Appendix 1. Parameters of the Main Phytochemicals of CS.

Components	Canonical SMILS	Chemical group	OB	DL	targets
Adenosin	C1=NC(=C2C(=N1)N(C=N2)C3C(C(C(O3)CO)O)O)N	Nucleoside	0.55	0.49	10
Capparilosid A	C1=CC2=C(C(=C1)OC3C(C(C(C(O3)CO)O)O)O)C(=CN2)CC#N	Alkaloide	0.55	0.50	1
Flazin	C1=CC=C2C(=C1)C3=CC(=NC(=C3N2)C4=CC=C(O4)CO)C(=O)O	Alkaloide	0.56	0.54	10
Capparin B	COC1=CC2=C(C=C1)C(=C(N2)SC)C=O	Alkaloide	0.55	0.64	1
Capparin A	COC1=CC2=C(C=C1)C3(CN=C(S3)SC)C(=O)N2	Alkaloide	0.55	0.85	2
5,5'-[Oxybis(methylene)] bis[2-furancarboxaldehyde]	O1C(C=O)=CC=C1COCC1=CC=C(C=O)O1	Pyrrole (Furan)	0.55	0.71	1
Capparisine C	C1C(C(NNC1=O)C(=O)C2=CC=CO2)C(=O)N	Pyrrole (Furan)	0.55	0.58	1
Kaempferol	C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O	Flavonoid	0.55	0.54	93
Apigenin	C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O	Flavonoid	0.55	0.63	130
Rutin (Quercetin-3-O-rutinoside)	CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC(=C(C=C5)O)O)O)O)O)O)O)O	Flavonoid	0.17	0.14	15
Oroxylin A	COC1=C(C2=C(C=C1O)OC(=CC2=O)C3=CC=CC=C3)O	Flavonoid	0.55	0.75	4
Wogonin	COC1=C(C=C(C2=C1OC(=CC2=O)C3=CC=CC=C3)O)O	Flavonoid	0.55	0.75	18
Sakuranetin	COC1=CC(=C2C(=O)CC(OC2=C1)C3=CC=C(C=C3)O)O	Flavonoid	0.55	0.88	7
Astragalin	C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)OC4C(C(C(C(O4)CO)O)O)O)O	Flavonoid	0.17	0.27	17
Isorhamnetin	COC1=C(C=CC(=C1)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O	Flavonoid	0.55	0.57	29
Quercetin 3-O glucoside-7-O-rhamnoside	CC1C(C(C(C(O1)OC2=CC(=C3C(=C2)OC(=C(C3=O)OC4C(C(C(C(O4)CO)O)O)O)C5=CC(=C(C=C5)O)O)O)O)O)O	Flavonoid	0.17	0.13	9
Ginkgetin	COC1=C(C=C(C=C1)C2=CC(=O)C3=C(C=C(C=C3O2)OC)O)C4=C(C=C(C5=C4OC(=CC5=O)C6=CC=C(C=C6)O)O)O	Flavonoid	0.55	0.20	6
Isoginkgetin	COC1=CC=C(C=C1)C2=CC(=O)C3=C(O2)C(=C(C=C3O)O)C4=C(C=CC(=C4)C5=CC(=O)C6=C(C=C(C=C6O5)O)O)OC	Flavonoid	0.55	0.20	5
Gallic acid	C1=C(C=C(C(=C1O)O)O)C(=O)O	Phenolic acid	0.56	0.46	51
Protocatechuic acid (3,4-Dihydroxybenzoic acid)	C1=CC(=C(C=C1C(=O)O)O)O	Phenolic acid	0.56	0.52	20
Chlorogenic Acid	C1C(C(C(CC1(C(=O)O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)O)O	Phenolic acid	0.11	0.23	6
2,5-Dihydroxybenzoic acid (gentisic acid)	C1=CC(=C(C=C1O)C(=O)O)O	Phenolic acid	0.56	0.52	15
Vanillic acid	COC1=C(C=CC(=C1)C(=O)O)O	Phenolic acid	0.85	0.69	3

