

LAMPIRAN

Lampiran 1. Validasi dan Visualisasi Model Farmakofoor

Model	Validasi Model	2D	3D
1	2007 hits TP: 27 FP: 1989 AUC₁₂: 0.8009, AUC₂₀₀₀: 0.8044 RF₁₂: 0.8009, RF₂₀₀₀: 0.804		
2	3048 hits TP: 48 FP: 2991 AUC₁₂: 0.8027, AUC₂₀₀₀: 0.811 RF₁₂: 0.8027, RF₂₀₀₀: 0.811		
3	3950 hits TP: 49 FP: 2901 AUC₁₂: 0.7927, AUC₂₀₀₀: 0.8042 RF₁₂: 0.7927, RF₂₀₀₀: 0.8042		
4	2662 hits TP: 35 FP: 2627 AUC₁₂: 0.8020, AUC₂₀₀₀: 0.8038 RF₁₂: 0.8020, RF₂₀₀₀: 0.8038		
5	1570 hits TP: 21 FP: 1549 AUC₁₂: 0.8020, AUC₂₀₀₀: 0.8043 RF₁₂: 0.8020, RF₂₀₀₀: 0.8043		

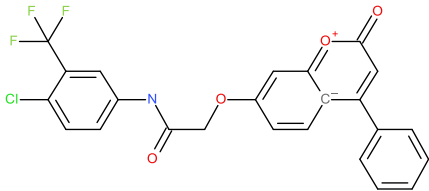
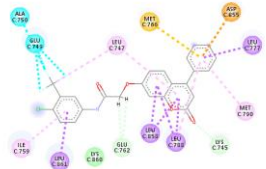
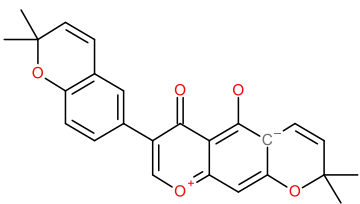
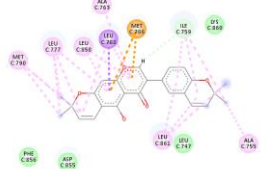
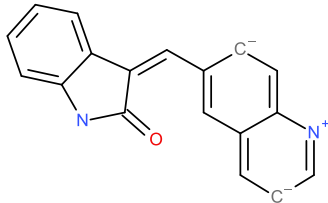
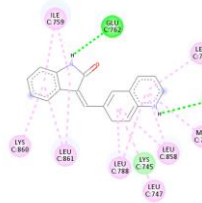
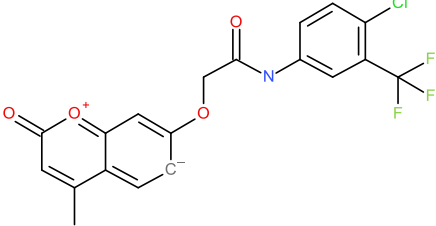
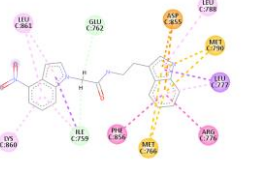
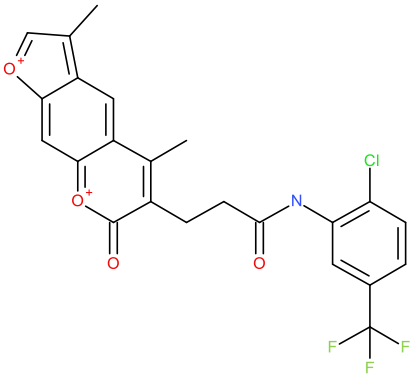
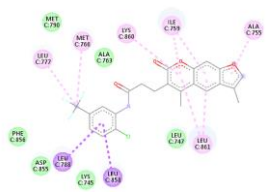
6	2789 hits TP: 45 FP: 2742 AUC: 0.710300, 0.710300, 48.039 PF: 0.500000, 0.500000, 0.500000		
7	2781 hits TP: 39 FP: 2742 AUC: 0.600000, 0.600000, 08.038 PF: 0.500000, 0.500000, 0.500000		
8	2752 hits TP: 44 FP: 2708 AUC: 0.600000, 0.600000, 08.035 PF: 0.500000, 0.500000, 0.500000		
9	4897 hits TP: 31 FP: 1564 AUC: 0.600000, 0.600000, 10.048 PF: 0.500000, 0.500000, 0.500000		
10	4800 hits TP: 46 FP: 2754 AUC: 0.600000, 0.600000, 10.046 PF: 0.500000, 0.500000, 0.500000		

