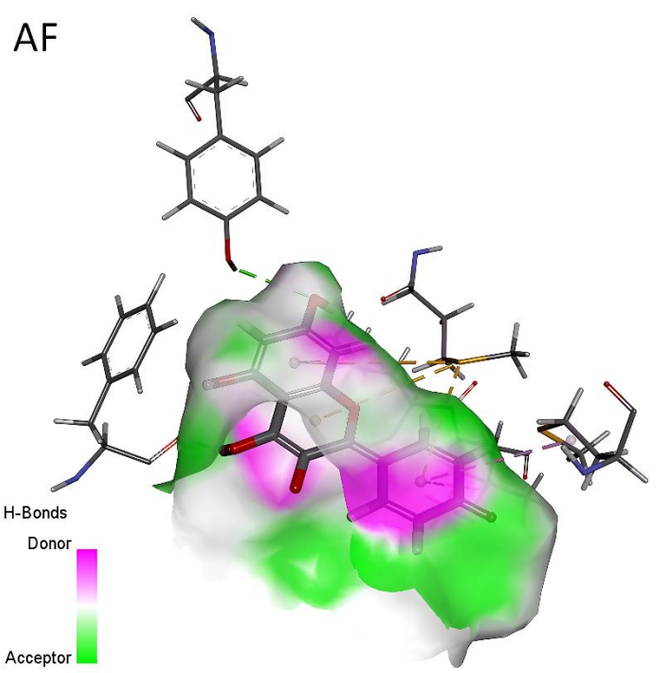
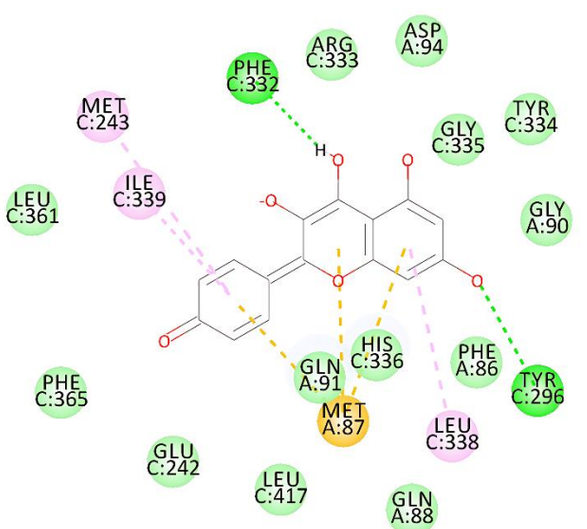
GLN A:88
Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Sulfur
Pi-Alkyl

AF


H-Bonds
Donor
Acceptor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MET C:243
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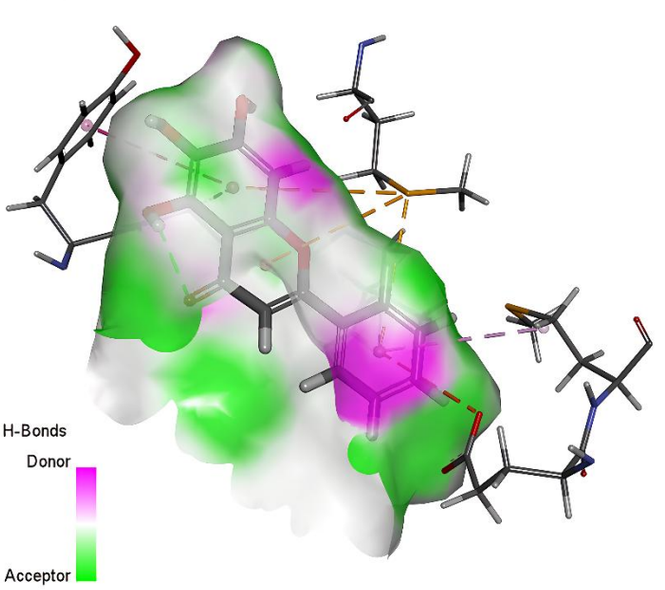
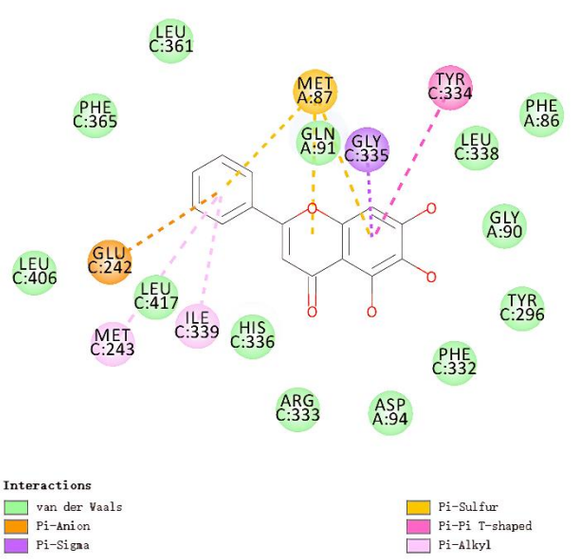
PHE A:86
GLN A:91
TYR C:296
PHE C:365
MET A:87
LEU C:338
GLU C:242
LEU C:417
GLN A:88
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Sulfur
Pi-Alkyl

