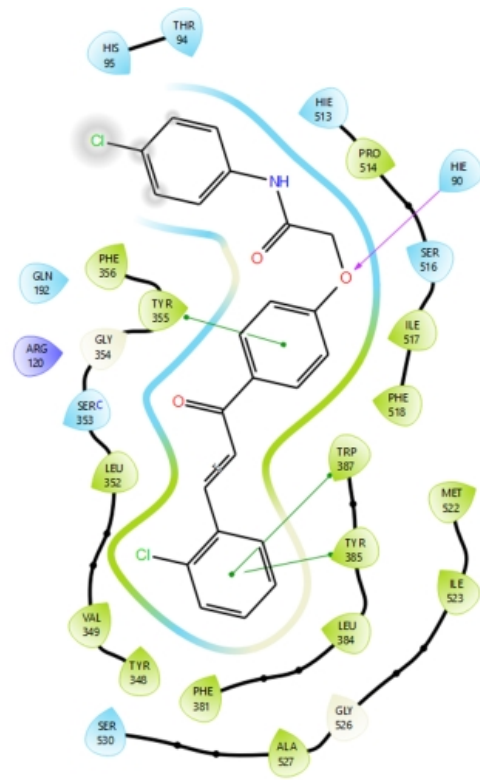


AS1 series docking tiff images

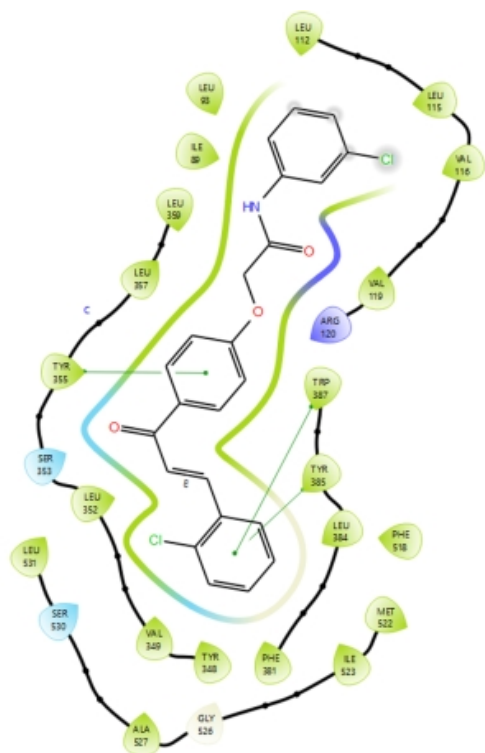
COX-1

AS1-1



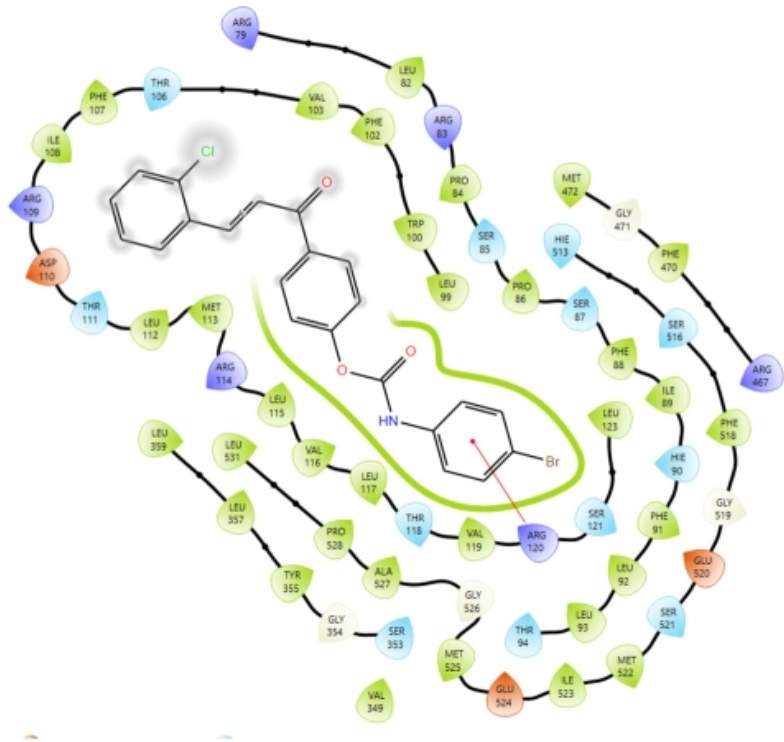
- | | | | |
|--------------------|----------------------------|--------------------|------------------|
| Charged (negative) | Polar | Distance | Pi-cation |
| Charged (positive) | Unspecified residue | H-bond | Salt bridge |
| Glycine | Water | Halogen bond | Solvent exposure |
| Hydrophobic | Hydration site | Metal coordination | |
| Metal | Hydration site (displaced) | Pi-Pi stacking | |

