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Appendices

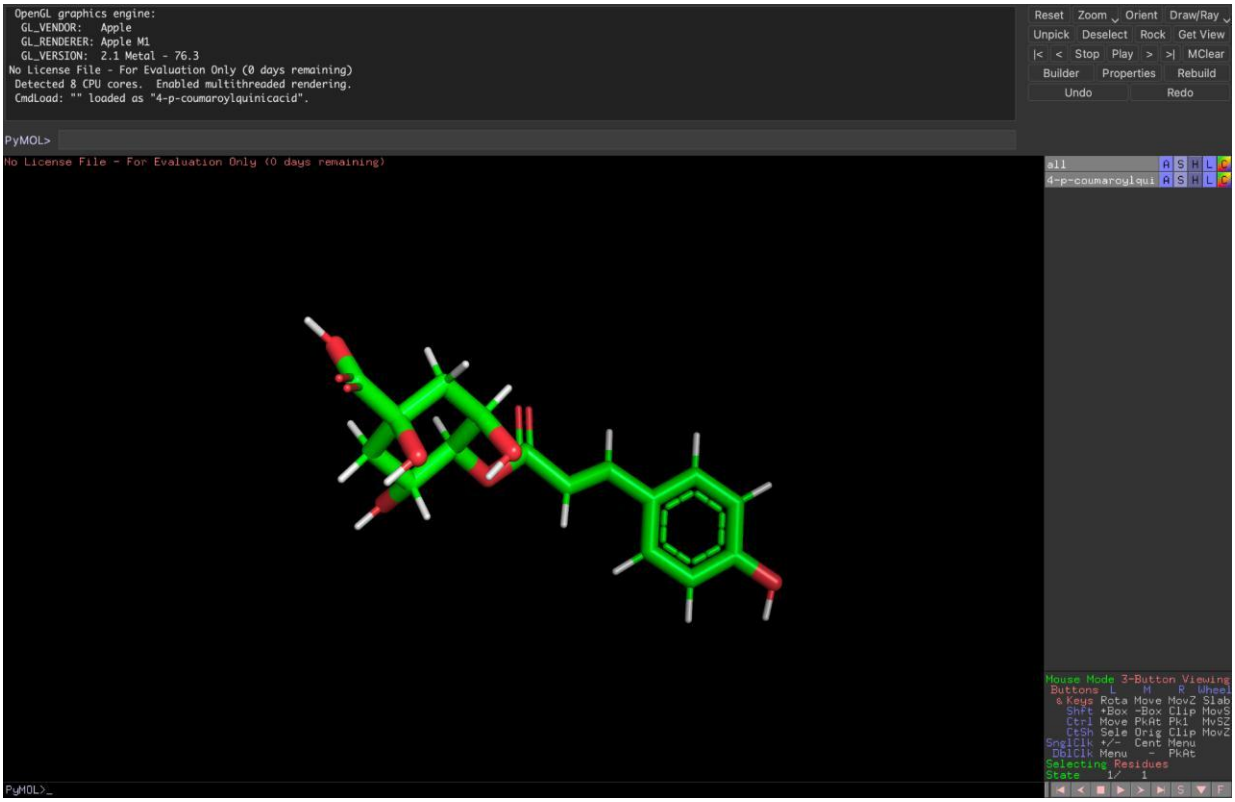
Docked protein visualization

3D structures were obtained from pubchem

Table containing results from SCF Bio's Lipinski's rule of five web tool

Number	Name	Hydrogen Bond Donor	Hydrogen Bond Acceptor	Lipophilicity (LOG*P*)	Molar Refractivity	PubChem CID
1	5-O-Caffeoylquinic acid	6	9	-0.645900	82.518768	5280633
2	Quercetin	5	7	2.010900	74.050476	5280343
3	3-O-Feruloylquinic acid	5	9	-0.342900	87.405968	9799386
4	4-O-Feruloylquinic acid	5	9	-0.342900	87.405968	10177048
5	5-O-Feruloylquinic acid	5	9	-0.342900	87.405968	73210496
6	4,5-Di-O-caffeoylquinic acid	5	6	-0.053101	77.145782	6474309
7	4-P-Coumaroylquinic acid	5	8	-0.351500	80.853966	5281766
8	5-P-Coumaroylquinic acid	5	8	-0.351500	80.853966	164893
