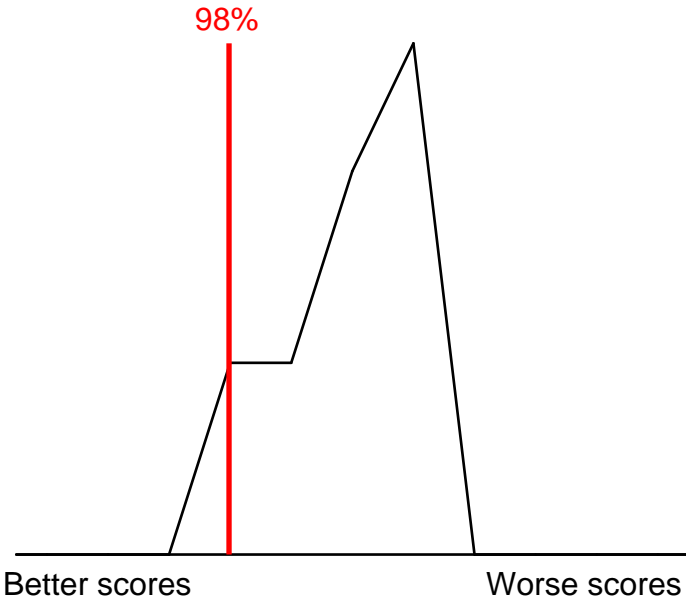
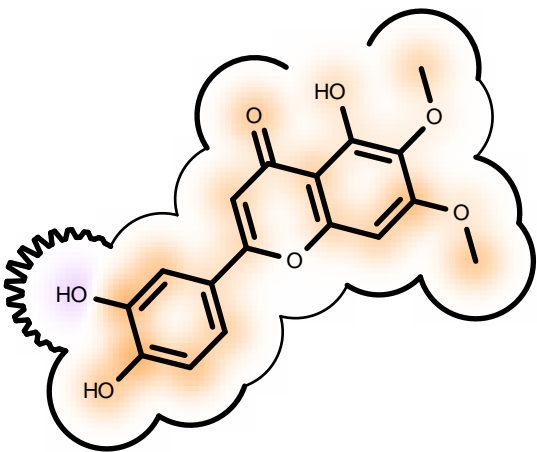


Molecule Name omega_1_4
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 1

Total Score -10.70

Score compared to other molecules



Protein Contact

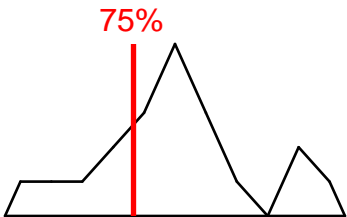
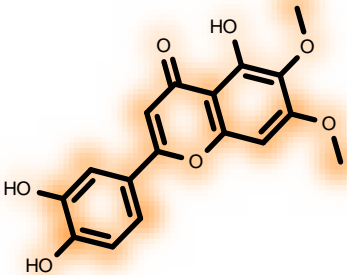


Protein Cavity

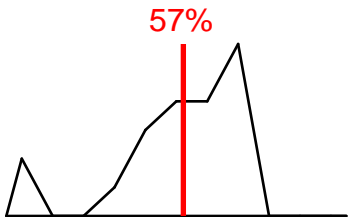
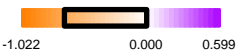
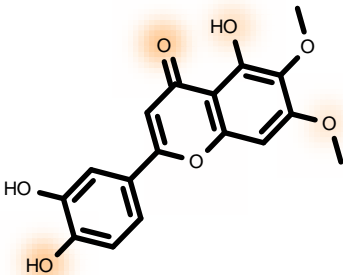
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

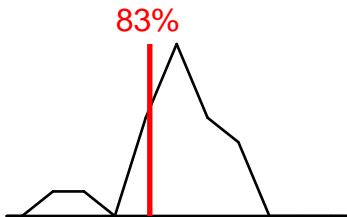
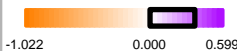
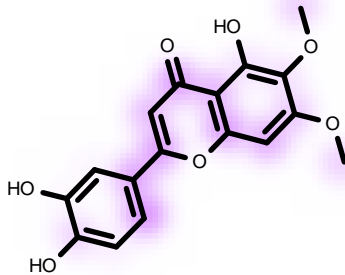
Shape -14.75



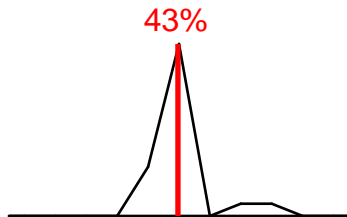
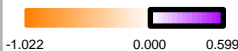
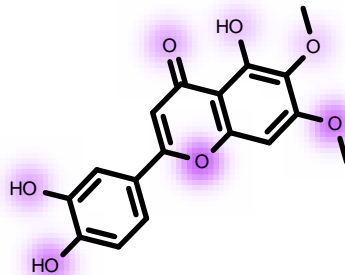
Hydrogen Bond -1.97



Protein Desolvation 3.33



Ligand Desolvation 2.69



Acceptor

Metal

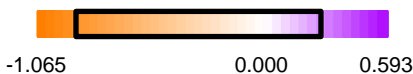
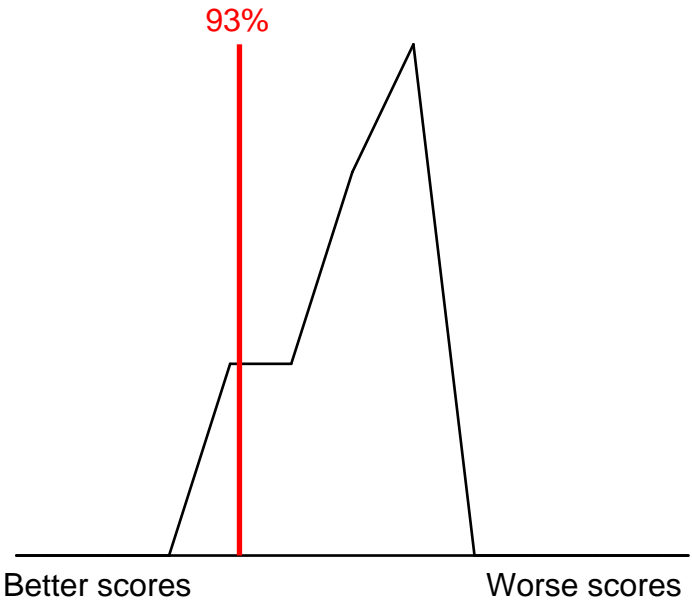
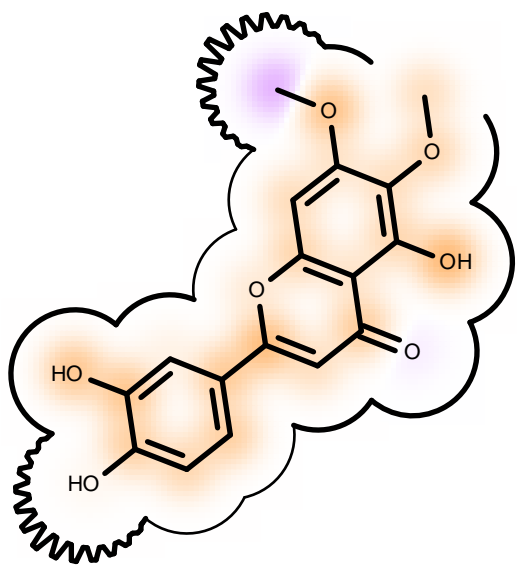
Donor

Contact

Molecule Name omega_1_10
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 2

Total Score -10.65

Score compared to other molecules

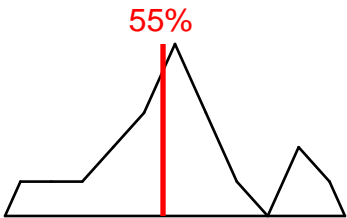
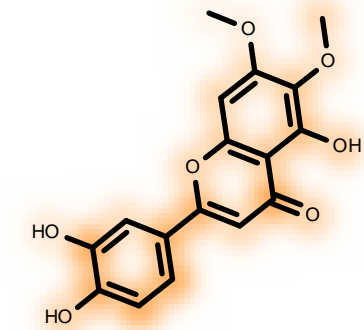


Protein Contact Protein Cavity

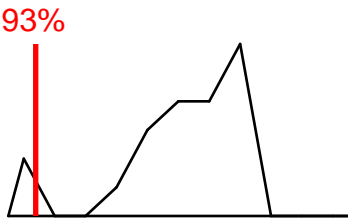
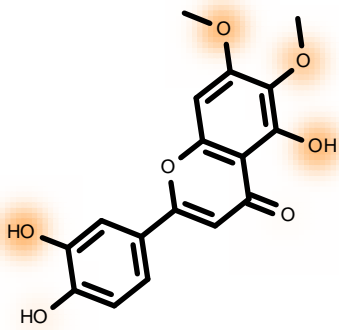
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

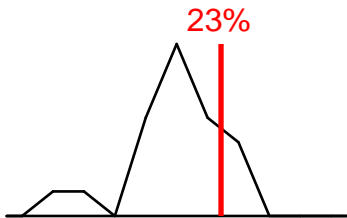
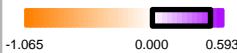
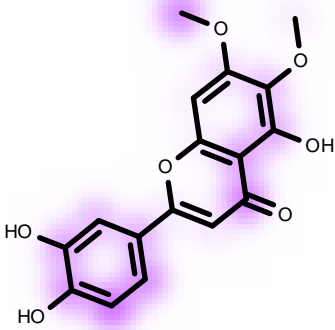
Shape -14.44



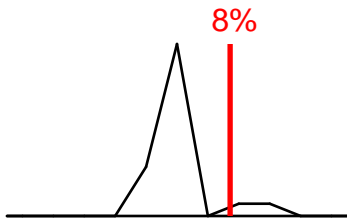
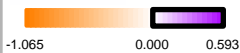
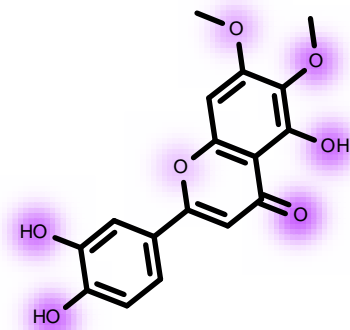
Hydrogen Bond -3.58



Protein Desolvation 4.10



Ligand Desolvation 3.27

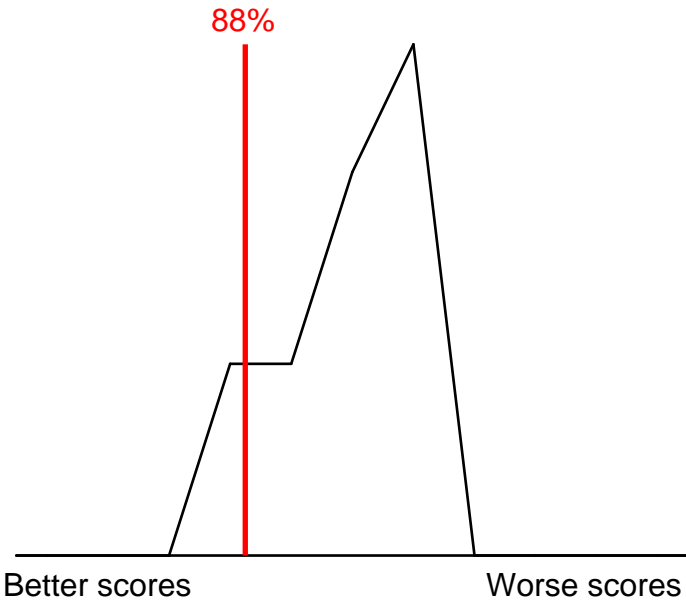
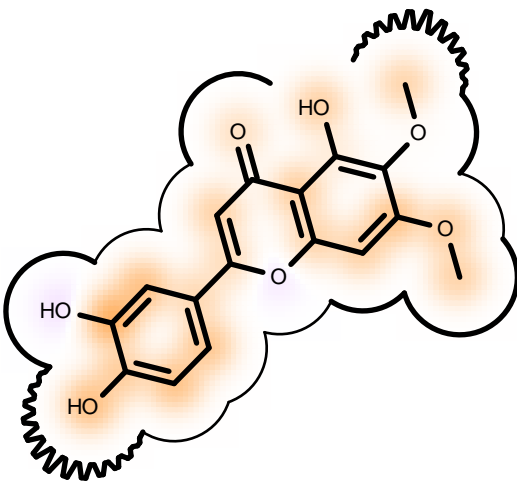


Acceptor **Donor**
Metal Contact

Molecule Name omega_1_4
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 3

Total Score -10.61

Score compared to other molecules

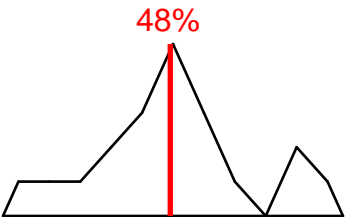
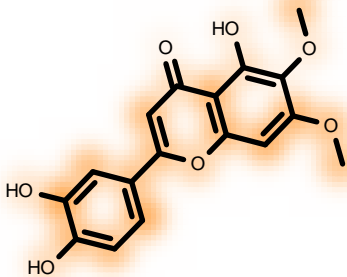