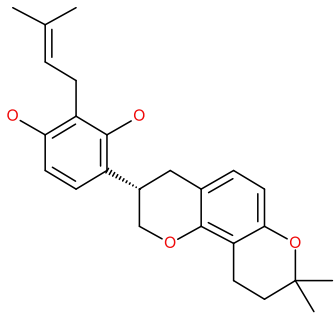
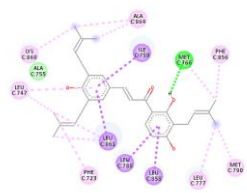
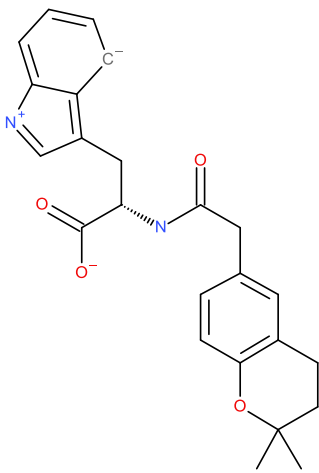
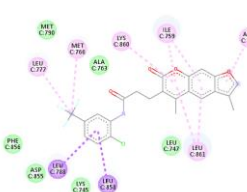
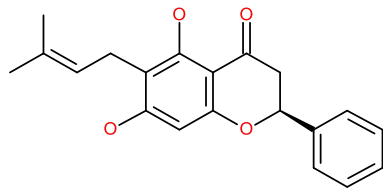
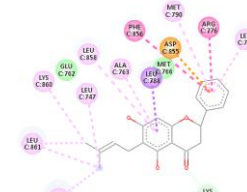
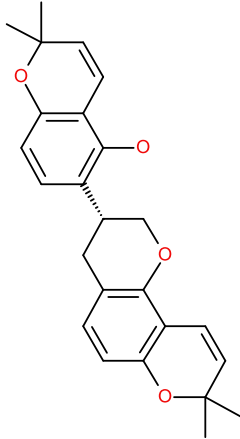
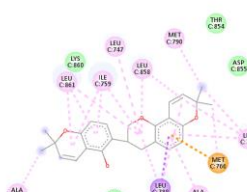
Lampiran 2. Hasil Virtual Screening Autodock Vina