9	16-O-Methylcafestol	1	3	4.060699	90.884766	68103163
10	16-O-Methyl Kahweol	1	3	4.141299	91.597771	68103165
11	Cafestol	2	3	3.406599	86.094566	108052
12	Kahweol	2	3	3.487199	86.807571	114778
13	Dehydrocafestol	1	2	4.211799	84.610771	101468593
14	Dehydro Kahweol	1	2	4.525099	86.256775	101468592

All 3D Structures then was cleaned from hydrogen bonds using PyMOL software



The image above is the PyMOL software, used to clean any hydrogen bonds prior to docking.

The molecule in view is 4-p-coumaroylquinic acid.

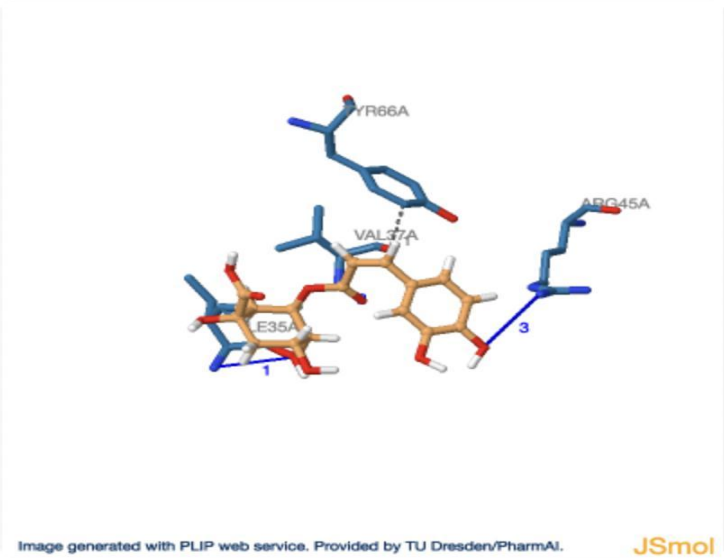
The following are the docked proteins with their interaction report from PLIP

SMALLMOLECULE

UNK (alpha-aminobutyric acid)

UNK-Z-0

Interacting chains: A



- Protein
- Ligand
- Water
- Charge Center
- Aromatic Ring Center
- Metal Ion
- Hydrophobic Interaction
- Hydrogen Bond
- Water Bridge