Sinapinic acid	COC1=CC(=CC(=C1O)OC)C=CC(=O)O	Phenolic acid	0.56	0.75	2
Syringic acid	COC1=CC(=CC(=C1O)OC)C(=O)O	Phenolic acid	0.56	0.76	25
Corchoionoside C	CC1=CC(=O)CC(C1(C=CC(C)OC2C(C(C(C(O2)CO)O)O)O)O)(C)C	Terpene	0.55	0.39	3
Spionoside A	CC(C=CC1(C(=CC(=O)CC1(C)C)CO)O)OC2C(C(C(C(O2)CO)O)O)O	Terpene	0.55	0.28	6
Spionoside B	CC(C=CC1(C2(CC(=O)CC1(OC2)C)C)O)OC3C(C(C(C(O3)CO)O)O)O	Terpene	0.55	0.35	10
Phaseic acid	CC(=CC(=O)O)C=CC1(C2(CC(=O)CC1(OC2)C)C)O	Terpene	0.56	0.60	10
Beta-Sitosterol	CCC(CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C	Terpene	0.55	0.43	9
Alpha- Tocopherol	CC1=C(C2=C(CCC(O2)(C)CCCC(C)CCCC(C)CCCC(C)C)C(=C1O)C)C	Terpene	0.55	0.35	12

Appendix 2. Network Node Parameters of the Overlapping Cancer Targets.

	Target	degree	Betweenness	closeness
1	AKT1	185	0.070177	0.552526
2	EGFR	170	0.04203	0.539969
3	SRC	163	0.042691	0.538281
4	ESR1	93	0.008753	0.505132
5	GSK3B	78	0.020212	0.468389
6	IGF1R	75	0.007068	0.480809
7	CDK2	51	0.00375	0.425834
8	AR	50	0.013463	0.461487
9	LCK	47	0.00246	0.434975
10	FLT3	46	0.002261	0.436076
11	PTGS2	41	0.004721	0.456594
12	MMP2	39	0.002253	0.443087
13	CDK6	32	0.001307	0.418336
14	MAP2K1	29	6.01E-04	0.432246
15	PGR	29	5.38E-04	0.441384
16	XIAP	29	0.003569	0.415561
17	ESR2	21	1.42E-04	0.421665
18	CALM1	20	0.0015	0.416063
19	CDK9	19	8.64E-04	0.40458
20	MMP1	19	3.17E-04	0.395977
21	BMP2	16	3.04E-04	0.388826
22	PDPK1	15	8.97E-05	0.400581
23	CASP7	14	1.74E-04	0.384487
24	PLAU	14	5.28E-05	0.373037
25	CSNK2A1	14	1.66E-04	0.395977
26	CCNT1	12	2.27E-04	0.362441
27	NOS2	12	2.03E-05	0.392593
28	MPO	10	8.33E-05	0.367859
29	ELANE	9	4.70E-05	0.358108
30	GSTP1	9	6.66E-04	0.373644
31	NQO1	9	9.31E-04	0.393714
32	DAPK1	8	3.68E-04	0.388388
33	PIM1	5	0.002904	0.372432
34	CTSL	4	1.89E-04	0.340247
25	CYP1B1	3	5.46E-06	0.303792
36	ABCB1	2	0.002903	0.35189

Appendix 3. Molecular Docking Results of Capparis spinosa Compounds with Predicted Targets