Protein Contact Protein Cavity

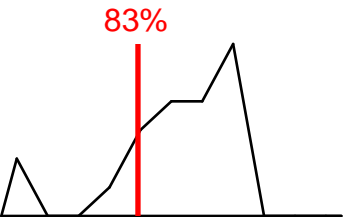
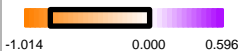
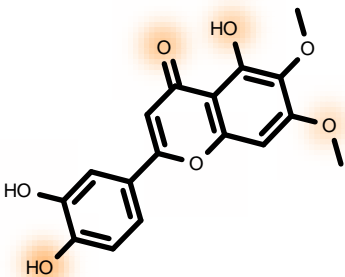
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

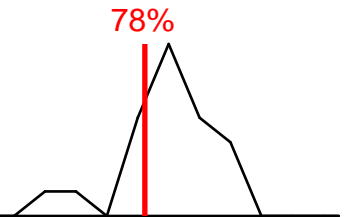
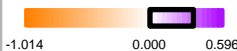
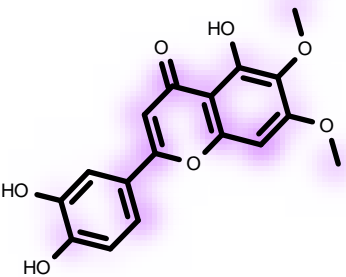
Shape -14.34



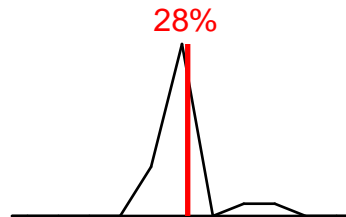
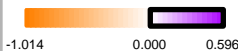
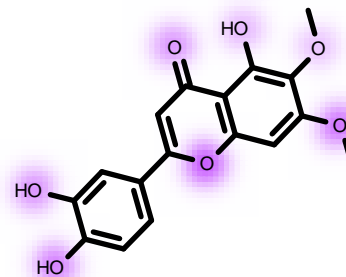
Hydrogen Bond -2.40



Protein Desolvation 3.36



Ligand Desolvation 2.76

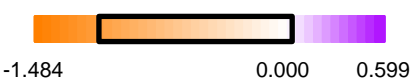
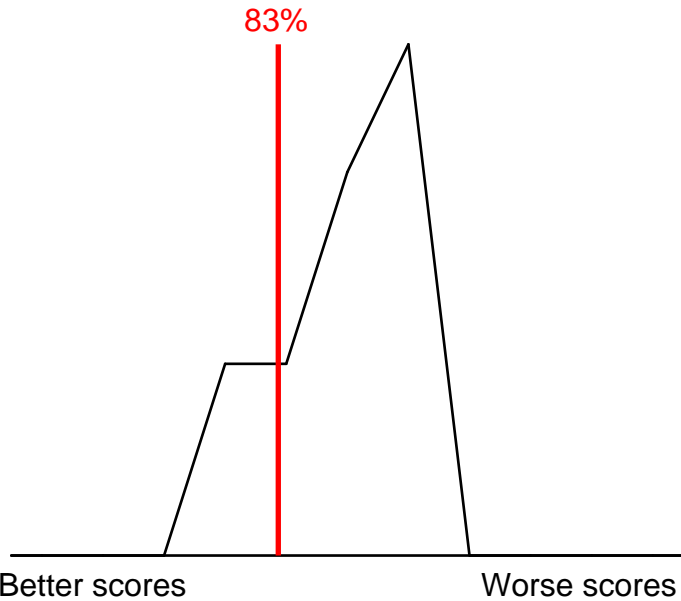
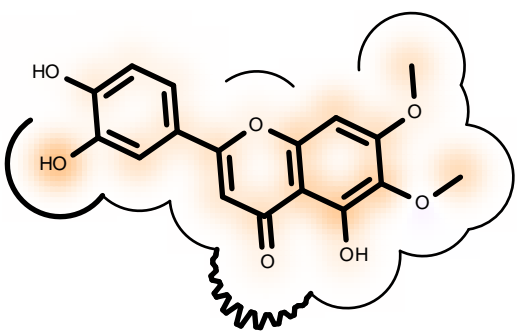


Acceptor Donor
Metal Contact

Molecule Name omega_1_13
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 4

Total Score -10.41

Score compared to other molecules

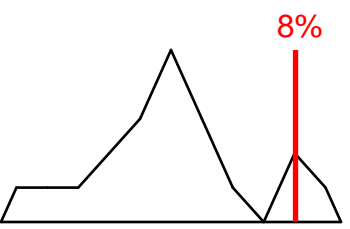
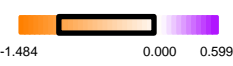
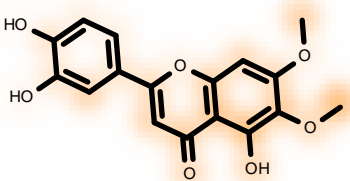


Protein Contact Protein Cavity

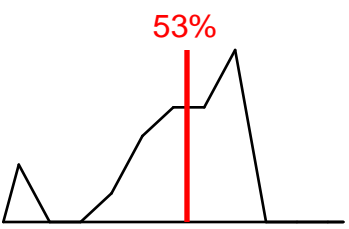
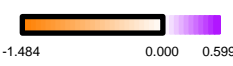
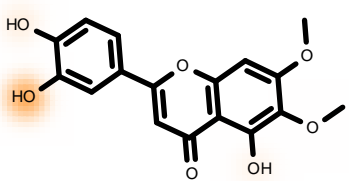
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

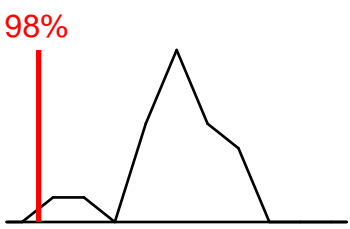
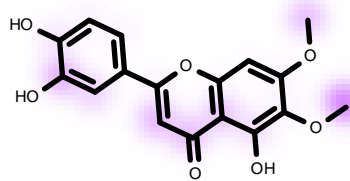
Shape -12.97



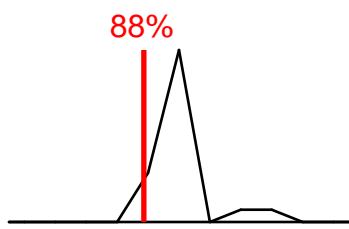
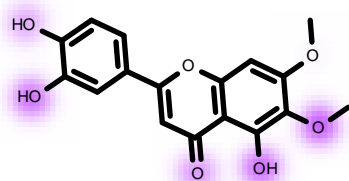
Hydrogen Bond -1.90



Protein Desolvation 2.14



Ligand Desolvation 2.32

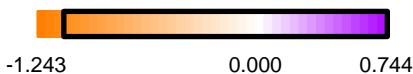
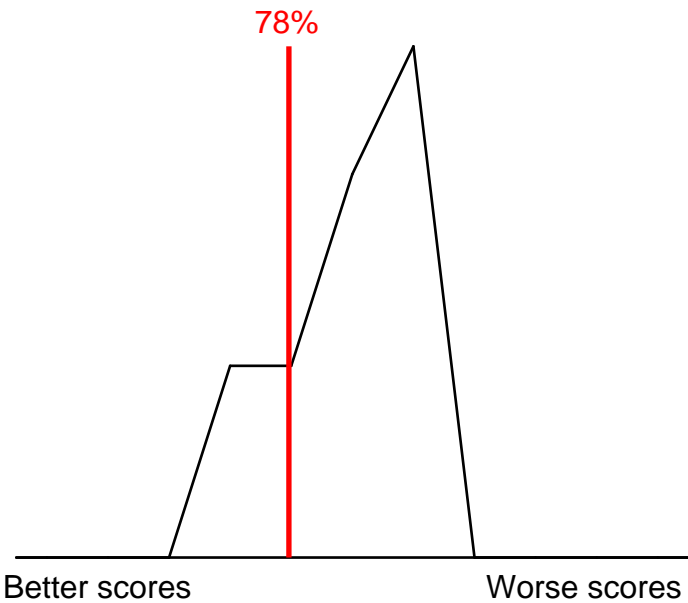
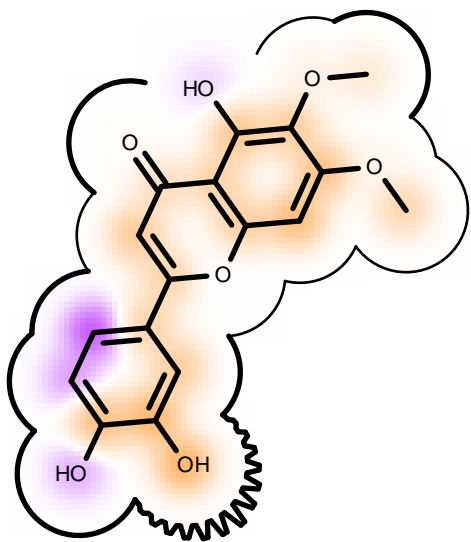


Acceptor Donor
Metal Contact

Molecule Name omega_1_1
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 5

Total Score -10.38

Score compared to other molecules

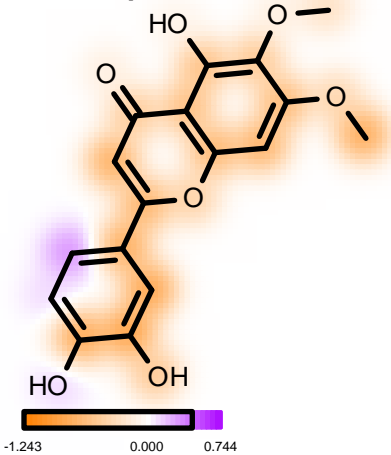


Protein Contact Protein Cavity

Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

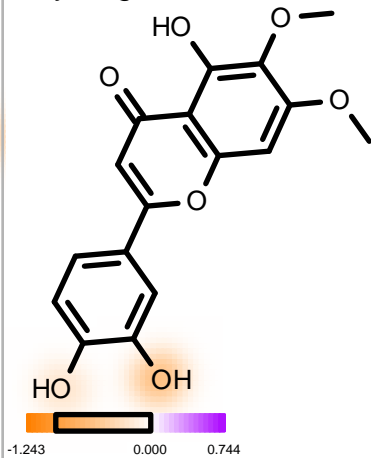
Shape -15.83



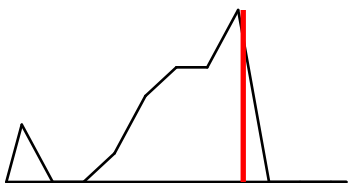
98%



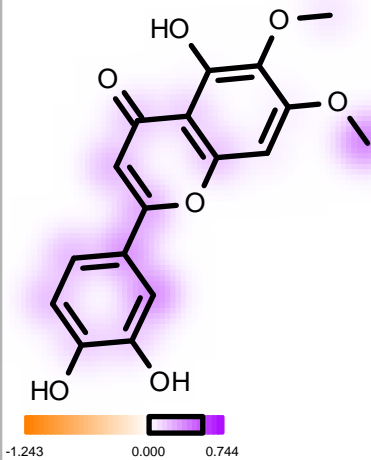
Hydrogen Bond -1.32



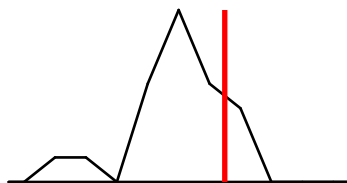
13%



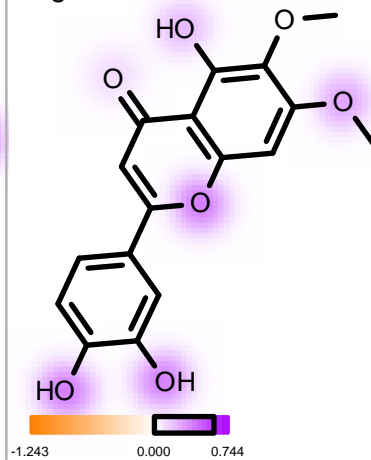
Protein Desolvation 4.11



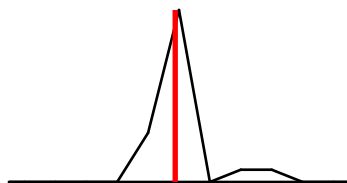
18%



Ligand Desolvation 2.66



63%

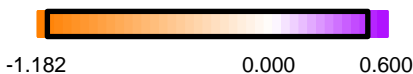
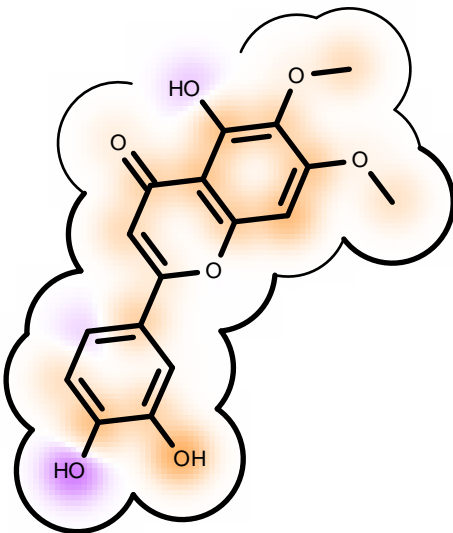