AS1-2



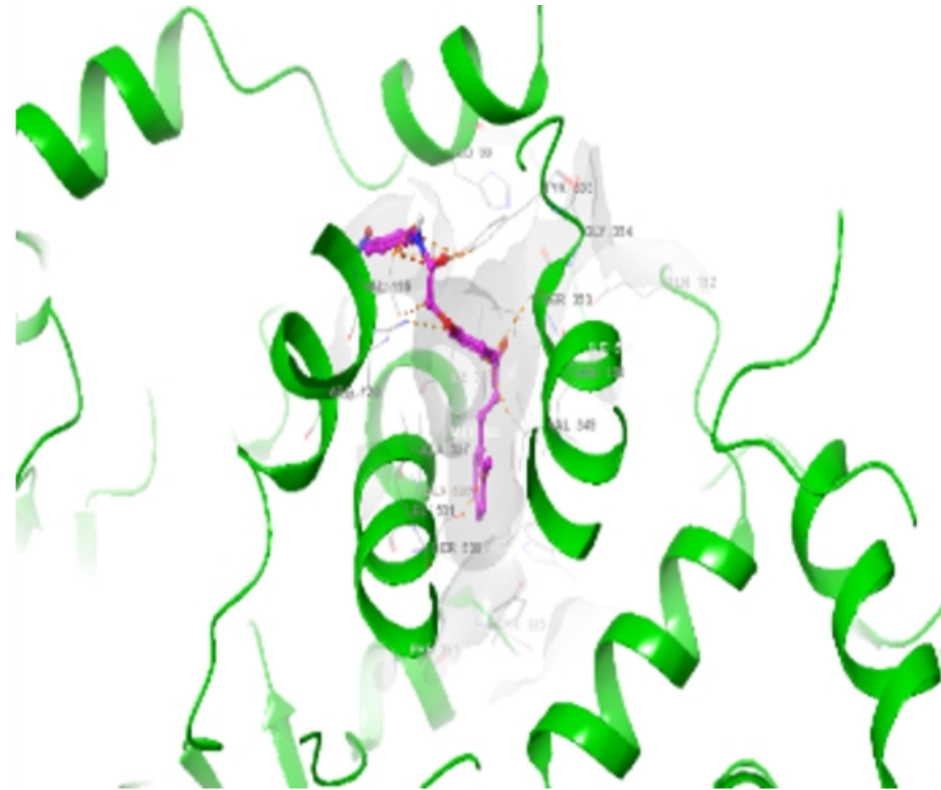
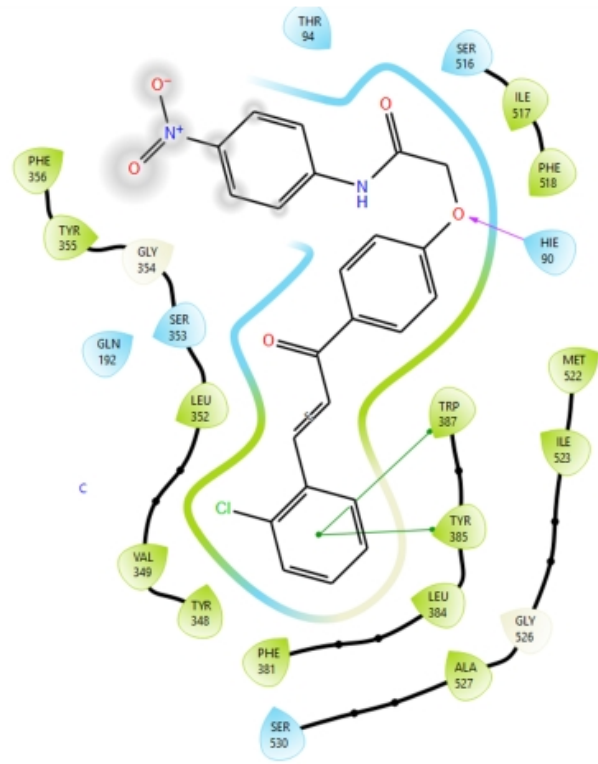
- | | | | |
|--------------------|----------------------------|--------------------|------------------|
| Charged (negative) | Polar | Distance | Pi-cation |
| Charged (positive) | Unspecified residue | H-bond | Salt bridge |
| Glycine | Water | Halogen bond | Solvent exposure |
| Hydrophobic | Hydration site | Metal coordination | |
| Metal | Hydration site (displaced) | Pi-Pi stacking | |