Hydrophobic Interactions ····

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	66A	TYR	2.99	19	596

Hydrogen Bonds —

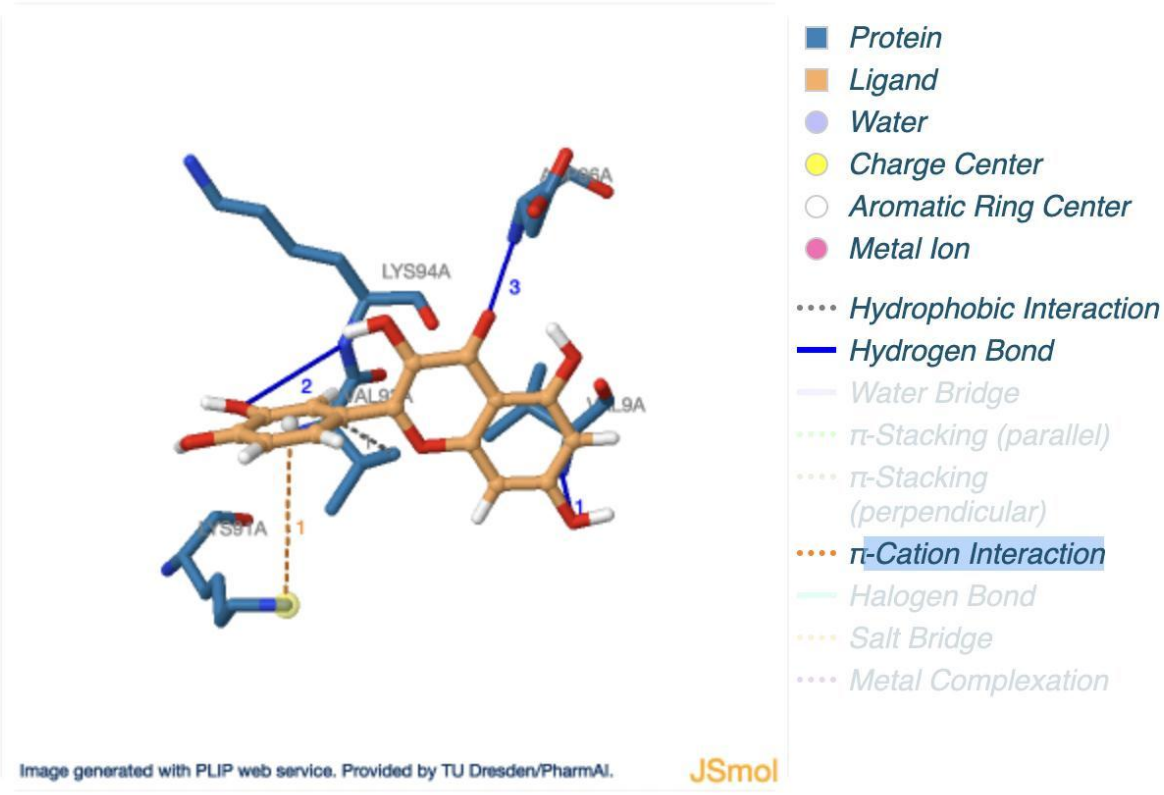
Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	35A	ILE	2.79	3.39	119.41	✔	✖	326 [Nam]	3 [O3]
2	37A	VAL	2.23	3.18	159.53	✔	✖	343 [Nam]	7 [O2]
3	45A	ARG	3.44	3.95	114.56	✔	✔	414 [Ng+]	9 [O2]

5-Caffeoylquinicacid

UNK (alpha-aminobutyric acid)

UNK-Z-0

Interacting chains: A



Hydrophobic Interactions ····

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	93A	VAL	3.38	17	809

Hydrogen Bonds —

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	9A	VAL	2.58	3.16	118.30	✓	×	109 [Nam]	5 [O2]
2	94A	LYS	3.03	3.89	147.32	✓	×	811 [Nam]	6 [O2]
3	96A	ASP	2.98	3.49	113.06	✓	×	834 [Nam]	4 [O2]

π-Cation Interactions ····

Index	Residue	AA	Distance	Offset	Protein charged?	Ligand Group	Ligand Atoms
1	91A	LYS	5.80	1.63	✓	Aromatic	11, 17, 19, 20, 21, 22

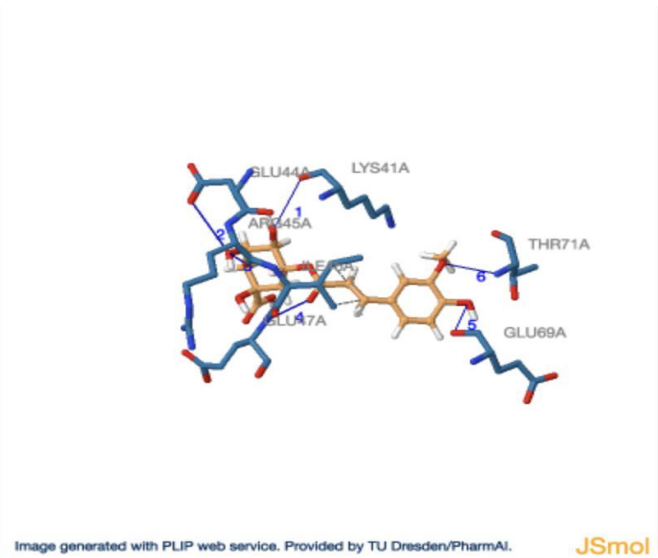
Quercetin

SMALLMOLECULE

UNK (alpha-aminobutyric acid)