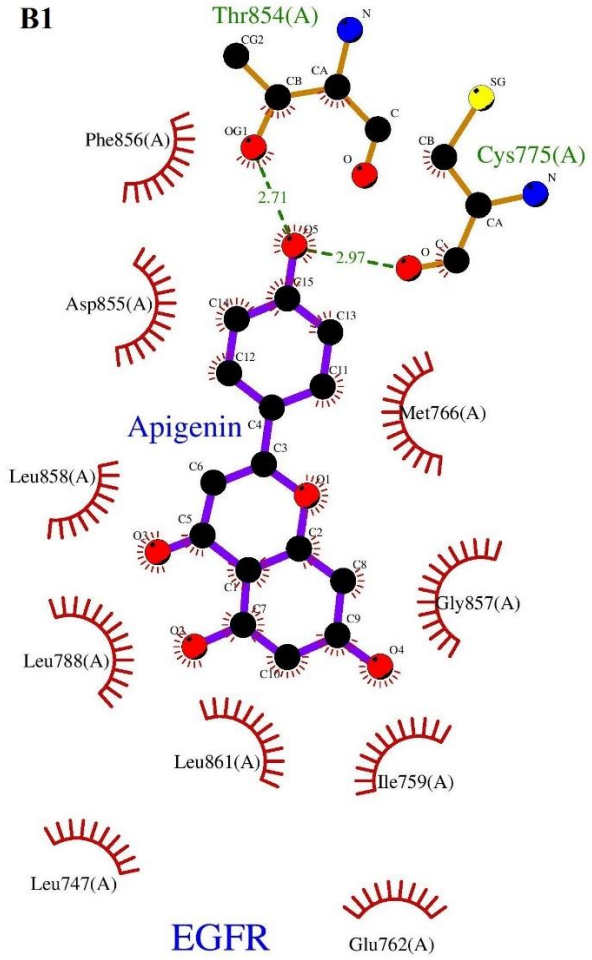
Compound	Target	Binding Energy (ΔG, kcal/mol)	Inhibition Constant (Ki, μM)	Key Interactions (Residues)	Interaction Types
Rutin	AKT1	-5.18	159.28	Lys158 (H-bond), Glu234 (H-bond), Tyr229 (hydrophobic)	H-bond, hydrophobic
Apigenin	EGFR	-8.1	1.17	Thr766 (H-bond), Met769 (π-π), Leu694 (hydrophobic)	H-bond, π-π, hydrophobic
Kaempferol	EGFR	-7.83	1.83	Thr766 (H-bond), Met769 (π-π), Leu820 (hydrophobic)	H-bond, π-π, hydrophobic
Flazin	SRC	-8.08	1.19	Asp404 (H-bond), Ile336 (hydrophobic), Tyr340 (π-π)	H-bond, π-π, hydrophobic
Gallic acid	CA II	-6.8	10.2	His94 (H-bond), Thr199 (H-bond), Gln92 (H-bond)	H-bond
Syringic acid	CA V	-7.1	6.5	His64 (H-bond), Asn67 (H-bond), Gln92 (hydrophobic)	H-bond, hydrophobic
Capparine A	JNK3	-6.45	18.9	Met149 (H-bond), Lys93 (salt bridge), Ile70 (hydrophobic)	H-bond, salt bridge, hydrophobic
β-Sitosterol	ESR1	-7.2	5.01	Leu387 (hydrophobic), Phe404 (π-π), Arg394 (H-bond)	H-bond, π-π, hydrophobic
Quercetin	BACE1	-7.5	3.2	Asp32 (H-bond), Gly34 (H-bond), Tyr71 (π-π)	H-bond, π-π

Isorhamnetin	JNK1	-6.9	8.45	Met111 (H-bond), Lys55 (salt bridge), Val78 (hydrophobic)	H-bond, salt bridge, hydrophobic
Spionoside A	IGF1R	-7.3	4.5	Glu1050 (H-bond), Phe1049 (π-π), Val983 (hydrophobic)	H-bond, π-π, hydrophobic
Ginkgetin	BACE1	-7.8	2	Asp228 (H-bond), Gly230 (H-bond), Trp76 (π-π)	H-bond, π-π
Astragalin	NOX4	-6.6	13.5	Arg103 (H-bond), Phe115 (π-π), His95 (hydrophobic)	H-bond, π-π, hydrophobic
Protocatechuic acid	CA IX	-6.4	20.1	Gln67 (H-bond), His68 (H-bond), Tyr194 (hydrophobic)	H-bond, hydrophobic
Gentisic acid	PTPN1	-6.2	28.3	Cys215 (H-bond), Arg221 (H-bond), Phe182 (hydrophobic)	H-bond, hydrophobic
Oroxylin A	p38 MAPK	-7	7.2	Lys53 (H-bond), Met109 (hydrophobic), Tyr35 (π-π)	H-bond, π-π, hydrophobic
Adenosine	PDPK1	-6.8	10.5	Glu166 (H-bond), Leu172 (hydrophobic), Phe241 (π-π)	H-bond, π-π, hydrophobic
Stachydrine	MMP2	-5.9	45.6	Leu164 (hydrophobic), Ala165 (H-bond), Tyr223 (π-π)	H-bond, π-π, hydrophobic
δ-Tocopherol	AR	-7.1	6.3	Leu701 (hydrophobic), Trp741 (π-π), Asn705 (H-bond)	H-bond, π-π, hydrophobic