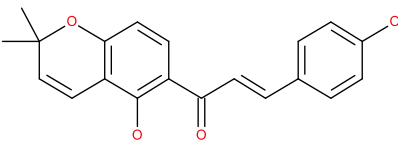
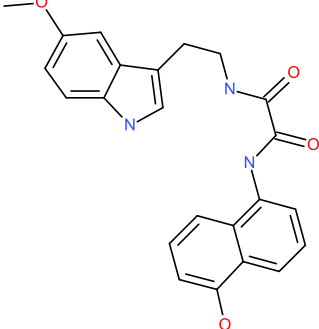
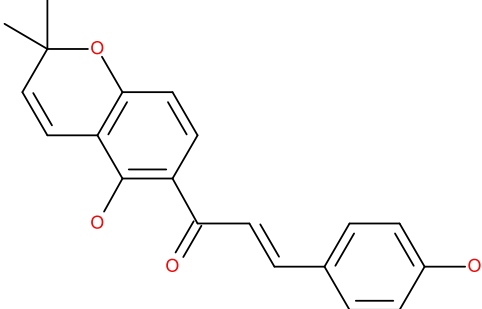
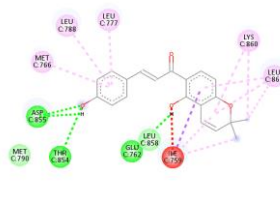
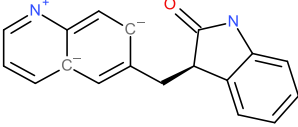
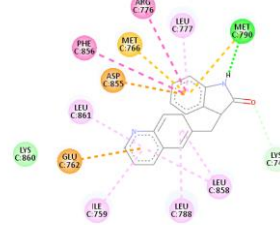
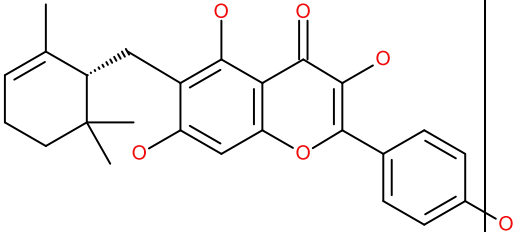
ZINC Natural Products	Kode Zinc	Kode Smiles	Binding Energy
IBScreen Natural Product	ZINC0209 4772	<chem>Clc4c(cc(NC(=O)COc2cc1oc(=O)cc(c1cc2)c3ccccc3)cc4)C(F)(F)F</chem>	-11,6
Specs Natural Product	ZINC1482 5188	<chem>o1c5c(c(=O)c(c1)c3cc2c(OC(C=C2)(C)C)cc3)c(O)c4c(OC(C=C4)(C)C)c5</chem>	-11,6
IBScreen Natural Product	ZINC4031 3335	<chem>O=c/1[nH]c4c(c/1=C/c3cc2c(nccc2)cc3)cccc4</chem>	-11,1
IBScreen Natural Product	ZINC9836 4057	<chem>o1coc2c1c(OC)cc(c2)[C@H](c3c(O)n[nH]c3Cc5cc4c(OC(CC4)(C)C)cc5)CC(=O)OC</chem>	-11
IBScreen Natural Product	ZINC0214 6796	<chem>Clc4c(NC(=O)CCc1c(oc3c(c1C)cc2c(occ2C)c3)=O)cc(cc4)C(F)(F)F</chem>	-10,9
Specs Natural Product	ZINC3383 1596	<chem>O4c2c1c(OC(CC1)(C)C)ccc2C[C@@H](c3c(O)c(c(O)cc3)CC=C(C)C)C4</chem>	-10,8
IBScreen Natural Product	ZINC9622 1977	<chem>O4c1c(cc(cc1)CC(=O)N[C@H](C(=O)[O-])Cc2c[nH]c3c2cccc3)CCC4(C)C</chem>	-10,6
IBScreen Natural Product	ZINC0402 6533	<chem>O2c1c(c(O)c(c(O)c1)CC=C(C)C)C(=O)C[C@H]2c3cccc3</chem>	-10,6
Specs Natural Product	ZINC1443 9706	<chem>O5c2c1c(OC(C=C1)(C)C)ccc2C[C@H](c4c(O)c3c(OC(C=C3)(C)C)c4)C5</chem>	-10,6
Afropan Natural Product	ZINC1455 7836	<chem>O3c1c(c(O)c(cc1)C(=O)\C=C\c2cc(O)cc2)C=CC3(C)C</chem>	-10,5
IBScreen Natural Product	ZINC3636 9853	<chem>O(c4cc1c([nH]cc1CCNC(=O)C(=O)Nc3c2c(c(O)ccc2)ccc3)cc4)C</chem>	-10,5
Specs Natural Product	ZINC1455 7836	<chem>O3c1c(c(O)c(cc1)C(=O)\C=C\c2cc(O)cc2)C=CC3(C)C</chem>	-10,5
IBScreen Natural Product	ZINC4031 3079	<chem>O=C2Nc1c(ccc1)[C@H]2Cc4cc3c(nccc3)cc4</chem>	-10,4
Specs Natural Product	ZINC1482 5106	<chem>o1c(c(O)c(=O)c2c1cc(O)c(c2O)C[C@H]3C(=CCCC3(C)C)C)c4ccc(O)cc4</chem>	-10,3
AnalytiCon Discovery Natural Product	ZINC0573 4356	<chem>O3c1c(c(O)c(cc1)C(=O)\C=C\c2ccc2)C=CC3(C)C</chem>	-10,2
IBScreen Natural Product	ZINC9611 6567	<chem>O=[N+](O-)]c4c1c(n(cc1)CC(=O)NCCc2c[nH]c3c2cccc3)ccc4</chem>	-10,2