UNK-Z-0

Interacting chains: A



- *Protein*
- *Ligand*
- *Water*
- *Charge Center*
- *Aromatic Ring Center*
- *Metal Ion*
- *Hydrophobic Interaction*
- *Hydrogen Bond*

Hydrophobic Interactions ····

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	46A	ILE	3.39	18	423
2	46A	ILE	3.27	19	424

Hydrogen Bonds —

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	41A	LYS	3.29	3.70	107.93	×	×	3 [O3]	380 [O2]
2	44A	GLU	2.89	3.80	164.94	✓	✓	405 [O3]	4 [O3]
3	45A	ARG	2.51	2.99	110.93	×	×	4 [O3]	410 [O2]
4	47A	GLU	2.36	3.03	125.00	✓	×	426 [Nam]	7 [O2]
5	69A	GLU	3.37	3.69	101.50	×	×	9 [O2]	625 [O2]
6	71A	THR	2.02	3.00	172.62	✓	×	642 [Nam]	8 [O2]

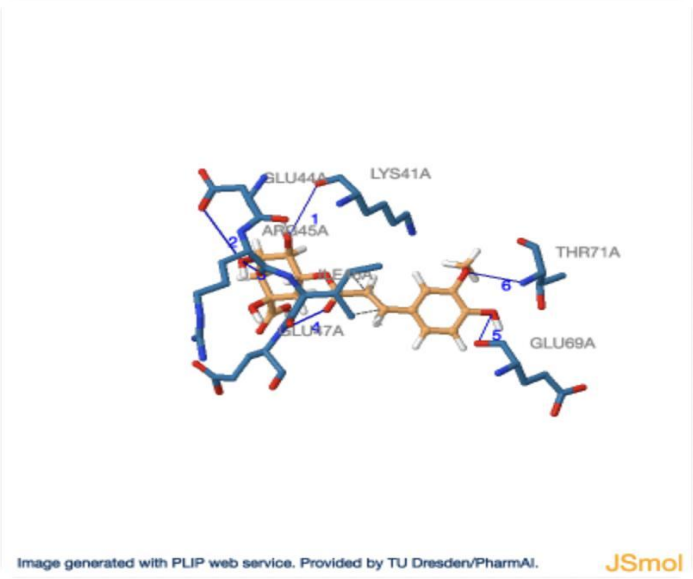
3-Feruloylquinic acid

SMALLMOLECULE

UNK (alpha-aminobutyric acid)

UNK-Z-0

Interacting chains: A



- *Protein*
- *Ligand*
- *Water*
- *Charge Center*
- *Aromatic Ring Center*
- *Metal Ion*
- *Hydrophobic Interaction*
- *Hydrogen Bond*

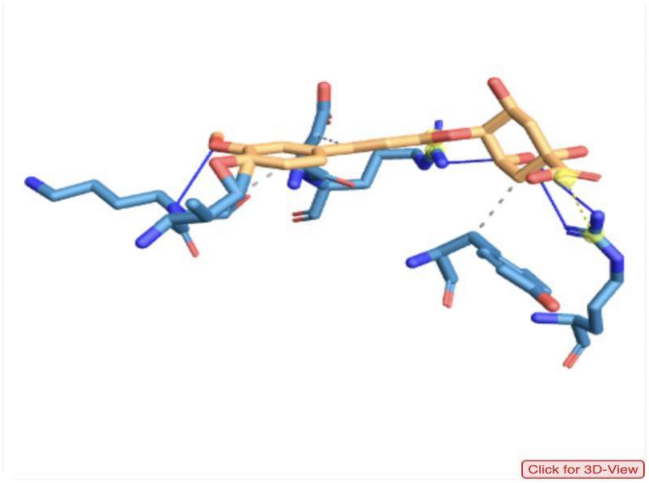
Hydrophobic Interactions ····

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	46A	ILE	3.39	18	423
2	46A	ILE	3.27	19	424