Glucocapperin	GSTP1	-5.7	65.2	Tyr108 (H-bond), Phe8 (hydrophobic), Val35 (hydrophobic)	H-bond, hydrophobic
Kaempferol-3-O-rutinoside	XIAP	-6.5	17.8	Trp323 (π-π), Lys297 (H-bond), Gly306 (H-bond)	H-bond, π-π
Quercetin-3-O-glucoside	PTGS2	-7.2	5.1	Tyr385 (H-bond), Ser530 (H-bond), Val349 (hydrophobic)	H-bond, hydrophobic
Isorhamnetin-3-O-glucoside	CDK2	-6.9	8.3	Glu81 (H-bond), Leu83 (hydrophobic), Phe82 (π-π)	H-bond, π-π, hydrophobic
Capparisine B	NOS2	-6.3	24.5	Trp372 (π-π), Glu377 (H-bond), Val346 (hydrophobic)	H-bond, π-π, hydrophobic
Oleic acid	PPARG	-6.7	12.4	Ser289 (H-bond), Leu330 (hydrophobic), Phe363 (π-π)	H-bond, π-π, hydrophobic
Linoleic acid	PPARA	-6.5	17.6	Tyr314 (H-bond), Leu321 (hydrophobic), Phe273 (π-π)	H-bond, π-π, hydrophobic
β-Carotene	CYP19A1	-6.8	10.8	Met374 (hydrophobic), Phe134 (π-π), Trp141 (π-π)	π-π, hydrophobic
Campesterol	PGR	-6.9	8.6	Leu715 (hydrophobic), Trp755 (π-π), Met756 (hydrophobic)	π-π, hydrophobic
Stigmasterol	ESR2	-7	7.4	Glu353 (H-bond), Leu387 (hydrophobic), Phe404 (π-π)	H-bond, π-π, hydrophobic

Saponarin	ABCB1	-6.4	20.8	Gln725 (H-bond), Phe728 (π-π), Val982 (hydrophobic)	H-bond, π-π, hydrophobic
Vitexin	DAPK1	-6.6	13.7	Lys42 (H-bond), Glu64 (H-bond), Phe67 (hydrophobic)	H-bond, hydrophobic