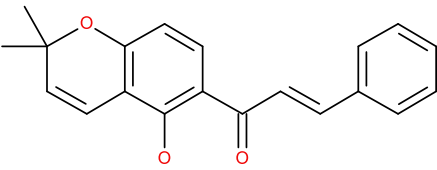
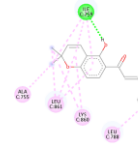
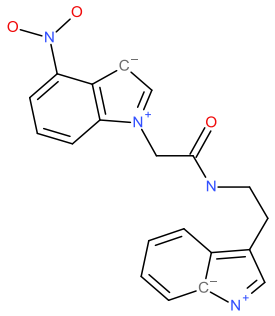
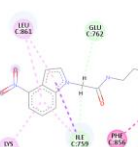
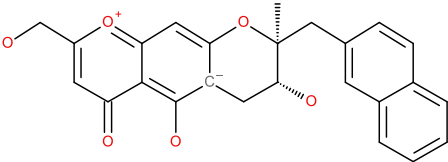
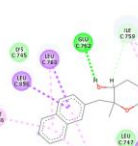
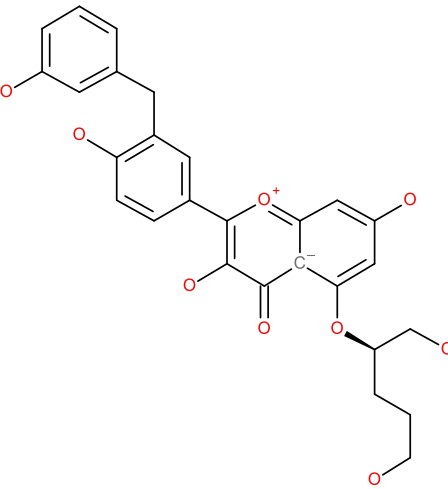
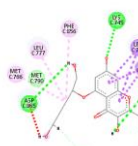
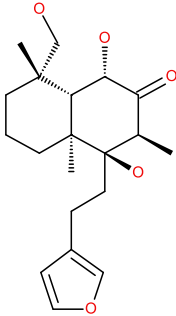
NuBBe Natural Product	ZINC3254 0719	O(c3c(c(O)c(c1n[nH]cc1c2ccc(OC) cc2)cc3)C)CC[NH+] 4CCCCC4	-10,2
Princeton Natural Product	ZINC8556 9412	o1c(c(O)c(=O)c2c1cc(O)cc2O[C@ @H])(CO)CCCO)c3cc(c(O)cc3)Cc 4cc(O)ccc4	-10,2
Specs Natural Product	ZINC1469 0579	O2c1c(c(O)cc(O)c1)C(=O)C[C@ H]2c4c(O)c3c(OC(C=C3)(C)C)cc 4	-10,2
Specs Natural Product	ZINC8554 6223	Oc4c(ccc(c1cc(ccc1)CCC(=O)[C @]23[C@](OC)(O)[C@H]([C@@ H])(CO)C2)C(C3(C)C)=C)c4)[C@ @H](c5ccc(O)cc5)C[NH2+] [C	-10,2
Specs Natural Product	ZINC1482 1540	Oc1c(c(O)ccc1C(=O)\C=C\c2cc(c(O)c(c2)CC=C(C)C)CC=C(C)C)C C=C(C)C	-10,1
Specs Natural Product	ZINC1481 4670	o2c(Oc1ccc(O)cc1)cc(=O)c3c2cc(O)c(c3O)CC=C(C)C	-10,1
Specs Natural Product	ZINC1334 0783	Oc1c(cc(cc1)CCc2cc(O)cc(O)c2)C C=C(C)C	-10,1
NPACT Database	ZINC0822 0175	O[C@@H]2CC(=C\C=C\C=C\C=C\ =C\C=C\C=C\C=C\C=C\C=C\C=C\ =C\C1=C(C[C@@H](O)CC1(C)C)C)/C)/C)\C)/C)C(C2)(C)C)C	-10
NuBBe Natural Product	ZINC3596 6135	O[C@H]3[C@]([C@@H]1[C@]([C@ @H])([C@@H])(CO)CC1)CCC 2C(=O)OCC=2)(CC3)C)(CO)C	-10
Specs Natural Product	ZINC9590 9542	Oc1c(cc(cc1)\C=C/c2cc(O)cc(O)c 2)CC=C(C)C	-10
Specs Natural Product	ZINC0089 9894	O4c1c(ccc(O)c1)C[C@@H](c3c(O)c2c(OC(C=C2)(C)C)cc3)C4	-10
Specs Natural Product	ZINC3139 4551	Oc1c(c(O)ccc1C(=O)\C=C/c2ccc(O)cc2)C\C=C(\CCC=C(C)C)/C	-10
Specs Natural Product	ZINC1348 5494	O[C@@@H]([C@@@H](O)C)\C=C\ C=C/CC\C=C\C=C(=O)NCC(O)(C)C	-10
Afropan Natural Product	ZINC1441 7338	o1c4c(c(=O)c(c1)c2ccc(O)cc2)c(O)c3c(OC(C=C3)(C)C)c4	-9,9
Protein Data Bank	Ligan Alami	-	-14.5