Hydrogen Bonds —

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	41A	LYS	3.29	3.70	107.93	×	×	3 [O3]	380 [O2]
2	44A	GLU	2.89	3.80	164.94	✓	✓	405 [O3]	4 [O3]
3	45A	ARG	2.51	2.99	110.93	×	×	4 [O3]	410 [O2]
4	47A	GLU	2.36	3.03	125.00	✓	×	426 [Nam]	7 [O2]
5	69A	GLU	3.37	3.69	101.50	×	×	9 [O2]	625 [O2]
6	71A	THR	2.02	3.00	172.62	✓	×	642 [Nam]	8 [O2]

4-feruloylquinic acid



- Protein
- Ligand
- Water
- Charge Center
- Aromatic Ring Center
- Metal Ion
- Hydrophobic Interaction
- Hydrogen Bond
- Water Bridge
- π-Stacking (parallel)
- π-Stacking (perpendicular)
- π-Cation Interaction
- Halogen Bond
- Salt Bridge

Hydrophobic Interactions ····

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	10A	TYR	3.25	12	134
2	93A	VAL	2.17	24	823
3	96A	ASP	3.99	19	852

Hydrogen Bonds —

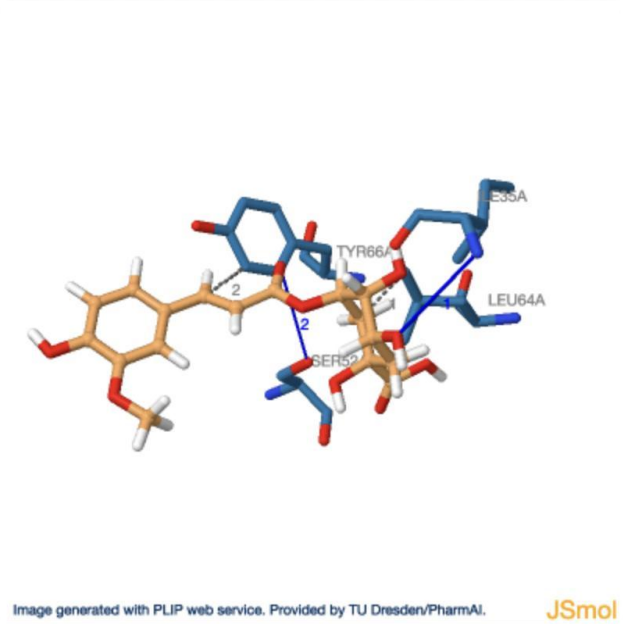
Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	12A	ARG	3.03	3.89	146.99	✓	✓	158 [Ng+]	3 [O3]
2	12A	ARG	2.68	3.62	161.03	✓	✓	157 [Ng+]	3 [O3]
3	94A	LYS	2.71	3.15	107.37	✓	×	825 [Nam]	8 [O2]
4	97A	ARG	3.22	3.89	127.19	✓	✓	866 [Ng+]	3 [O3]

Salt Bridges ····

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	12A	ARG	5.08	✓	Carboxylate	5, 6
2	97A	ARG	4.61	✓	Carboxylate	1, 7

5-Feruloylquinic acid

Interacting chains: A



- *Protein*
- *Ligand*
- *Water*
- *Charge Center*
- *Aromatic Ring Center*
- *Metal Ion*