AS1-3



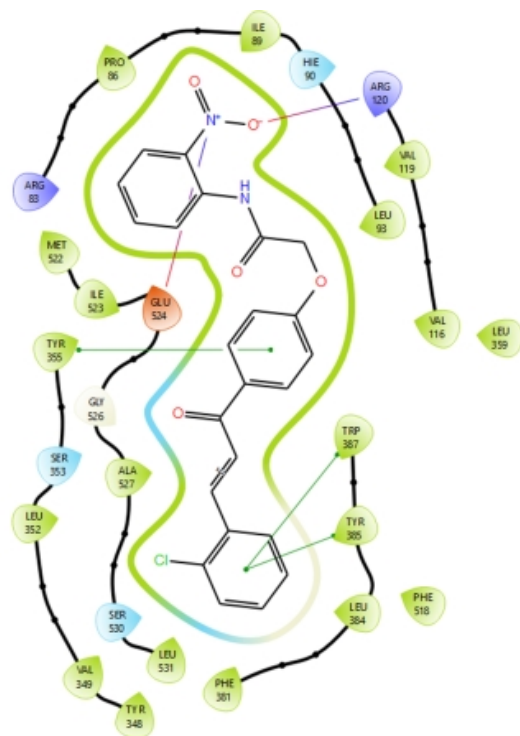
- | | | | |
|--|--|--|--|
|  Charged (negative) |  Polar |  Distance |  Pi-cation |
|  Charged (positive) |  Unspecified residue |  H-bond |  Salt bridge |
|  Glycine |  Water |  Halogen bond |  Solvent exposure |
|  Hydrophobic |  Hydration site |  Metal coordination | |
|  Metal |  Hydration site (displaced) |  Pi-Pi stacking | |

AS1-4



- | | | | |
|--------------------|----------------------------|--------------------|------------------|
| Charged (negative) | Polar | Distance | Pi-cation |
| Charged (positive) | Unspecified residue | H-bond | Salt bridge |
| Glycine | Water | Halogen bond | Solvent exposure |
| Hydrophobic | Hydration site | Metal coordination | |
| Metal | Hydration site (displaced) | Pi-Pi stacking | |

AS1-5

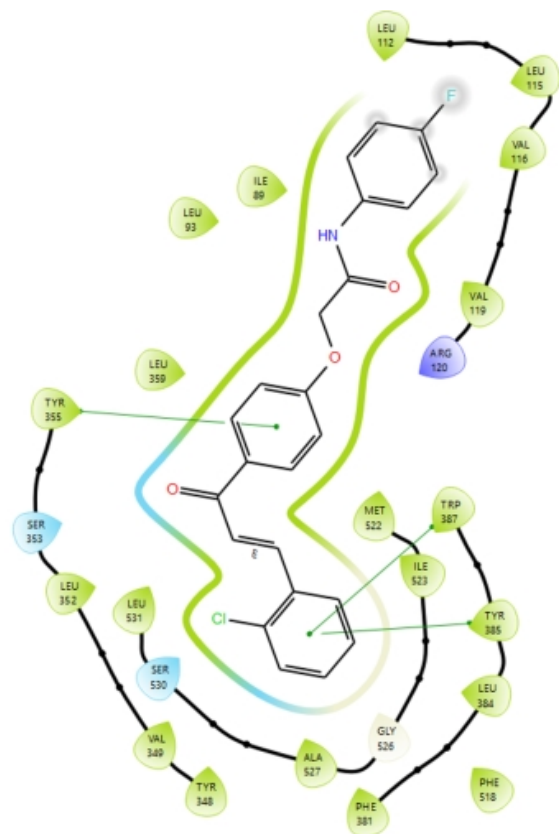


- Charged (negative)
- Charged (positive)
- Glycine
- Hydrophobic
- Metal

- Polar
- Unspecified residue
- Water
- Hydration site
- Hydration site (displaced)
- Distance
- H-bond
- Halogen bond
- Metal coordination
- Pi-Pi stacking