AG


H-Bonds
Donor
Acceptor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LEU C:338
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GLU C:242
LEU C:406
LEU C:417
TYR C:296
ILE C:339
HIS C:336
MET C:243
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ASP A:94
Interactions
van der Waals
Pi-Anion
Pi-Sigma
Pi-Sulfur
Pi-Pi T-shaped
Pi-Alkyl

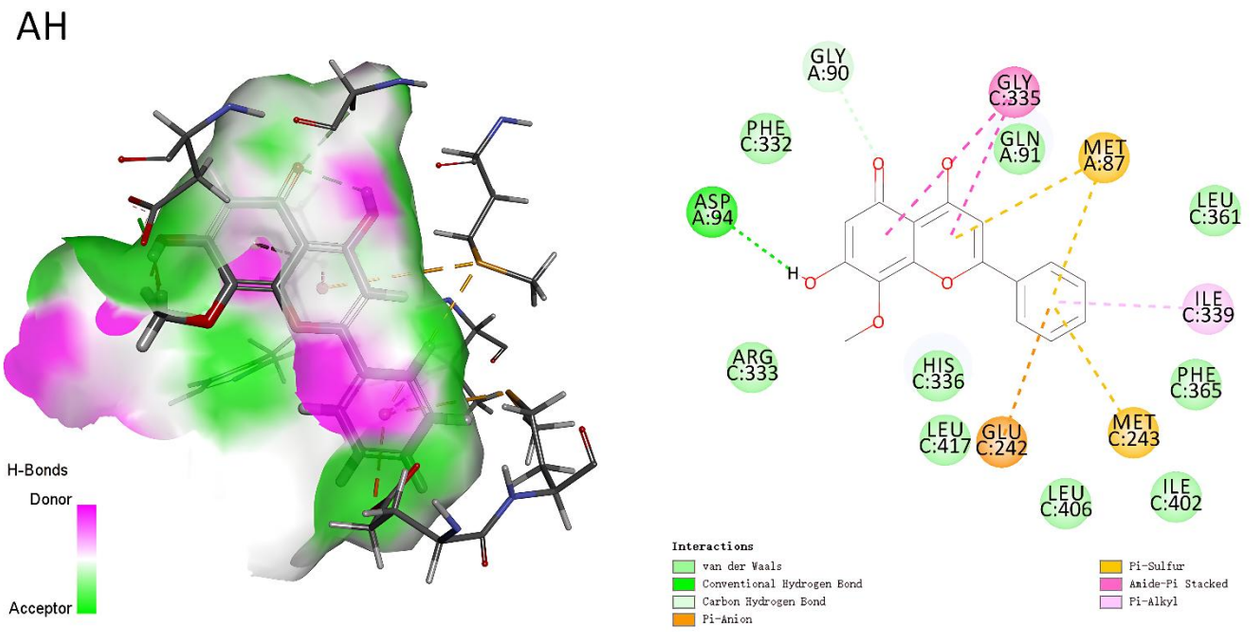

Figure S1. The interaction between the 12 predicted target and the active compound (LibDock score >110) at the optimal poses. The interactions (A-D) between NOS3 with squalene, baicalein, quercetin and kaempferol respectively; (E) between EGFR and squalene; (F) between IGF1R and squalene; (G-H) between GSK3β with squalene and baicalein respectively; (I) between BACE1 and squalene; (J-N) between PTGS2 with squalene, quercetin, kaempferol, baicalein and wogonin respectively; (O-S) between NOS2 with squalene, quercetin, kaempferol, baicalein and wogonin respectively; (T) between ESR1 and squalene; (U-Y) between PLAU with squalene, baicalein, kaempferol, wogonin and quercetin respectively; (Z) between ABCB1 and squalene; (AA-AC) between F2 with squalene, quercetin and baicalein respectively; (AD-AH) between MPO with squalene, quercetin, kaempferol, baicalein and wogonin respectively. The carbon atoms of compounds and proteases are represented as grey sticks, and oxygen atoms are shown in red. All the non-bonded interactions are shown in dotted lines with different colors according to their different interaction properties