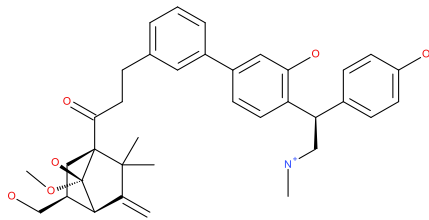
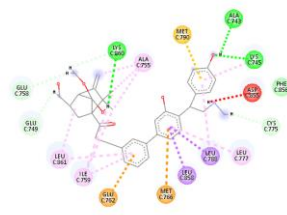
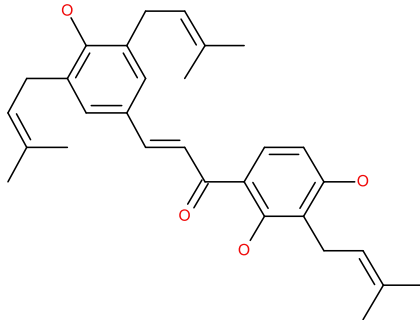
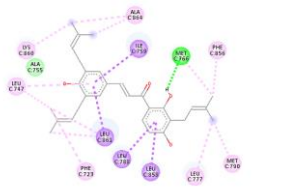
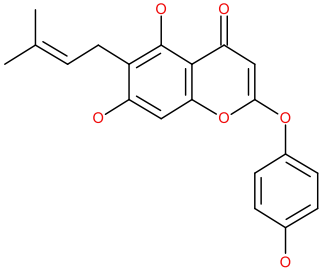
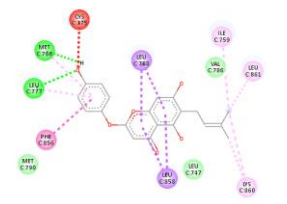
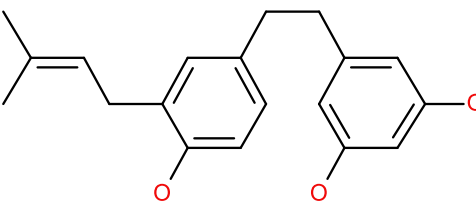
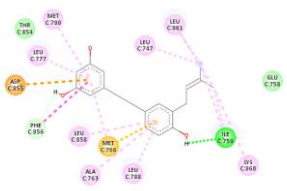
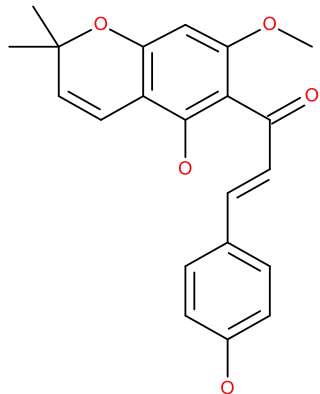
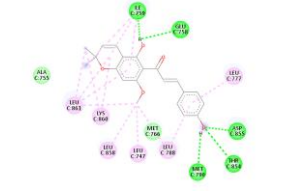
Lampiran 3. Visualisasi Interaksi Senyawa