Acceptor Donor
Metal Contact

Molecule Name omega_1_1
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 6

Total Score -10.23

Score compared to other molecules



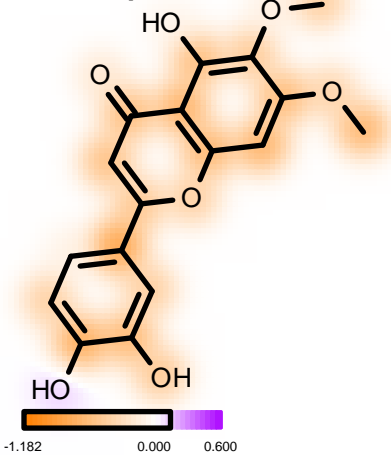
Protein Contact

Protein Cavity

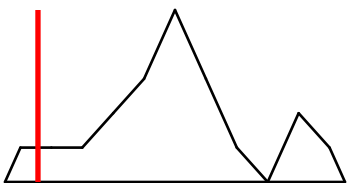
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

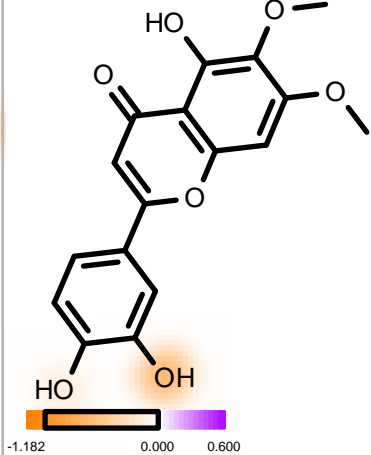
Shape -15.78



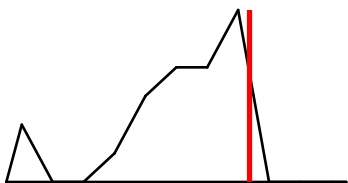
93%



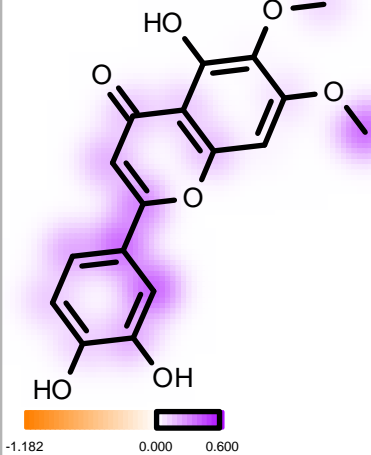
Hydrogen Bond -1.26



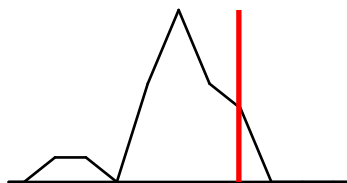
3%



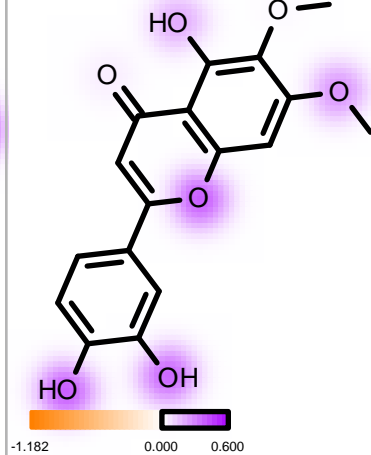
Protein Desolvation 4.27



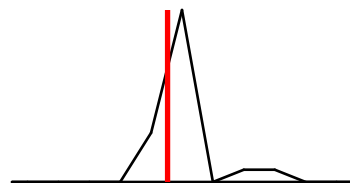
3%



Ligand Desolvation 2.55



78%



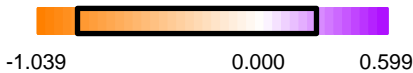
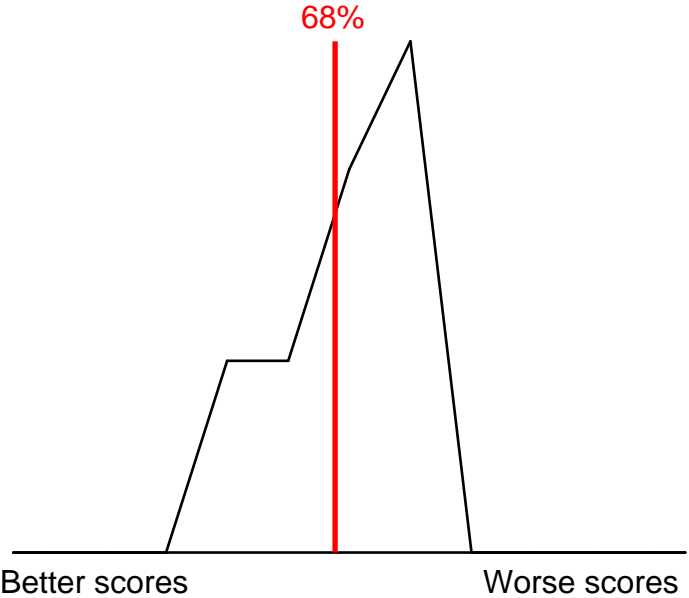
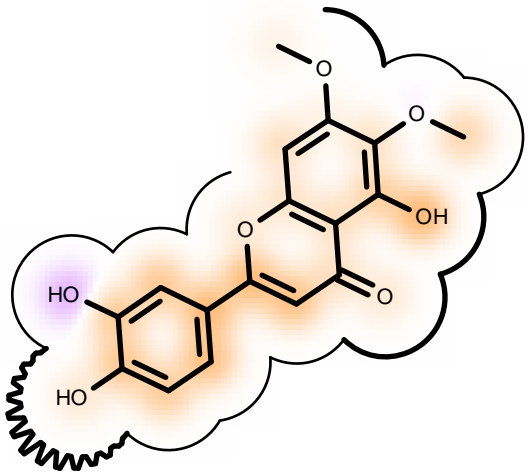
Acceptor
Metal

Donor
Contact

Molecule Name omega_1_16
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 7

Total Score -10.11

Score compared to other molecules



Protein Contact

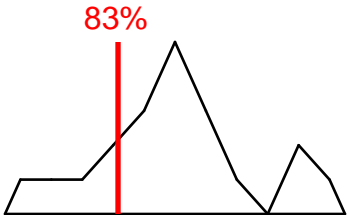
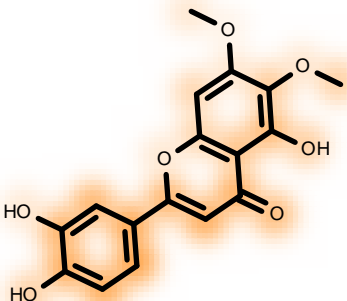


Protein Cavity

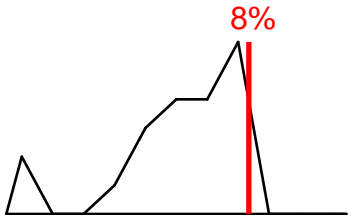
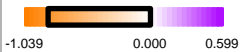
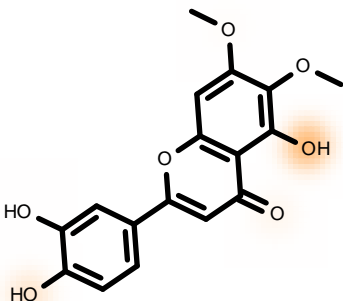
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

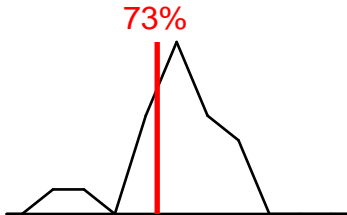
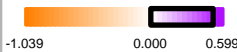
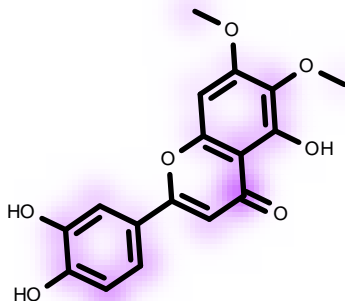
Shape -14.92



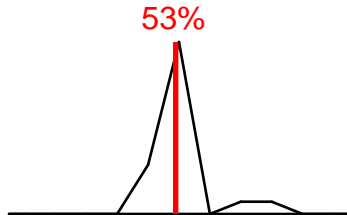
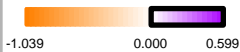
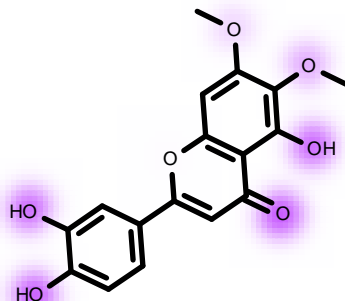
Hydrogen Bond -1.26



Protein Desolvation 3.41



Ligand Desolvation 2.67



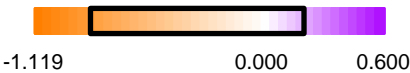
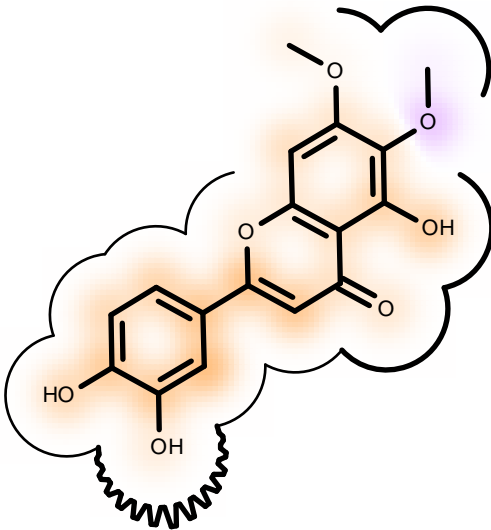
Acceptor
Metal

Donor
Contact

Molecule Name omega_1_14
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 8

Total Score -10.05

Score compared to other molecules



Protein Contact

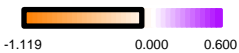
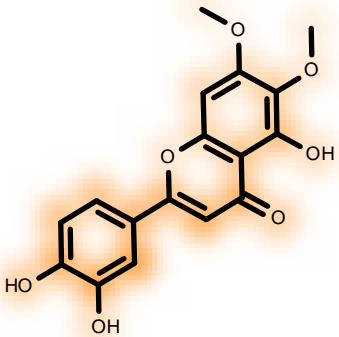


Protein Cavity

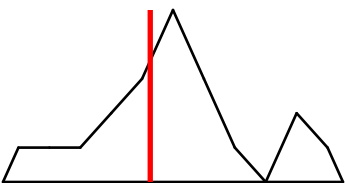
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

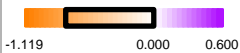
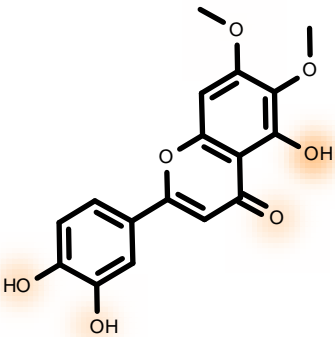
Shape -14.55



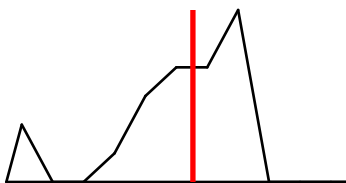
68%



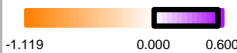
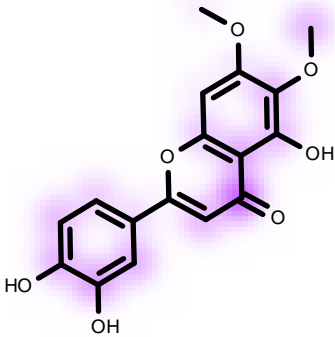
Hydrogen Bond -1.87



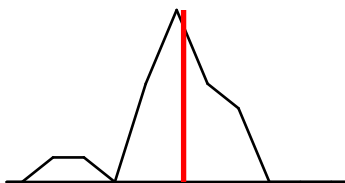
48%



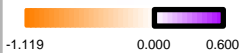
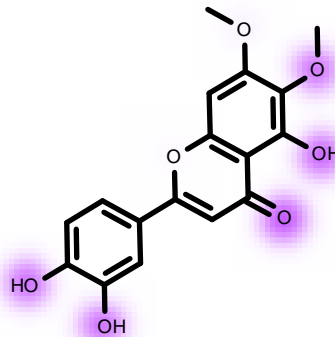
Protein Desolvation 3.69