Appendix 4. Molecular docking of CS phytochemicals on cancer hub-targets. Two-dimensional diagrams (1) and three-dimensional diagrams (2) were depicted. A, rutin binding to AKT1; B, apigenin binding to EGFR; C, flazin binding to EGFR; D, kaempferol binding to EGFR; E, flazin binding to Src.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2.97
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Apigenin
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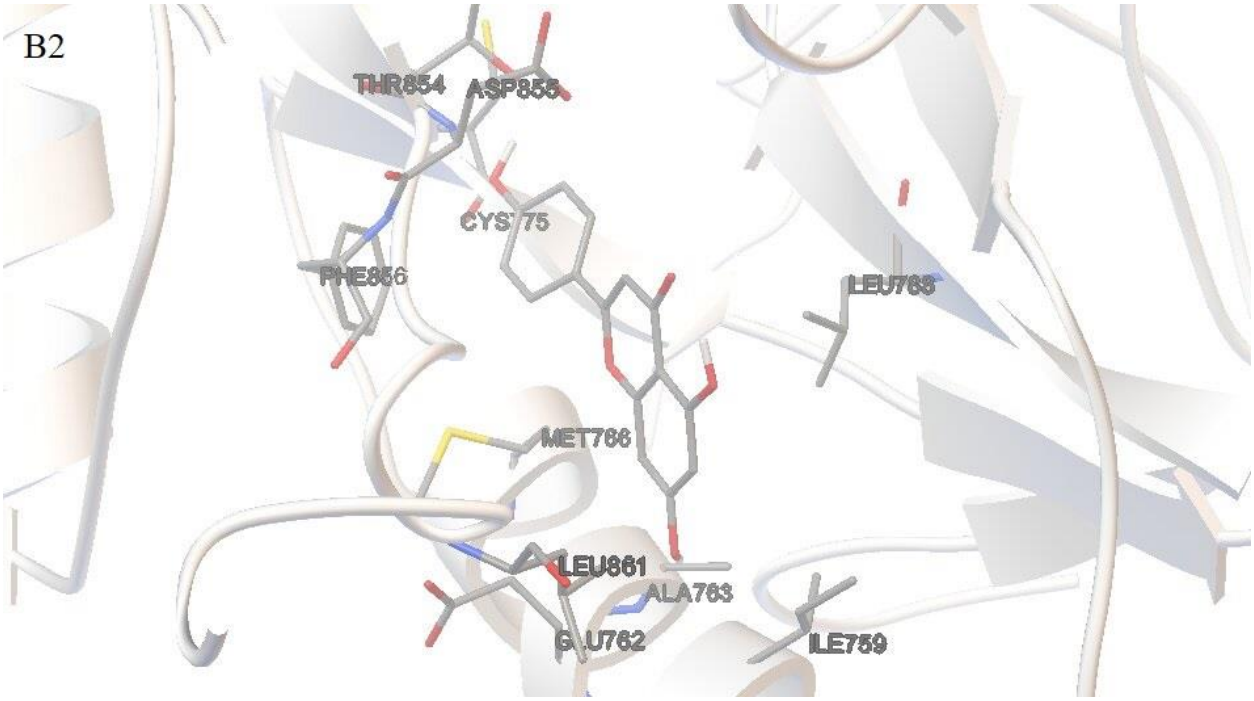
EGFR
Glu762(A)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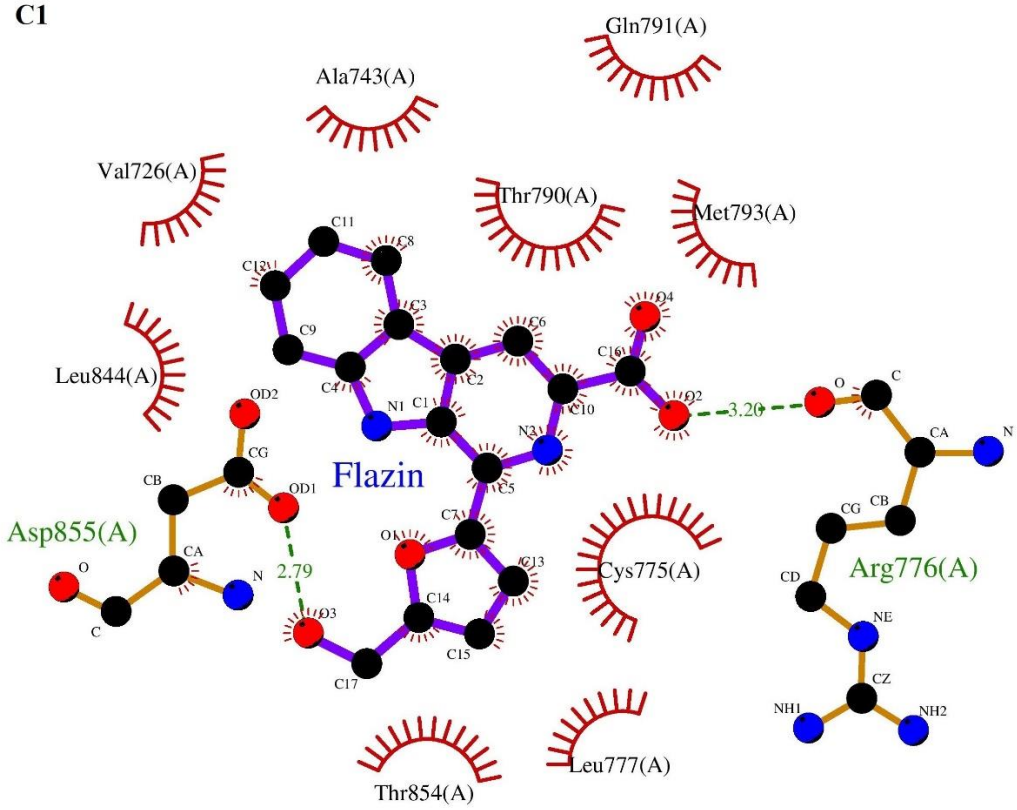
C1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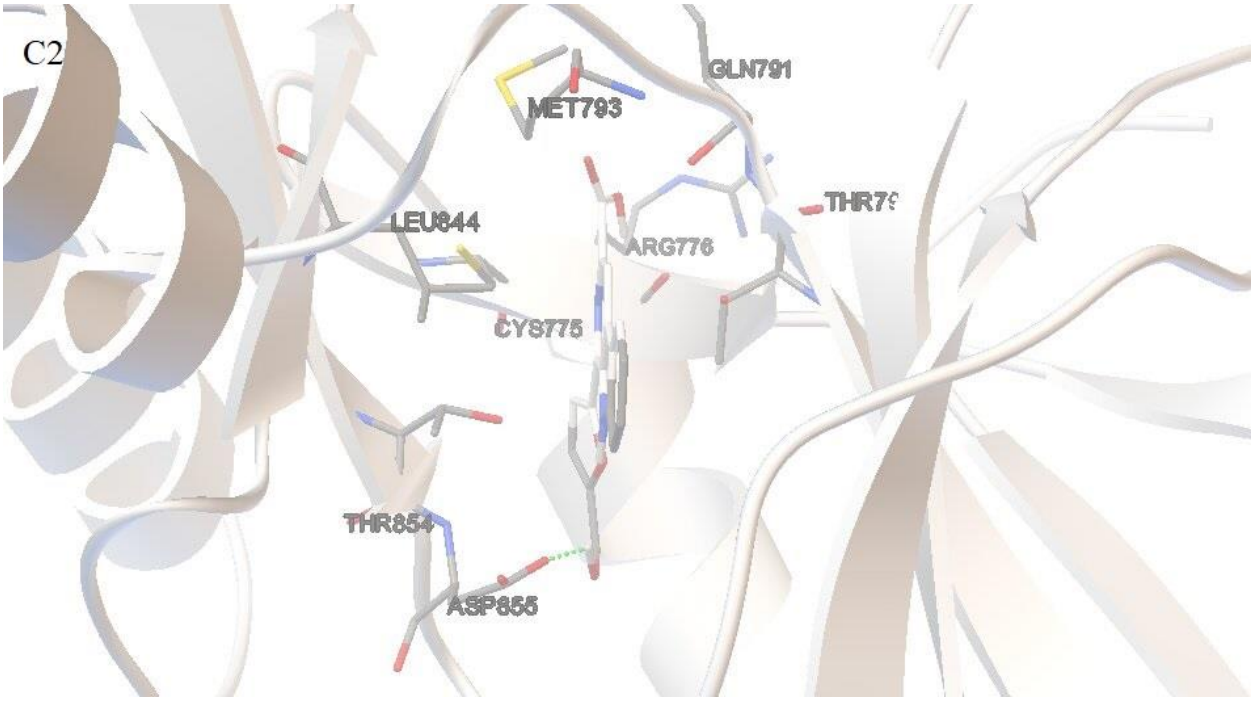
3.20