- *Hydrophobic Interaction*
- *Hydrogen Bond*
- *Water Bridge*

Hydrophobic Interactions ····

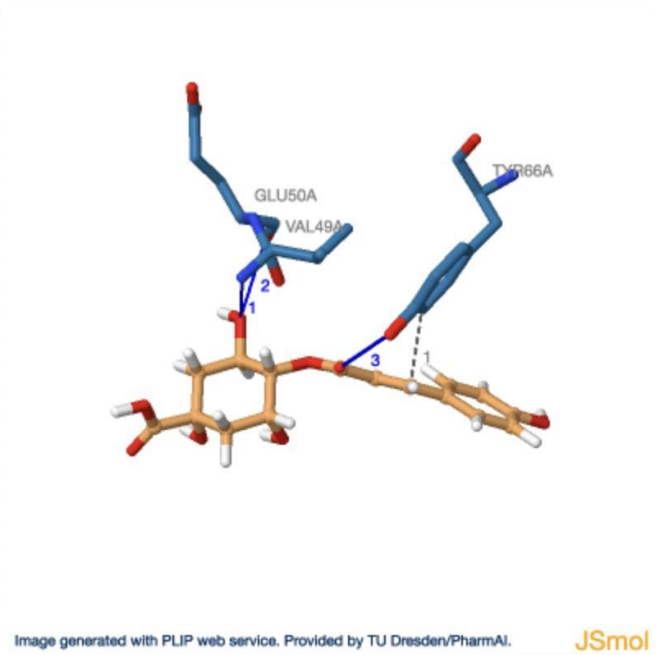
Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	64A	LEU	3.08	12	582
2	66A	TYR	3.36	19	599

Hydrogen Bonds —

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	35A	ILE	3.25	4.00	134.30	✓	×	329 [Nam]	4 [O3]
2	52A	SER	3.40	3.96	119.11	✓	✓	475 [O3]	7 [O2]

4-p-Coumaroylquinic acid

Interacting chains: A



- *Protein*
- *Ligand*
- *Water*
- *Charge Center*
- *Aromatic Ring Center*
- *Metal Ion*
- *Hydrophobic Interaction*
- *Hydrogen Bond*

Hydrophobic Interactions ····

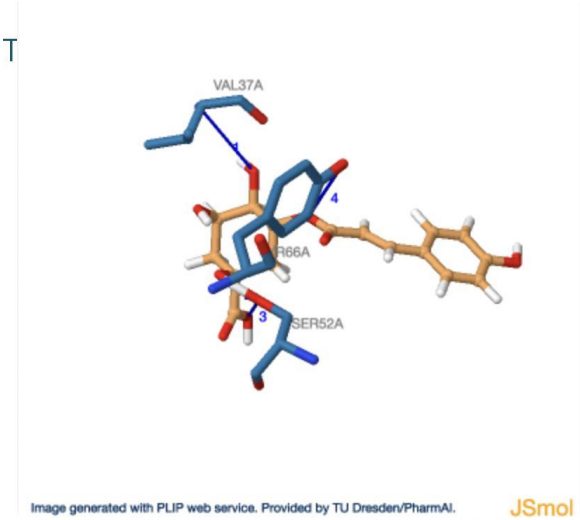
Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	66A	TYR	2.86	18	595

Hydrogen Bonds —

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	49A	VAL	3.39	3.82	108.34	✓	×	440 [Nam]	3 [O3]
2	50A	GLU	3.64	3.99	103.99	×	×	3 [O3]	450 [O2]
3	66A	TYR	1.63	2.49	150.83	✓	✓	598 [O3]	7 [O2]

5-p-Coumaroylquinic acid

T



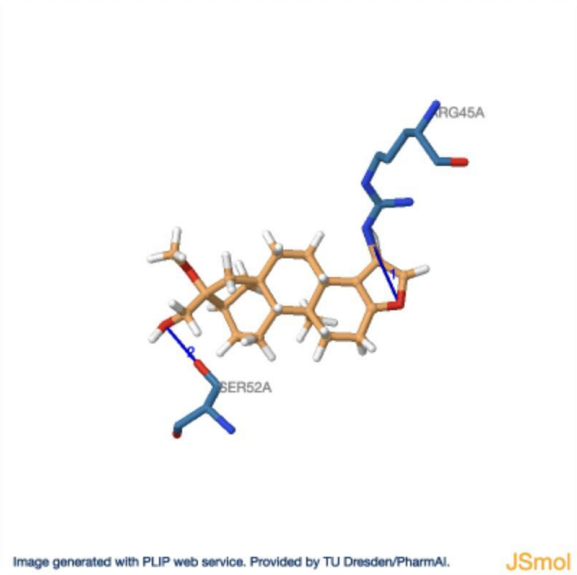
- *Protein*
- *Ligand*
- *Water*
- *Charge Center*
- *Aromatic Ring Center*
- *Metal Ion*
- *Hydrophobic Interaction*
- *Hydrogen Bond*