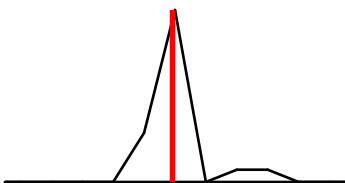
43%



Ligand Desolvation 2.67



48%



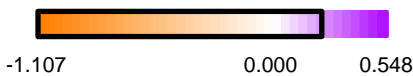
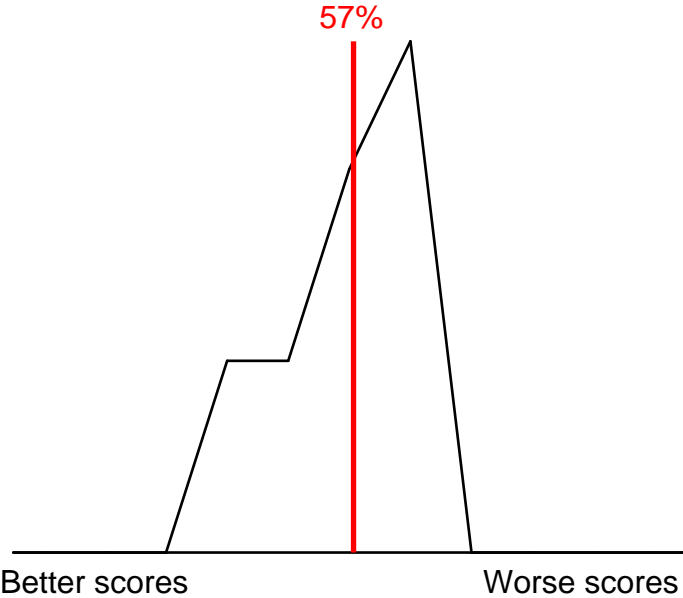
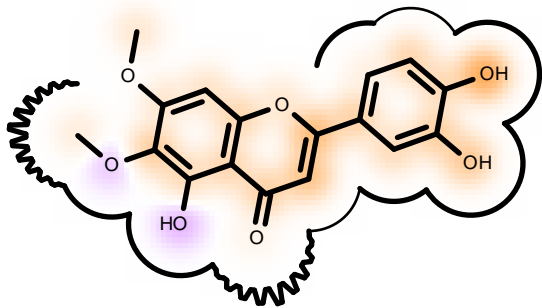
Acceptor
Metal

Donor
Contact

Molecule Name omega_1_3
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 9

Total Score -10.01

Score compared to other molecules

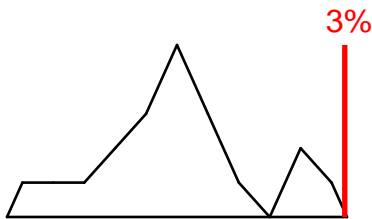
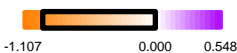
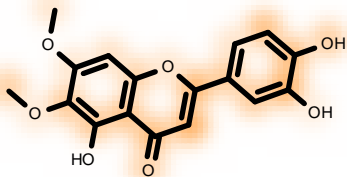


Protein Contact Protein Cavity

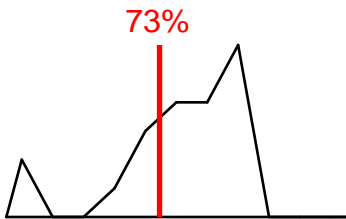
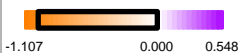
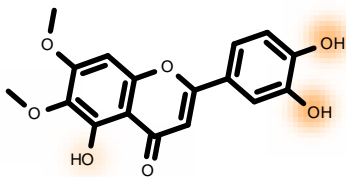
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

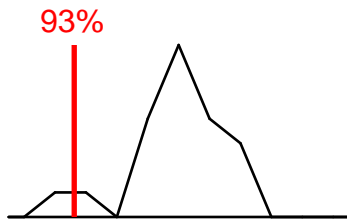
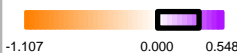
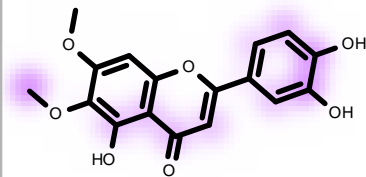
Shape -12.50



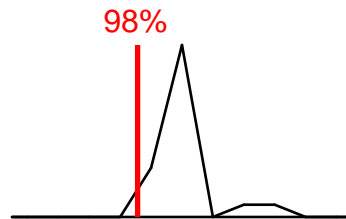
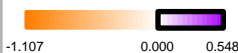
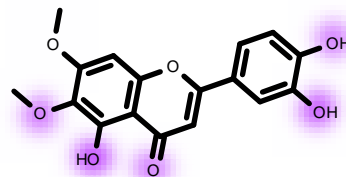
Hydrogen Bond -2.22



Protein Desolvation 2.50



Ligand Desolvation 2.22

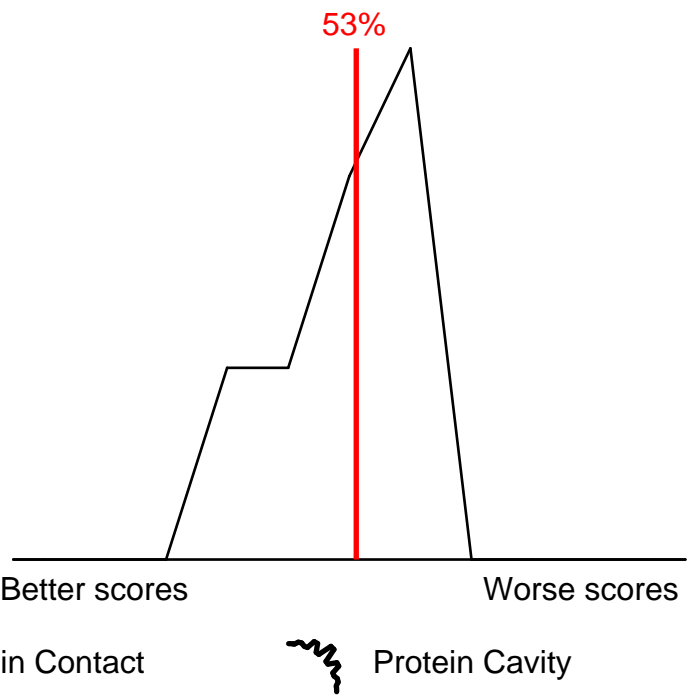
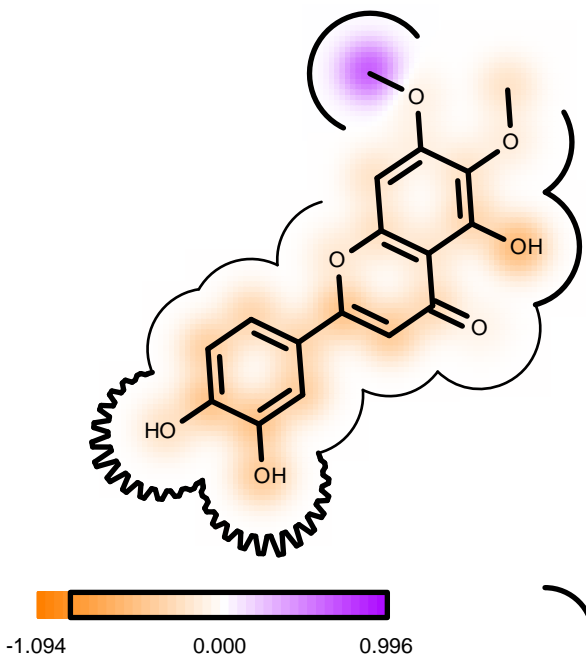


Acceptor Metal Donor Contact

Molecule Name omega_1_13
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 10

Total Score -9.99

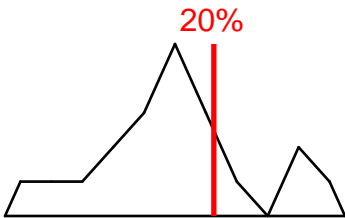
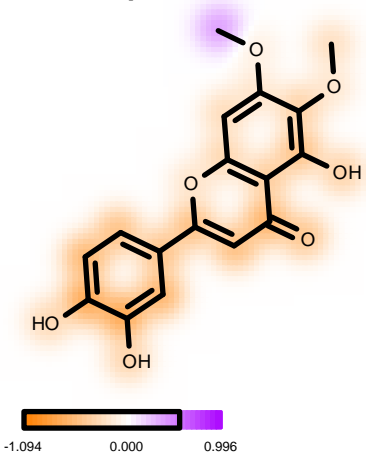
Score compared to other molecules



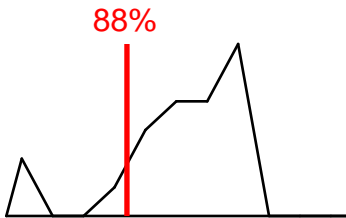
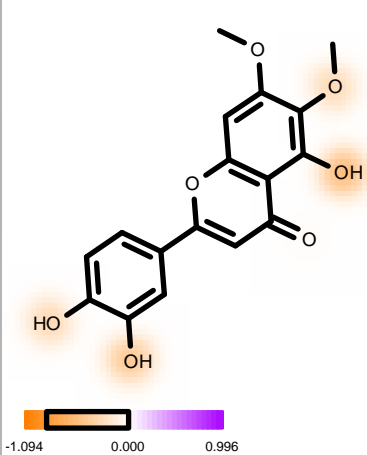
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

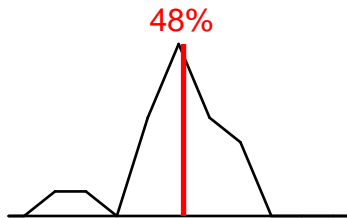
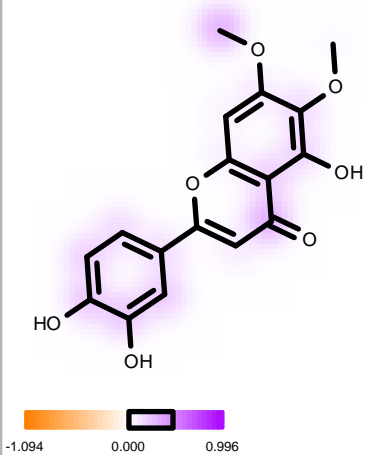
Shape -13.89



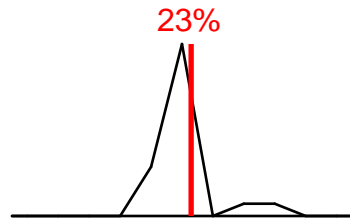
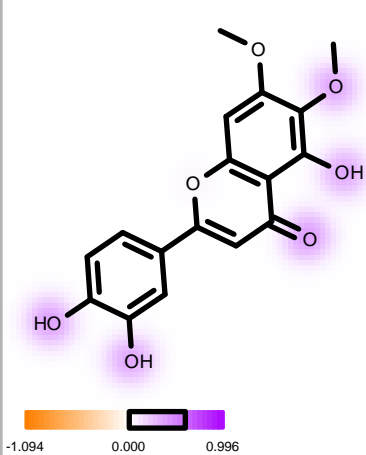
Hydrogen Bond -2.58



Protein Desolvation 3.67



Ligand Desolvation 2.80

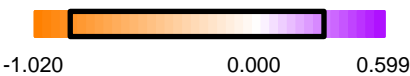
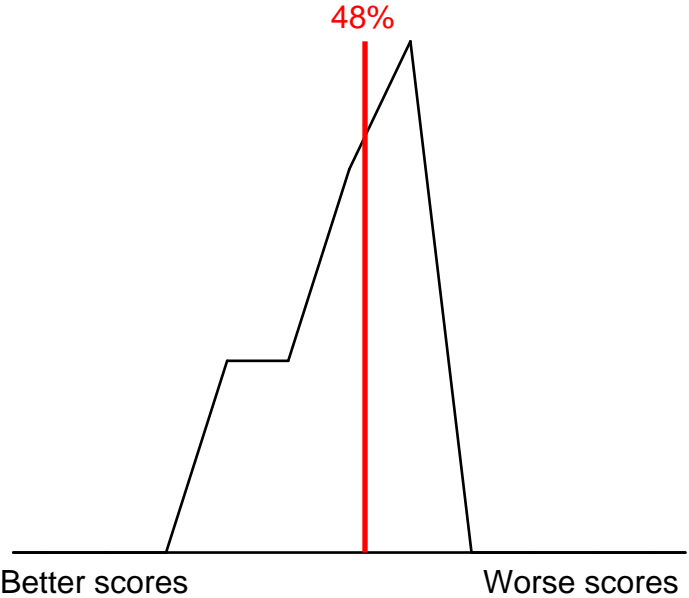
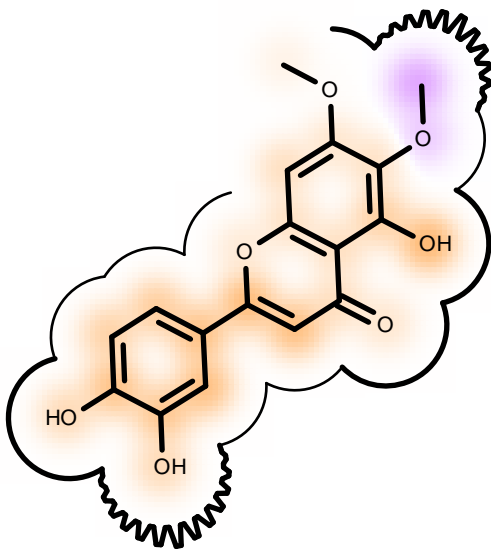