EGFR

C2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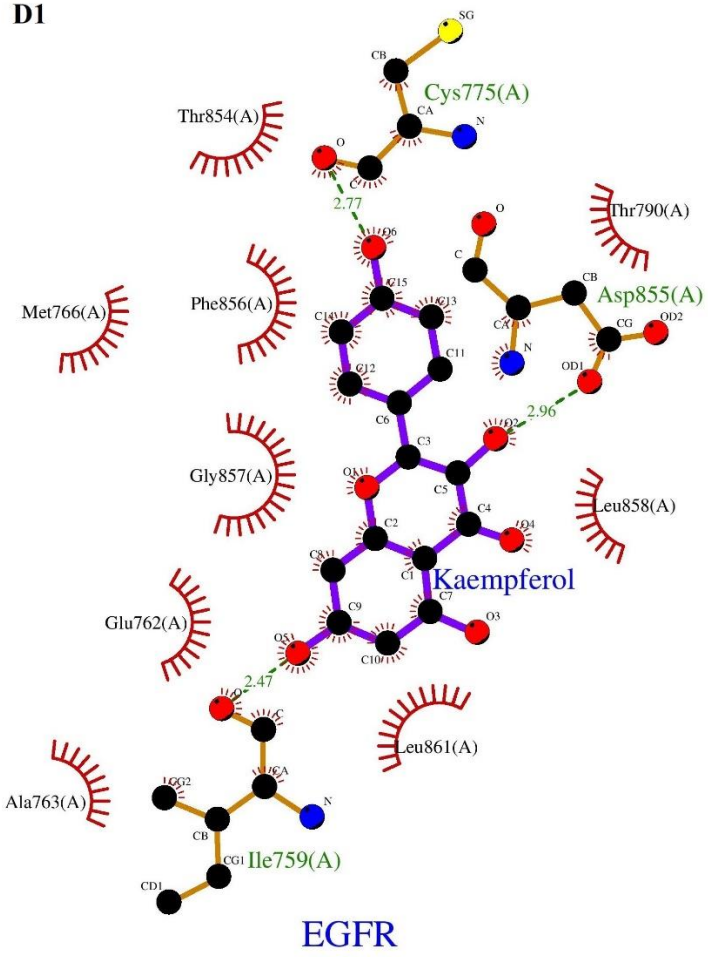
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Ile759(A)
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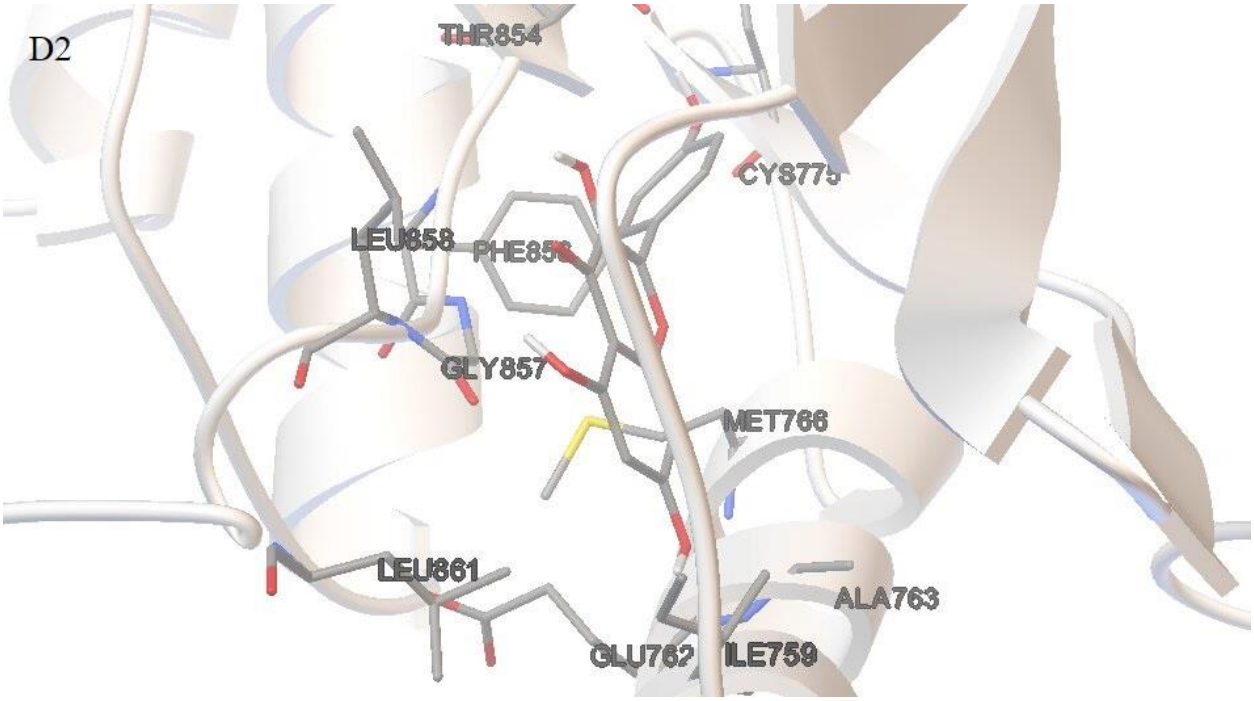
2.96
2.47