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	37A	VAL	2.73	3.67	161.60	✓	×	342 [Nam]	3 [O3]
2	52A	SER	1.12	1.95	137.71	×	✓	2 [O3]	471 [O3]
3	52A	SER	3.19	3.64	110.10	✓	✓	471 [O3]	5 [O.co2]
4	66A	TYR	3.20	3.85	127.88	✓	✓	598 [O3]	1 [O2]

16-methylcafestol

Interacting chains: A



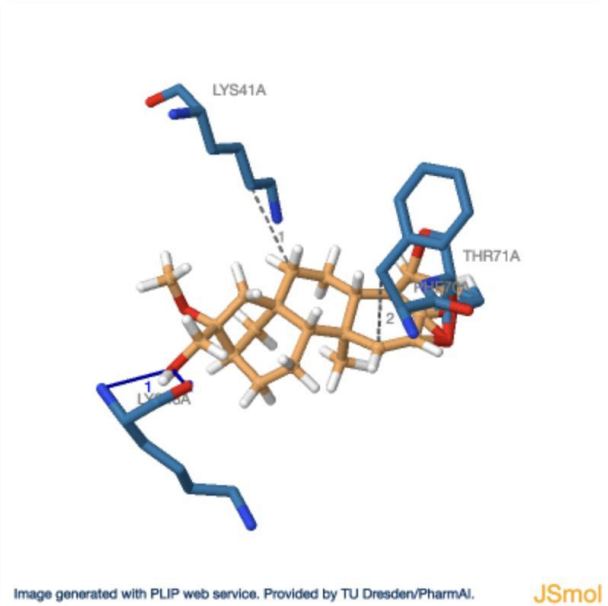
- *Protein*
- *Ligand*
- *Water*
- *Charge Center*
- *Aromatic Ring Center*
- *Metal Ion*
- *Hydrophobic Interaction*
- *Hydrogen Bond*

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	45A	ARG	3.05	3.86	140.01	✓	✓	425 [Ng+]	3 [O2]
2	52A	SER	2.87	3.39	114.71	✓	✓	483 [O3]	2 [O3]

16-Methylkahweol

Interacting chains: A



- *Protein*
- *Ligand*
- *Water*
- *Charge Center*
- *Aromatic Ring Center*
- *Metal Ion*

···· *Hydrophobic Interaction*

— *Hydrogen Bond*

Hydrophobic Interactions ····

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	41A	LYS	3.47	11	389
2	70A	PHE	3.93	18	641
3	71A	THR	2.75	22	653

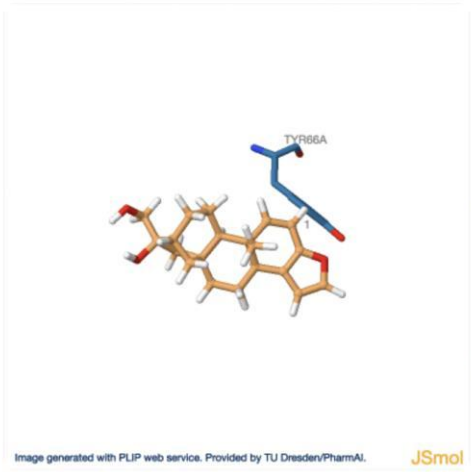
Hydrogen Bonds —

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	48A	LYS	2.98	3.84	146.84	✓	×	441 [Nam]	2 [O3]
2	48A	LYS	3.25	4.05	140.60	×	×	2 [O3]	444 [O2]