Acceptor Donor
Metal Contact

Molecule Name omega_1_14
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 11

Total Score -9.95

Score compared to other molecules



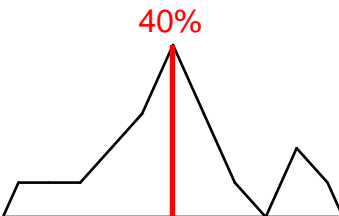
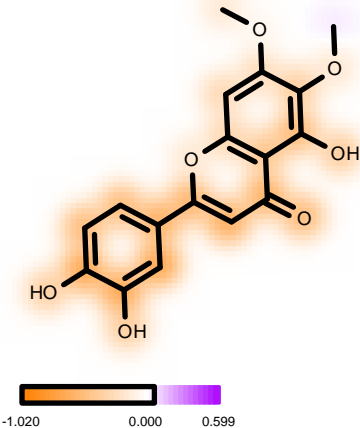
Protein Contact

Protein Cavity

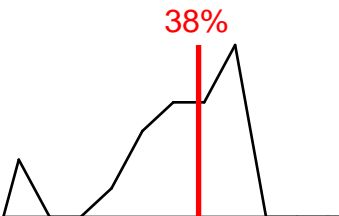
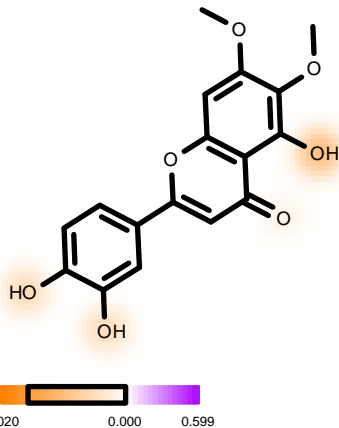
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

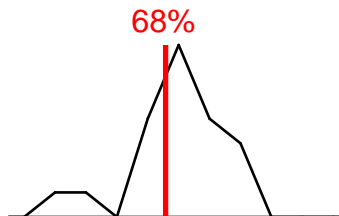
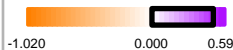
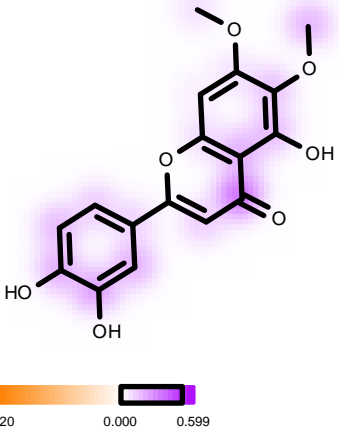
Shape -14.31



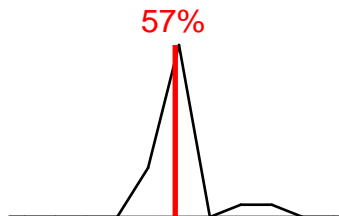
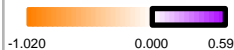
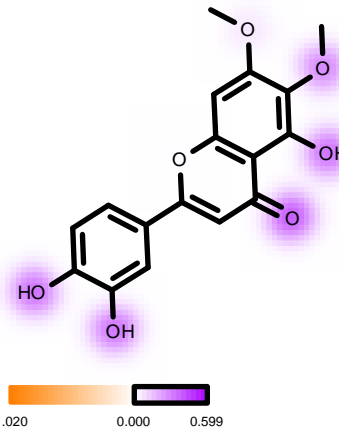
Hydrogen Bond -1.77



Protein Desolvation 3.48



Ligand Desolvation 2.66



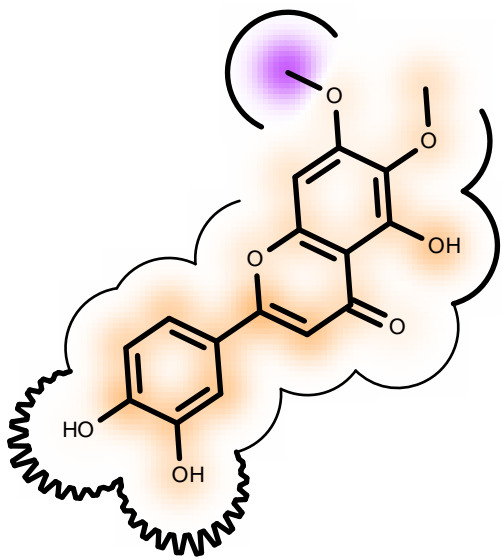
Acceptor
Metal

Donor
Contact

Molecule Name omega_1_13
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 12

Total Score -9.87

Score compared to other molecules

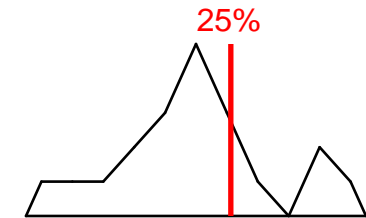
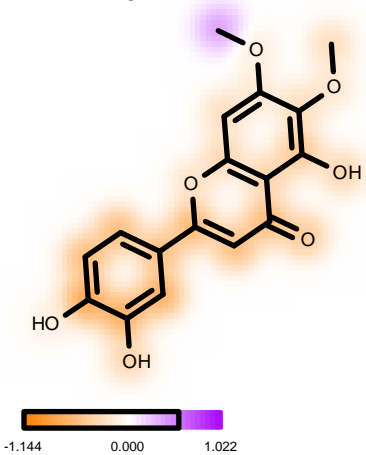


Protein Contact Protein Cavity

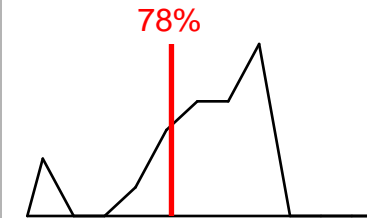
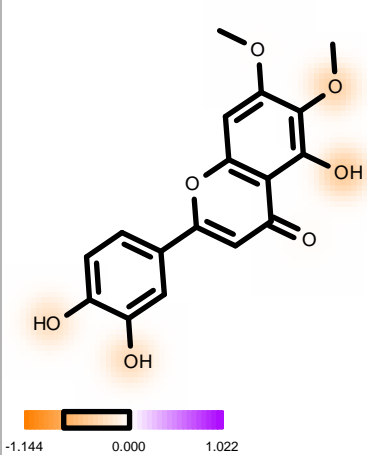
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

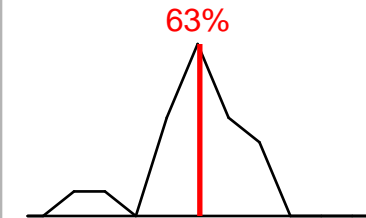
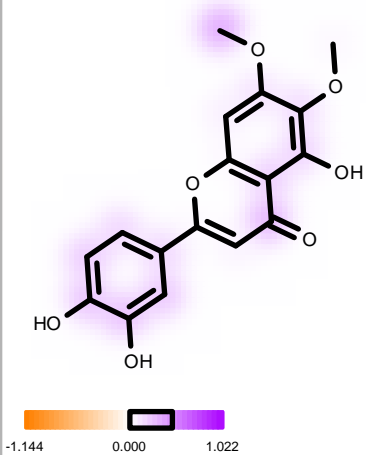
Shape -13.93



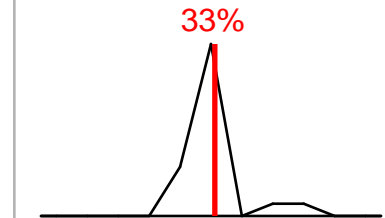
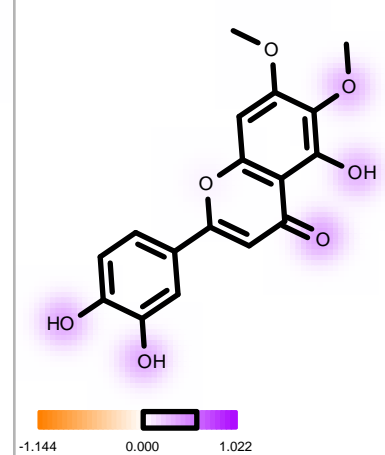
Hydrogen Bond -2.32



Protein Desolvation 3.64



Ligand Desolvation 2.74

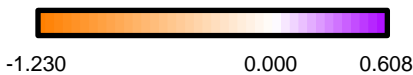
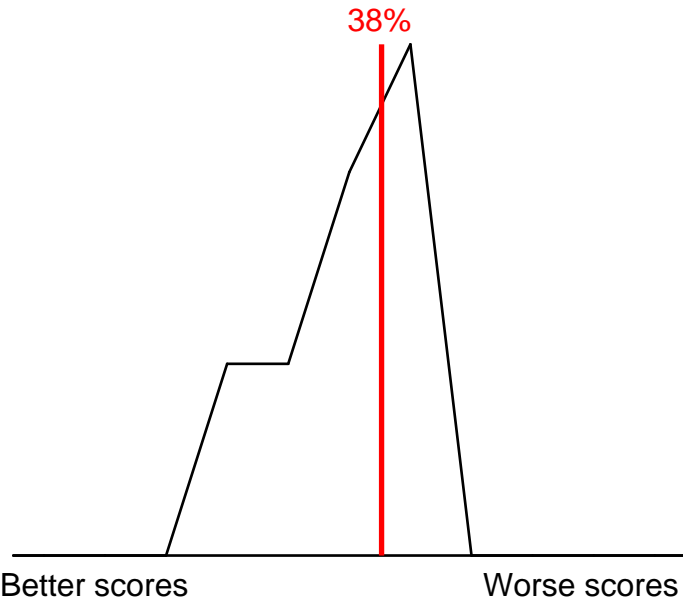
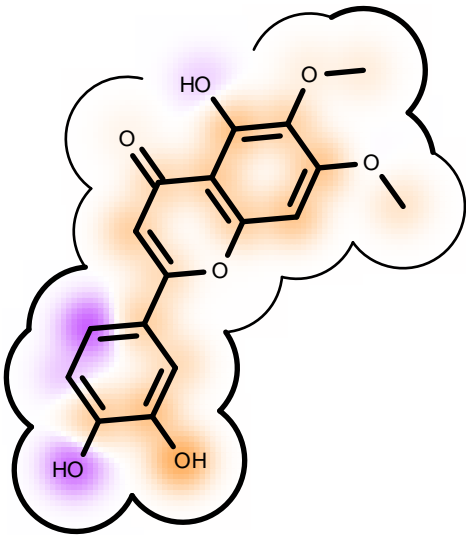


Acceptor Donor
Metal Contact

Molecule Name omega_1_1
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 13

Total Score -9.86

Score compared to other molecules



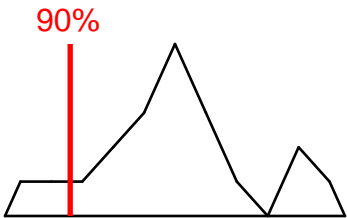
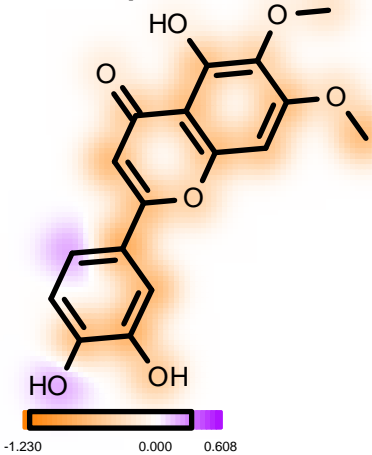
Protein Contact

Protein Cavity

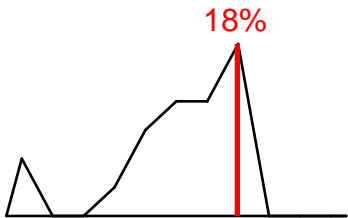
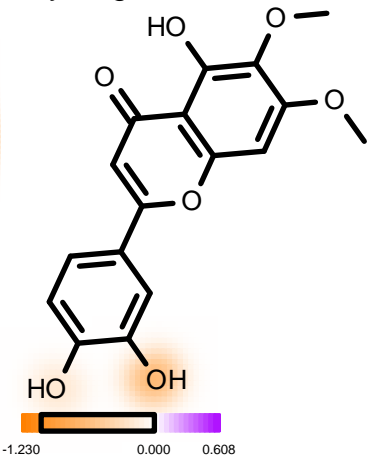
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