EGFR

D2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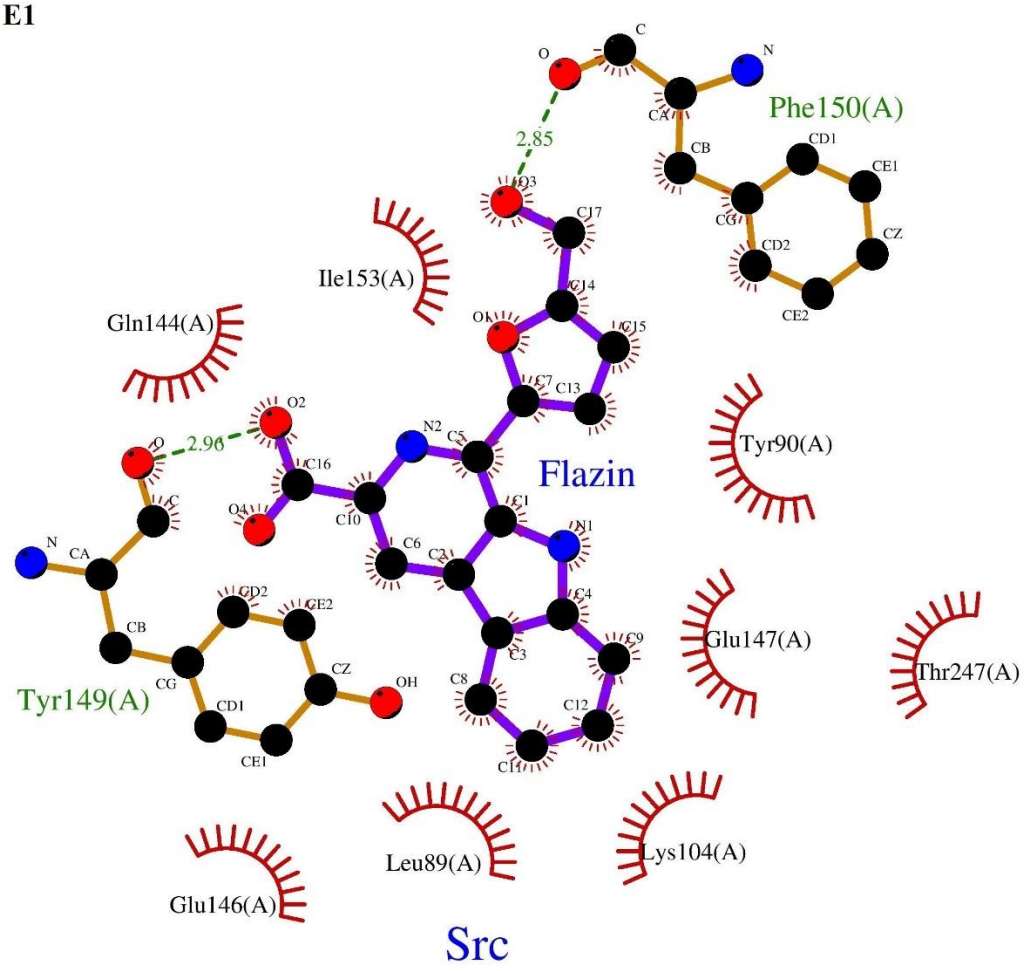
E1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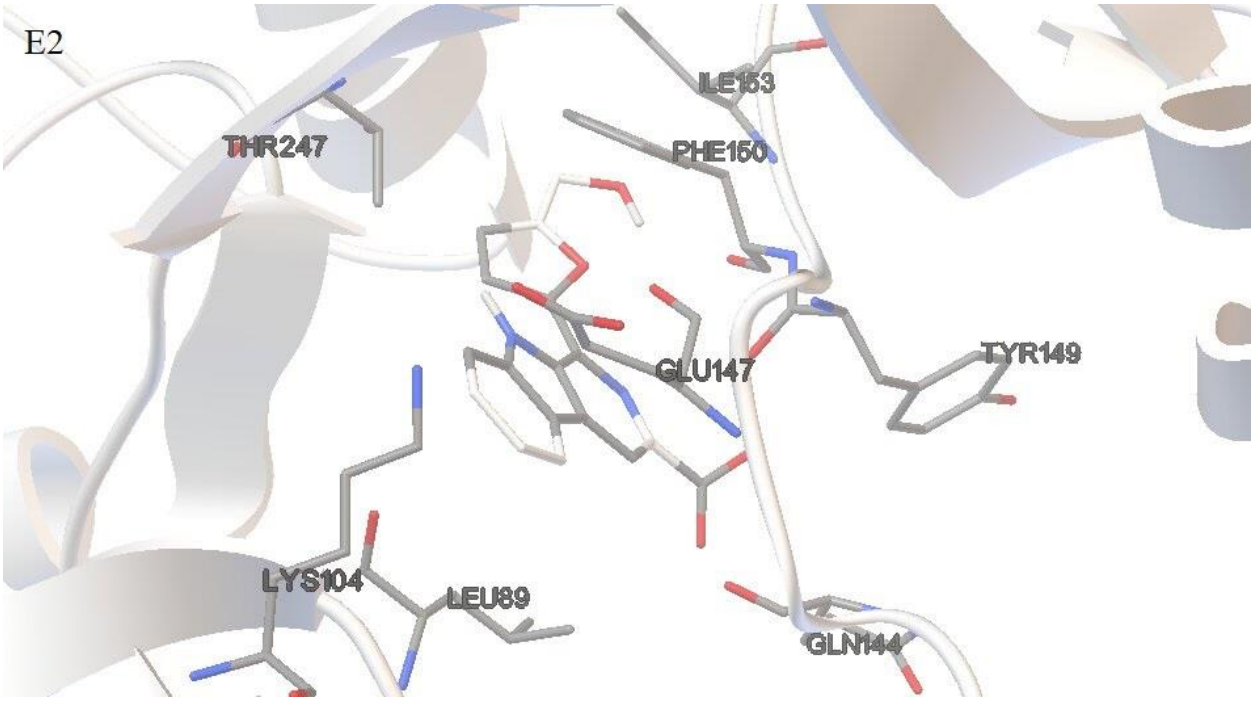
Src

E2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