Kahweol

UNK (alpha-aminobutyric acid)
UNK-Z-0

Interacting chains: A



- Protein
- Ligand
- Water
- Charge Center
- Aromatic Ring Center
- Metal Ion
- Hydrophobic Interaction
- Hydrogen Bond
- Water Bridge
- π-Stacking (parallel)
- π-Stacking (perpendicular)
- π-Cation Interaction
- Halogen Bond
- Salt Bridge
- Metal Complexation

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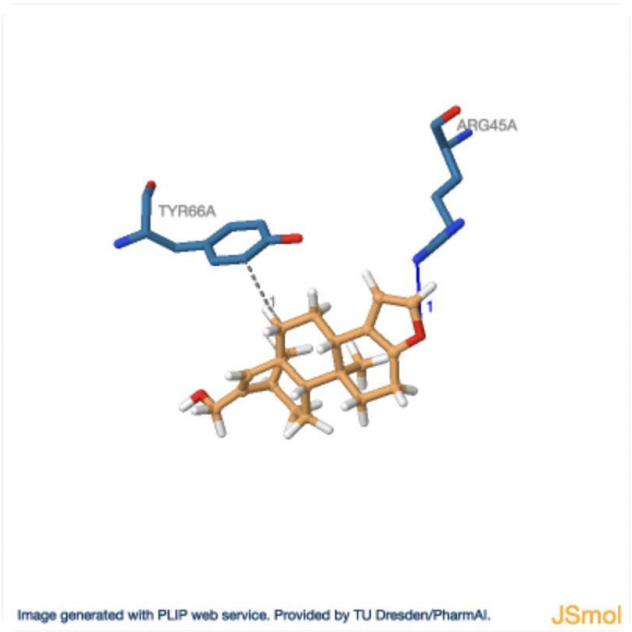
Download visualization as image (.png)

Hydrophobic Interactions ····

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	66A	TYR	2.51	20	602

Dehydrocafestol



- *Protein*
- *Ligand*
- *Water*
- *Charge Center*
- *Aromatic Ring Center*
- *Metal Ion*
- *Hydrophobic Interaction*
- *Hydrogen Bond*

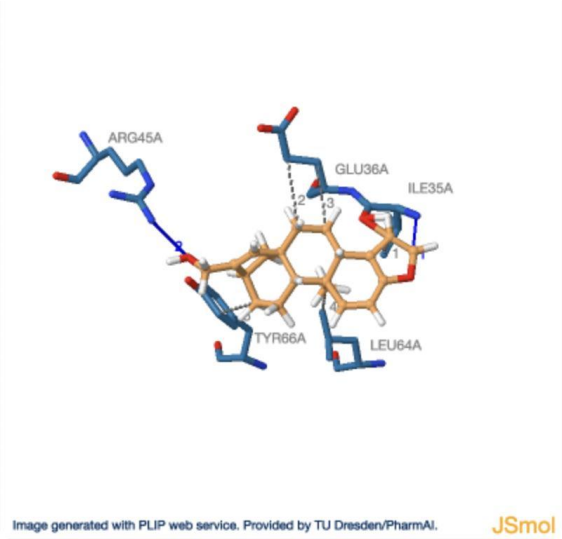
Hydrophobic Interactions ····

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	66A	TYR	3.39	8	601

Hydrogen Bonds —

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	45A	ARG	3.27	3.66	105.01	✓	✓	419 [Ng+]	1 [O2]

Dehydro Kahweol



- *Protein*
- *Ligand*
- *Water*
- *Charge Center*
- *Aromatic Ring Center*
- *Metal Ion*
- *Hydrophobic Interaction*
- *Hydrogen Bond*

Hydrophobic Interactions ····

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	35A	ILE	2.82	21	335
2	36A	GLU	3.85	8	342
3	36A	GLU	3.68	11	341
4	64A	LEU	3.90	15	582
5	66A	TYR	3.14	12	599

Hydrogen Bonds —

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	35A	ILE	2.71	3.31	119.48	✓	×	329 [Nam]	1 [O2]
2	45A	ARG	1.99	2.76	133.62	✓	✓	417 [Ng+]	2 [O3]