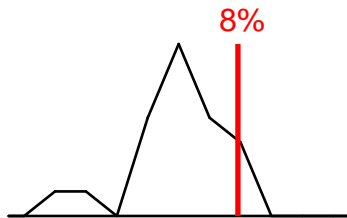
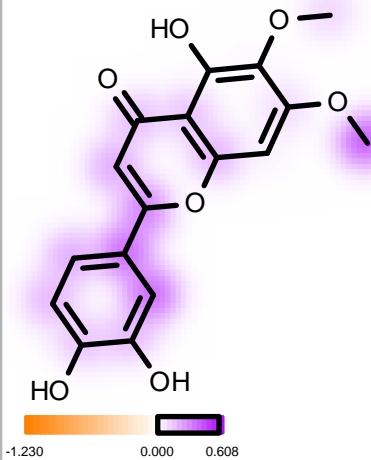
Shape -15.44



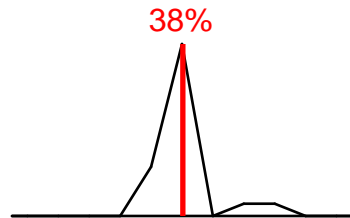
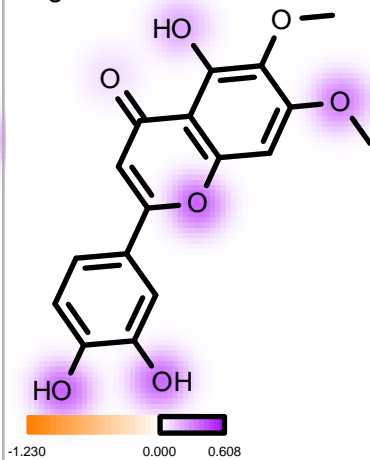
Hydrogen Bond -1.39



Protein Desolvation 4.26



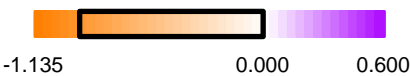
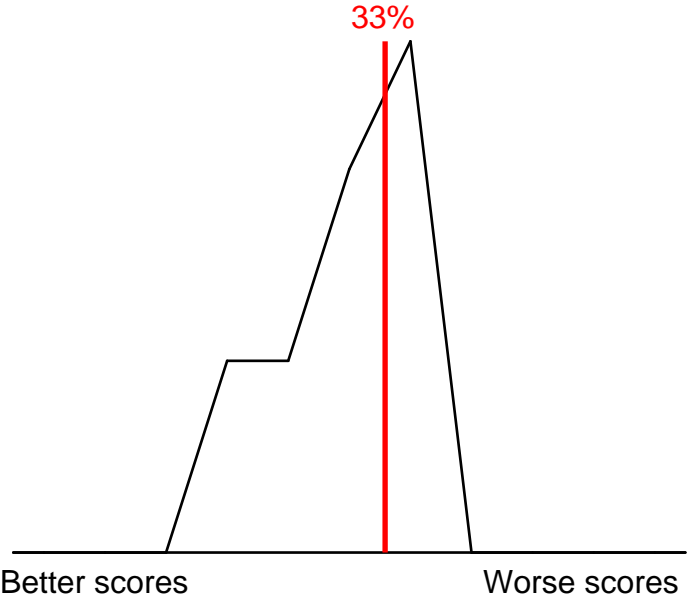
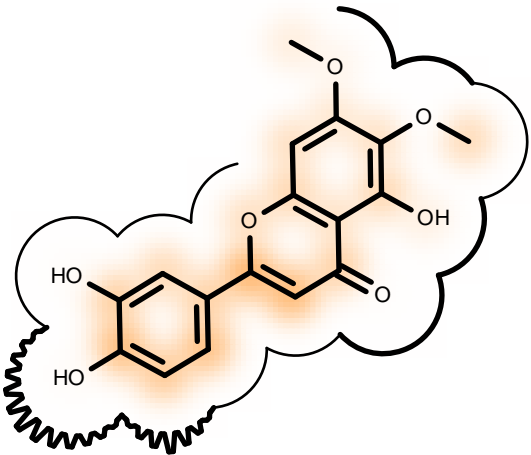
Ligand Desolvation 2.71



Acceptor Donor
Metal Contact

Molecule Name omega_1_16
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 14

Total Score -9.84 Score compared to other molecules

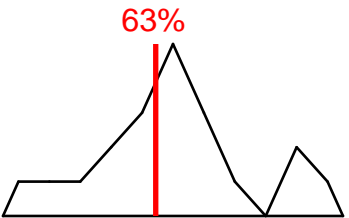
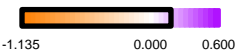
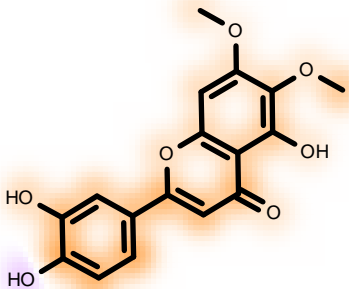


Protein Contact Protein Cavity

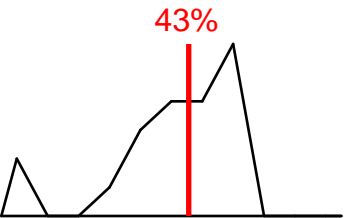
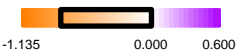
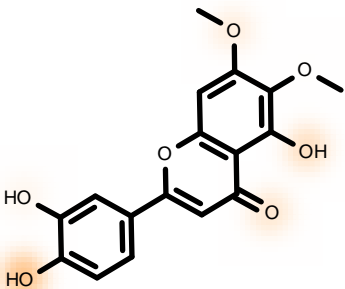
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

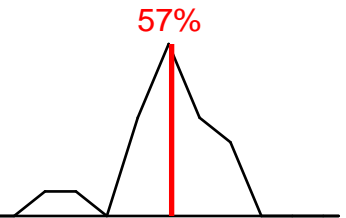
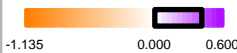
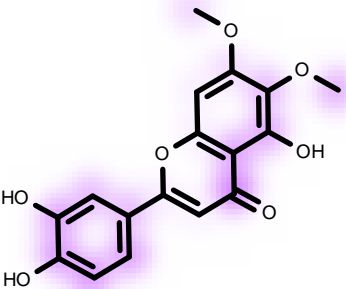
Shape -14.49



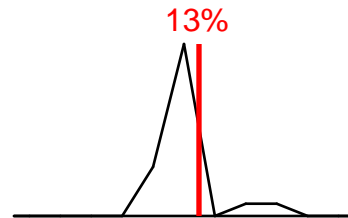
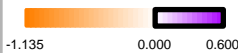
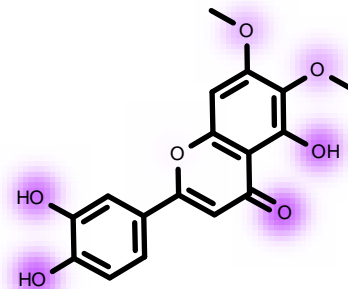
Hydrogen Bond -1.86



Protein Desolvation 3.65



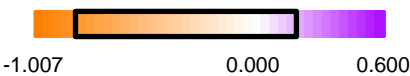
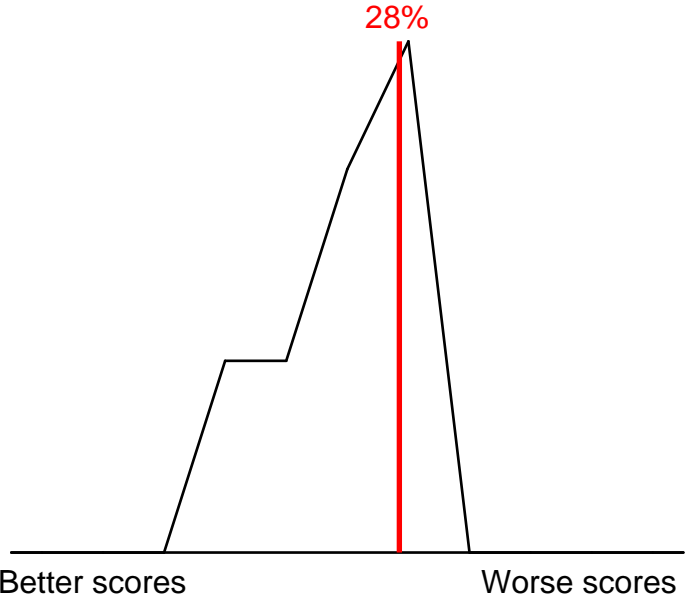
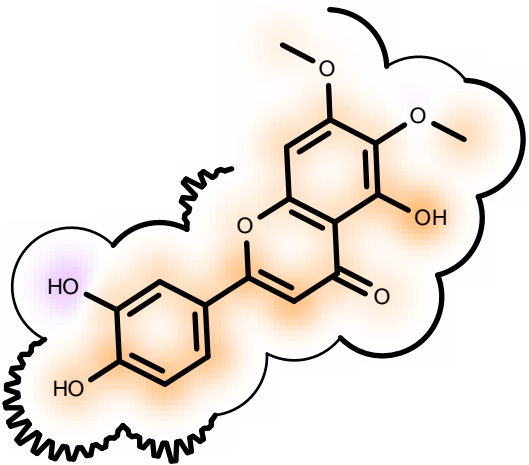
Ligand Desolvation 2.86



Acceptor Donor
Metal Contact

Molecule Name omega_1_16
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 15

Total Score -9.75 Score compared to other molecules

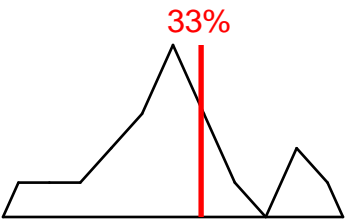
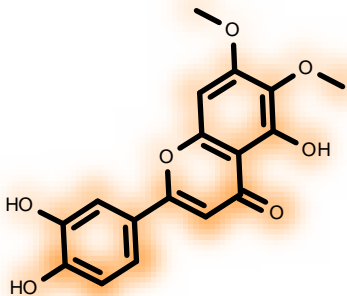


Protein Contact Protein Cavity

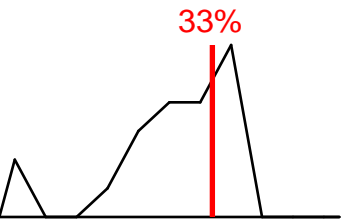
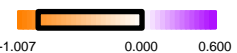
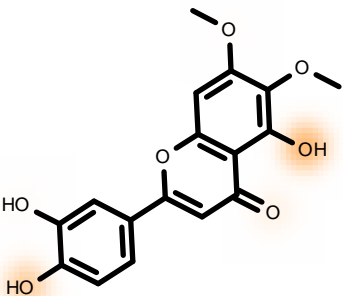
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

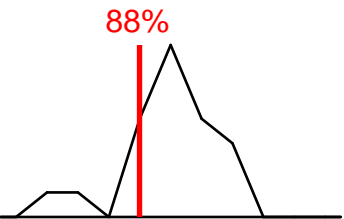
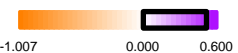
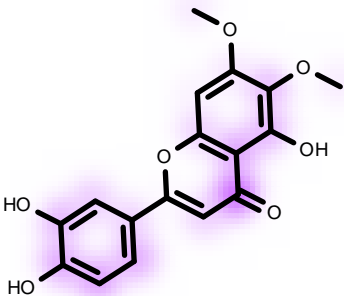
Shape -14.01



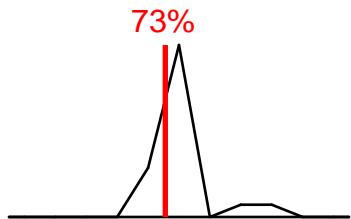
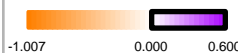
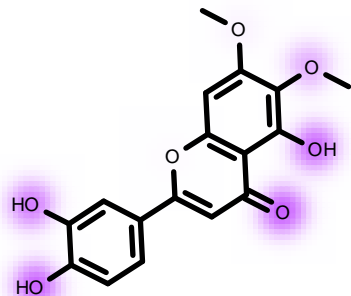
Hydrogen Bond -1.58



Protein Desolvation 3.28



Ligand Desolvation 2.55

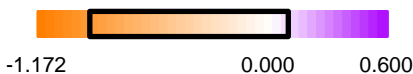
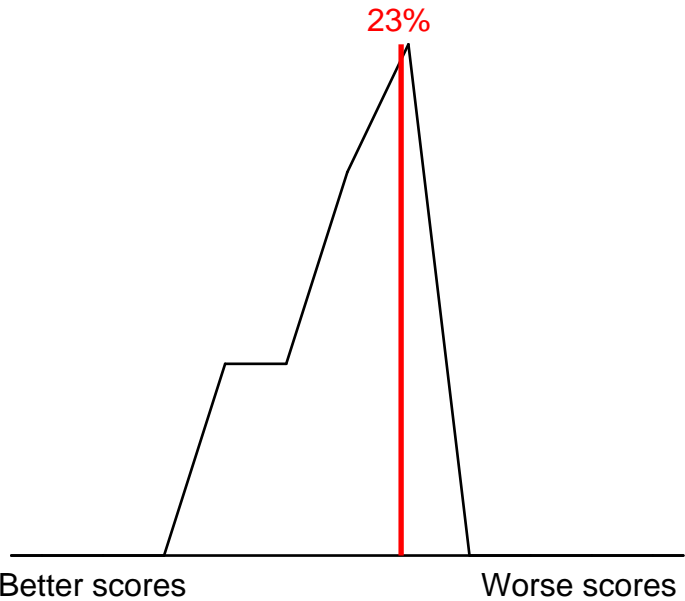
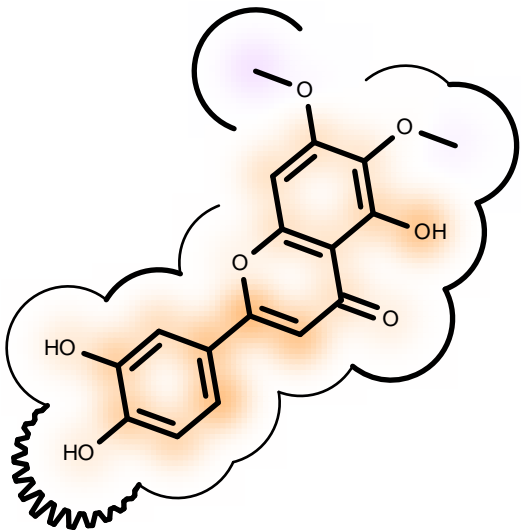