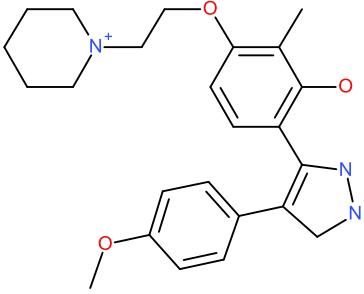
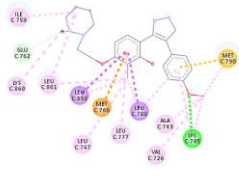
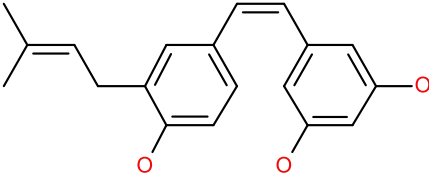
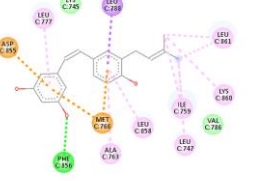
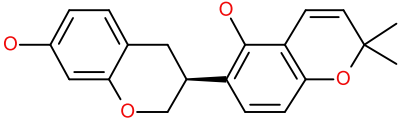
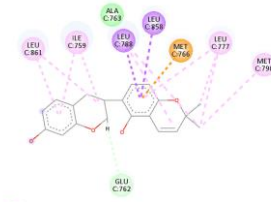
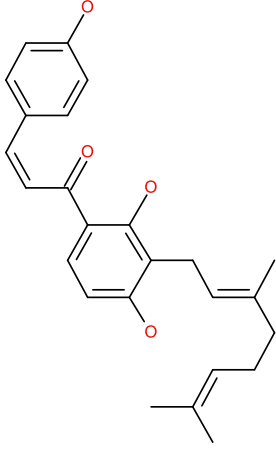
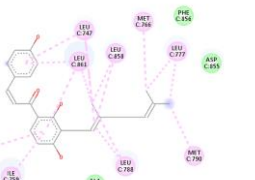
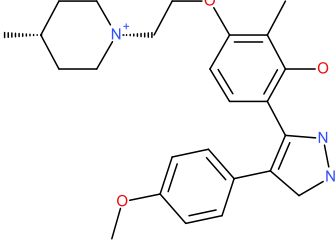
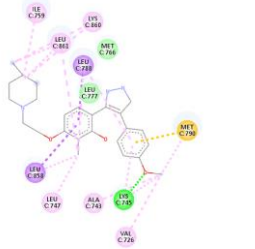
ZINC Natural Products	Struktur	Binding Energy	Interaksi
IBScreen Natural Product		-11,6	
Specs Natural Product		-11,6	
IBScreen Natural Product		-11,1	
IBScreen Natural Product		-11	
IBScreen Natural Product		-10,9	

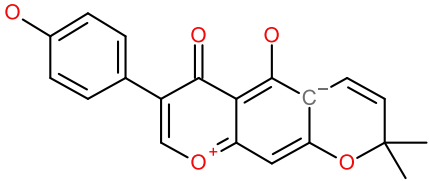
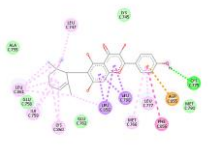
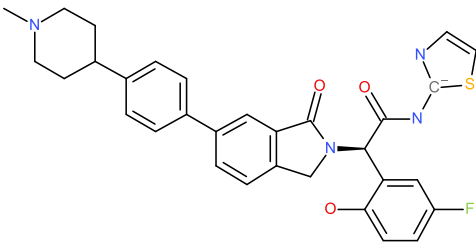
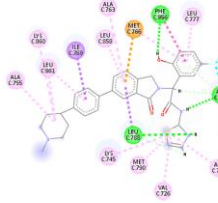
Specs Natural Product		-10,8	
IBScreen Natural Product		-10,6	
IBScreen Natural Product		-10,6	
Specs Natural Product		-10,6	

Afropan Natural Product		-10,5	
IBScreen Natural Product		-10,5	
Specs Natural Product		-10,5	
IBScreen Natural Product		-10,4	
Specs Natural Product		-10,3	

AnalytiC on Discover y Natural Product		-10,2	
IBScreen Natural Product		-10,2	
NuBBE Natural Product		-10,2	
Princeton Natural Product		-10,2	
Specs Natural Product		-10,2	

Specs Natural Product		-10,2	
Specs Natural Product		-10,1	
Specs Natural Product		-10,1	
Specs Natural Product		-10,1	
NPACT Database		-10	

NuBBe Natural Product		-10	
Specs Natural Product		-10	
Specs Natural Product		-10	
Specs Natural Product		-10	
Specs Natural Product		-10	

Afropan Natural Product	 <chem>O=C1C(=O)C(=C(C=C1)OC2C(C)C=CC2)C(=O)C3=CC=C(C=C3)OC4=CC=CC=C4</chem>	-9,9	 Molecular docking diagram showing the interaction of Afropan Natural Product with a protein binding site. The ligand is shown in stick representation, and the protein residues are shown as spheres. Dashed lines indicate hydrogen bonds and other interactions.
Ligan Alami	 <chem>CN1CCCCC1c2ccc(cc2)-c3ccc(cc3)-c4cc5c(cc4)nc(=O)c6cc(F)ccc6c5=O</chem>	-14,5	 Molecular docking diagram showing the interaction of Ligan Alami with a protein binding site. The ligand is shown in stick representation, and the protein residues are shown as spheres. Dashed lines indicate hydrogen bonds and other interactions.