Acceptor Donor
Metal Contact

Molecule Name omega_1_15
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 16

Total Score -9.74

Score compared to other molecules



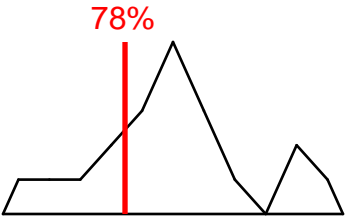
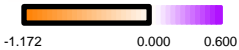
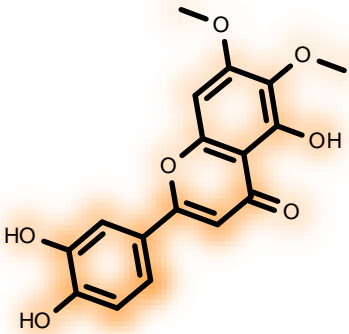
Protein Contact

Protein Cavity

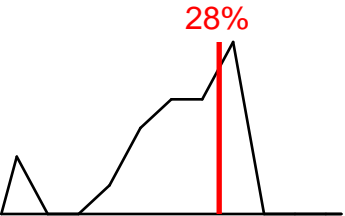
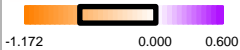
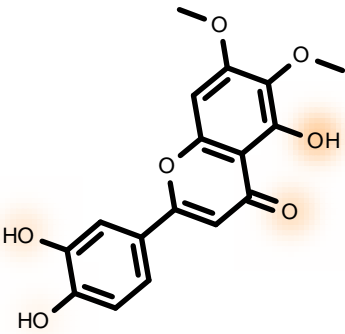
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

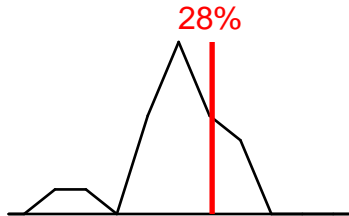
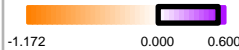
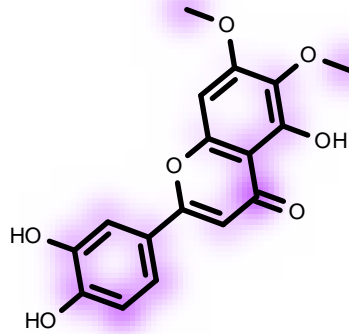
Shape -14.82



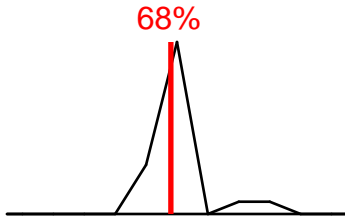
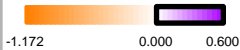
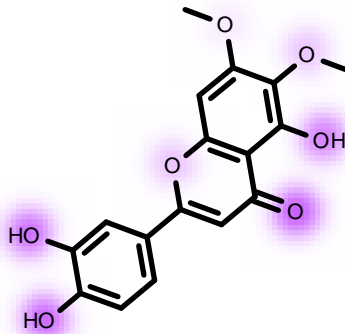
Hydrogen Bond -1.53



Protein Desolvation 3.98



Ligand Desolvation 2.64



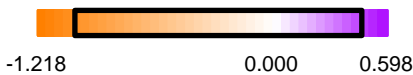
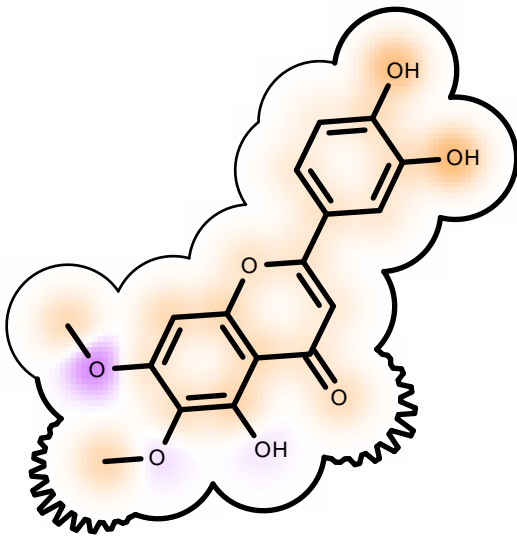
Acceptor
Metal

Donor
Contact

Molecule Name omega_1_13
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 17

Total Score -9.72

Score compared to other molecules

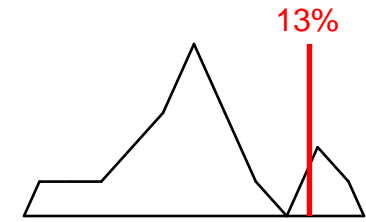
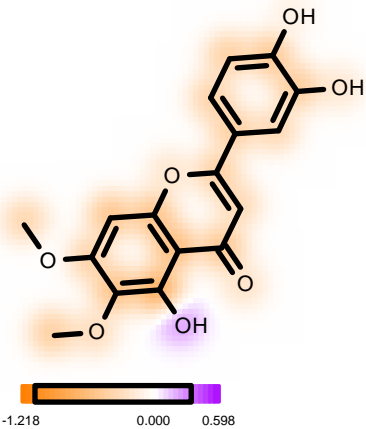


Protein Contact  Protein Cavity

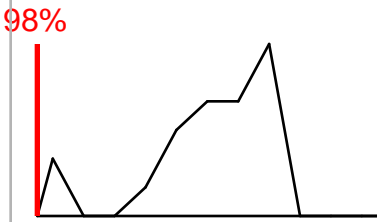
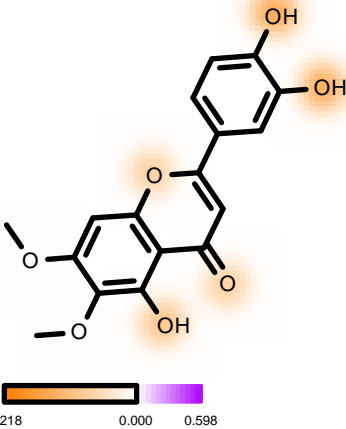
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

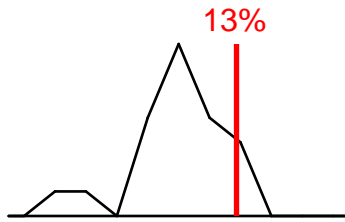
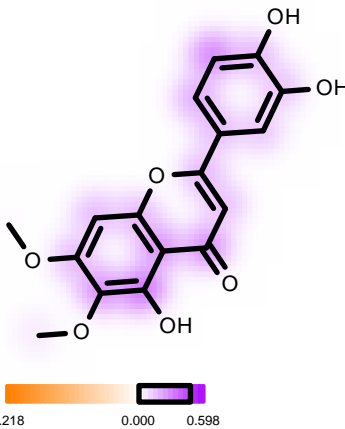
Shape -13.07



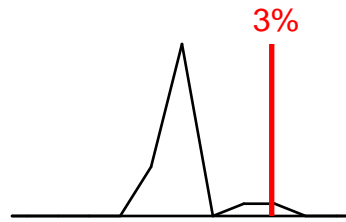
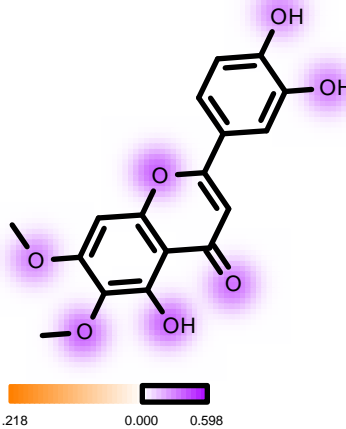
Hydrogen Bond -4.57



Protein Desolvation 4.24



Ligand Desolvation 3.67

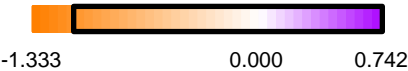
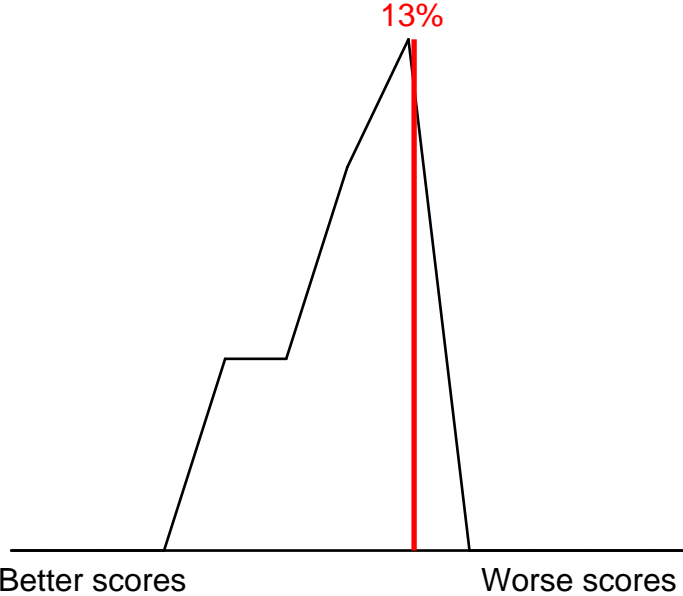
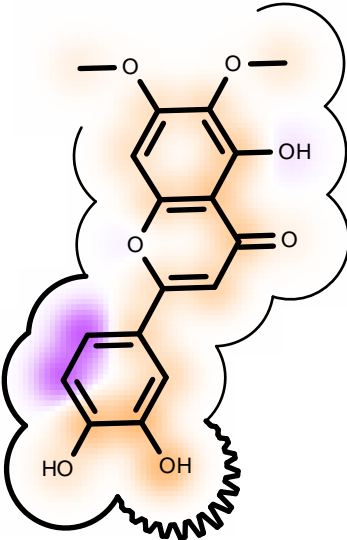


Acceptor Metal Donor Contact

Molecule Name omega_1_4
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 18

Total Score -9.67

Score compared to other molecules



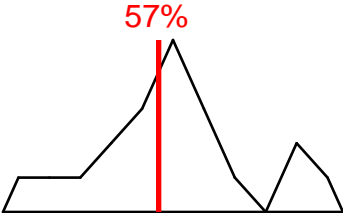
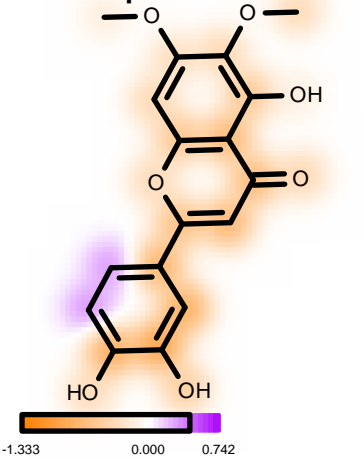
Protein Contact

Protein Cavity

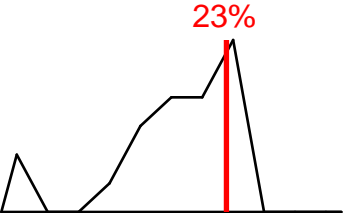
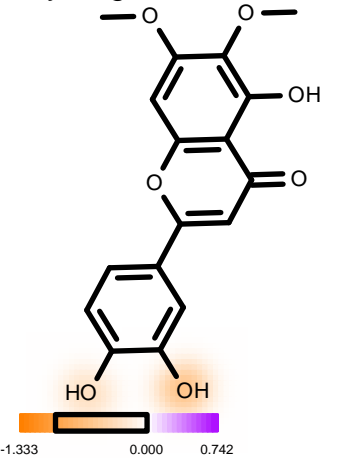
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

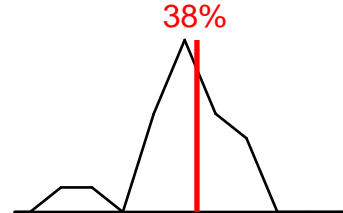
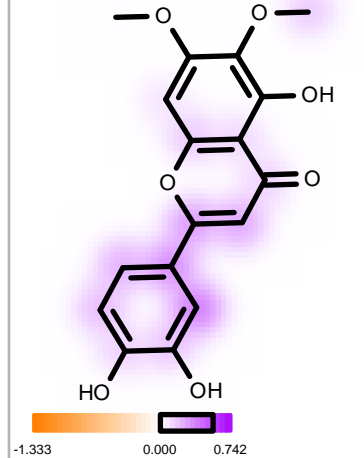
Shape -14.46



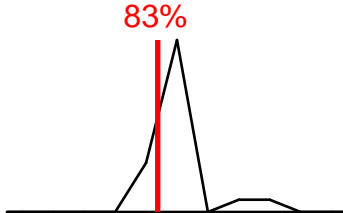
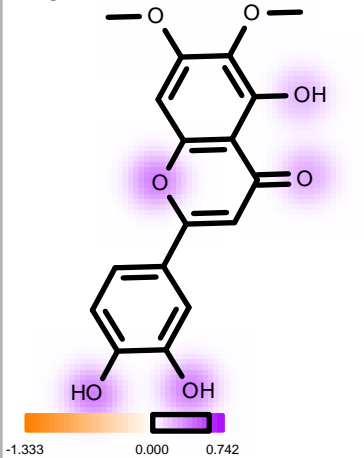
Hydrogen Bond -1.45



Protein Desolvation 3.75



Ligand Desolvation 2.49

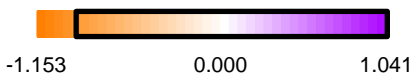
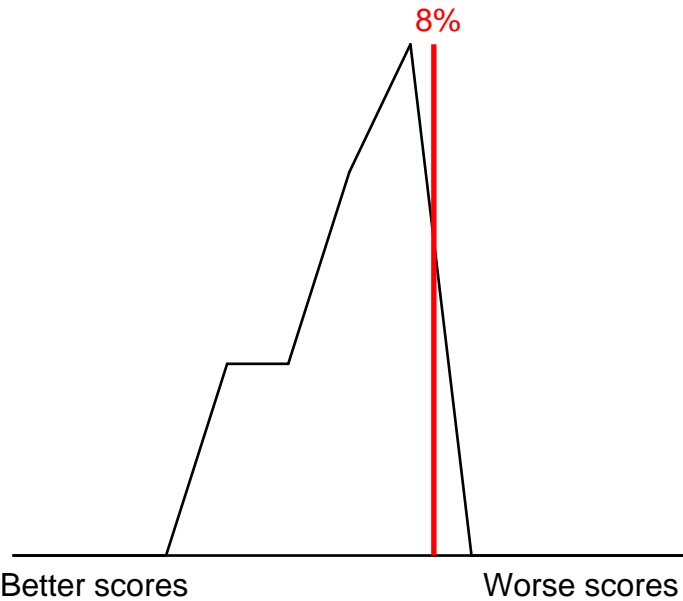
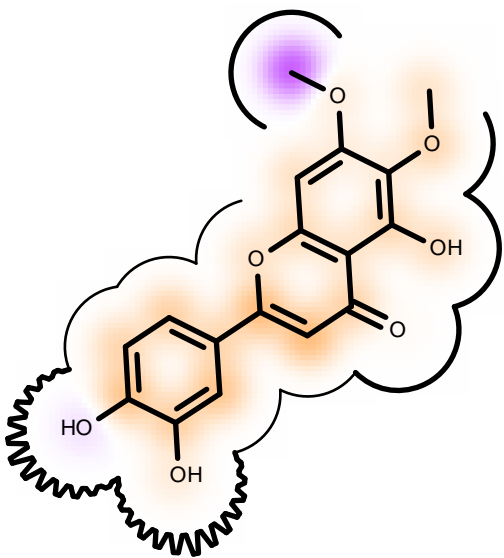


Acceptor
Metal

Donor
Contact

Molecule Name omega_1_13
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 19

Total Score -9.57 Score compared to other molecules

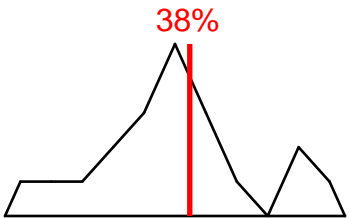
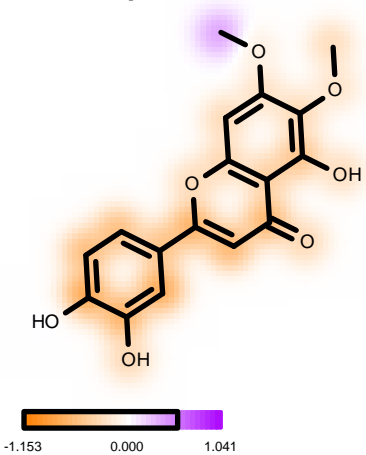


Protein Contact Protein Cavity

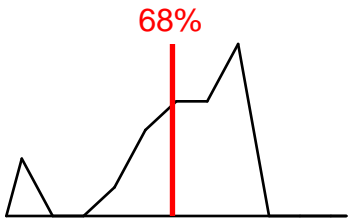
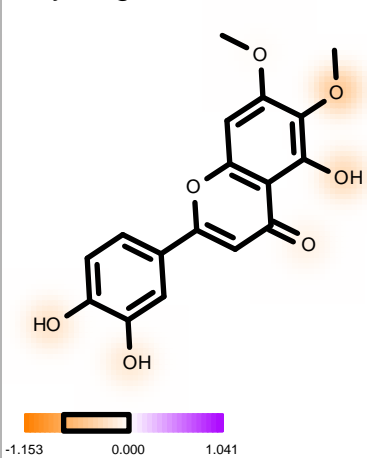
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

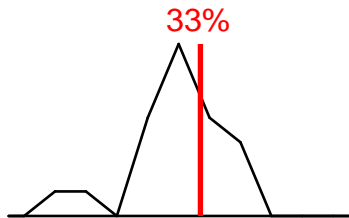
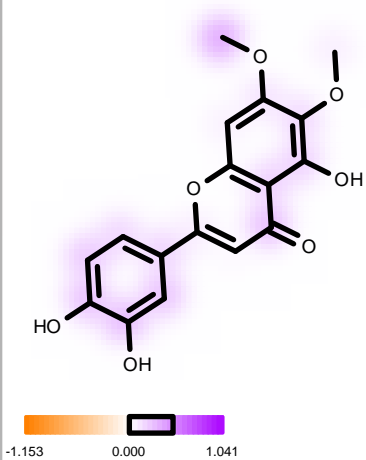
Shape -14.15



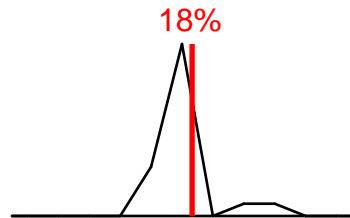
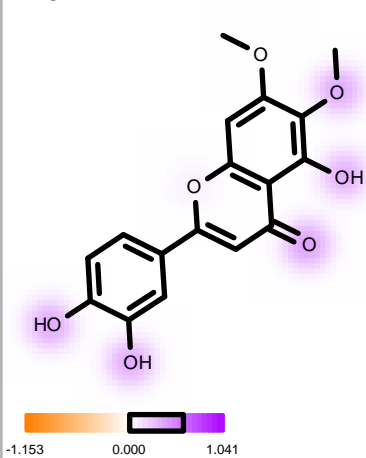
Hydrogen Bond -2.09



Protein Desolvation 3.85



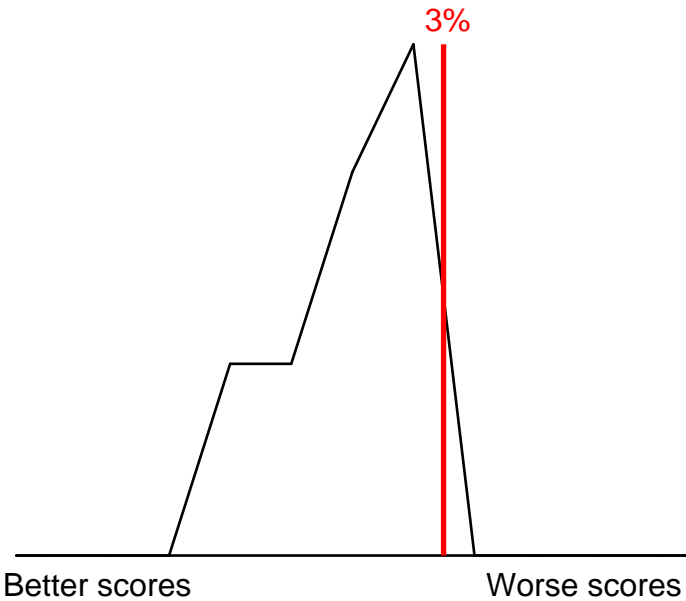
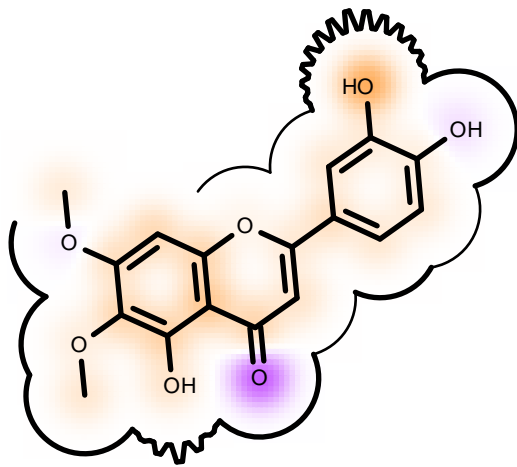
Ligand Desolvation 2.81



Acceptor Donor
Metal Contact

Molecule Name omega_1_2
Molecular Weight 330.3
XLogP 1.2
PSA 109.4
Heavy Atoms 24
Acceptor Count 7
Donor Count 3
Chelator Count 3
Pose Index 20

Total Score -9.54 Score compared to other molecules

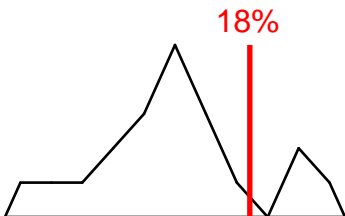
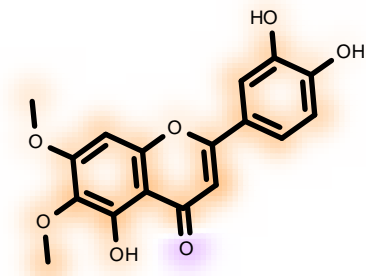


Protein Contact Protein Cavity

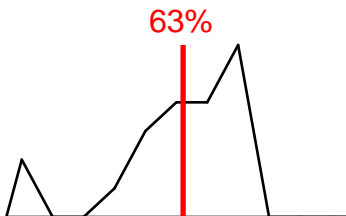
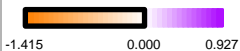
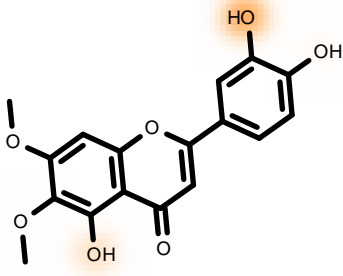
Residue Fingerprint

ALA256G	ALA278E
ALA278F	ALA293B
ALA293C	ALA336B
ARG252G	ARG279C
ARG291B	ASP316F
ASP333B	GLN255G
GLU264G	GLU292B
GLU292C	GLY290B
GLY290C	ILE263G
ILE338C	LYS260G
PRO276F	PRO289C
SER267G	SER277F
THR259G	TYR294C
VAL279E	VAL279F

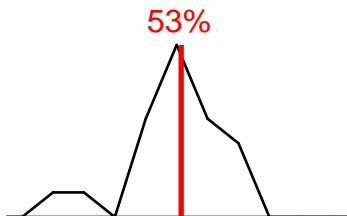
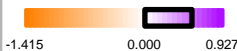
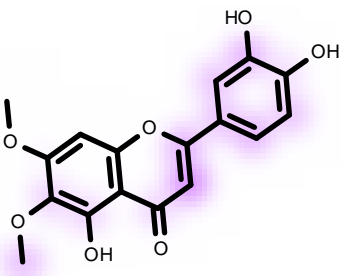
Shape -13.50



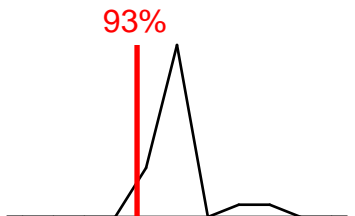
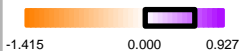
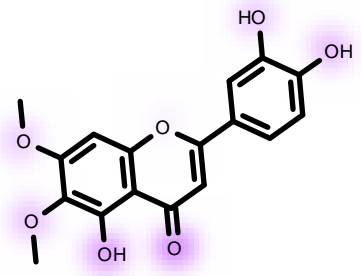
Hydrogen Bond -1.97



Protein Desolvation 3.67



Ligand Desolvation 2.27



Acceptor Donor
Metal Contact