- Pi-cation
- Salt bridge
- Solvent exposure

AS1-6

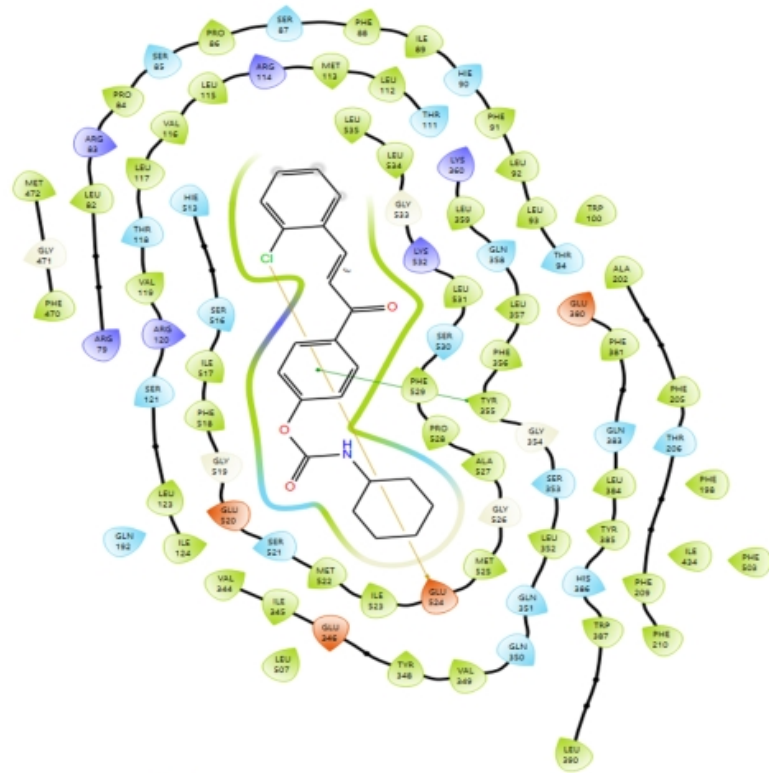


- Charged (negative)
- Charged (positive)
- Glycine
- Hydrophobic
- Metal

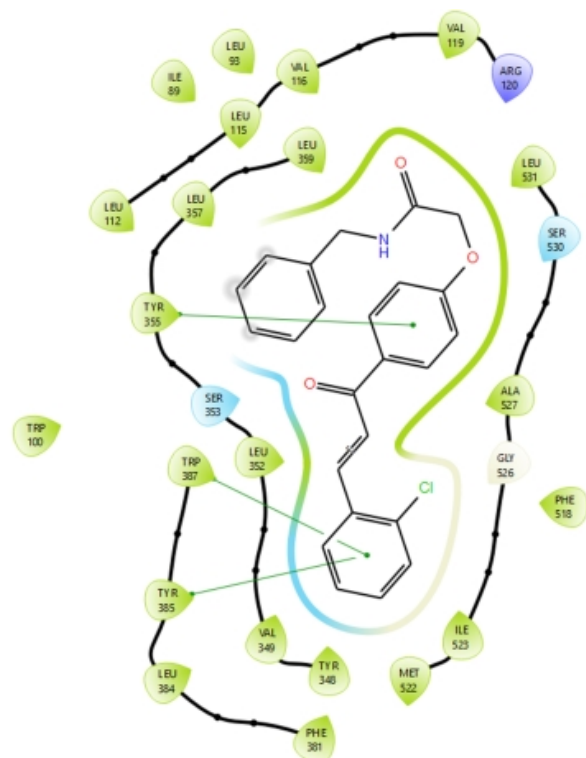
- Polar
- Unspecified residue
- Water
- Hydration site
- X Hydration site (displaced)
- Distance
- H-bond
- Halogen bond
- Metal coordination
- Pi-Pi stacking

- Pi-cation
- Salt bridge
- Solvent exposure

AS1-7

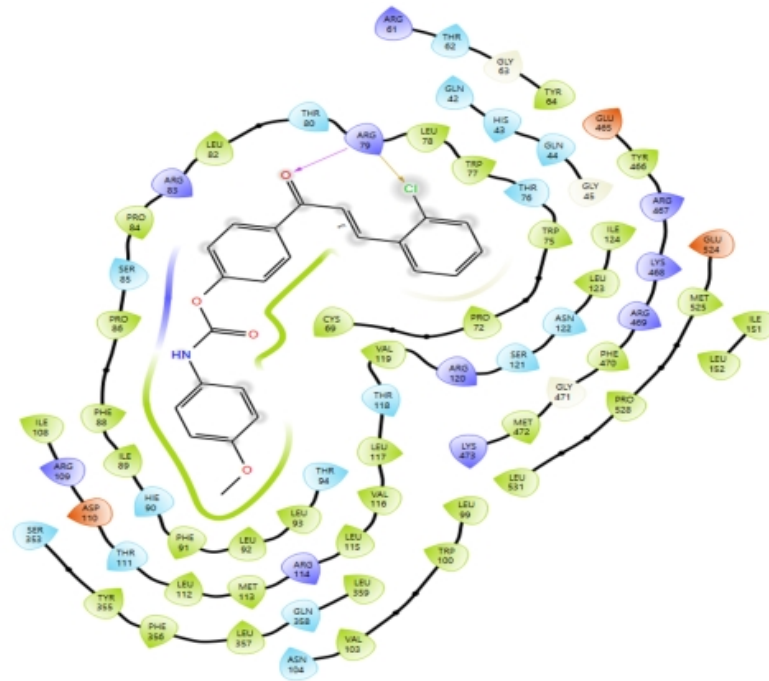


AS1-8



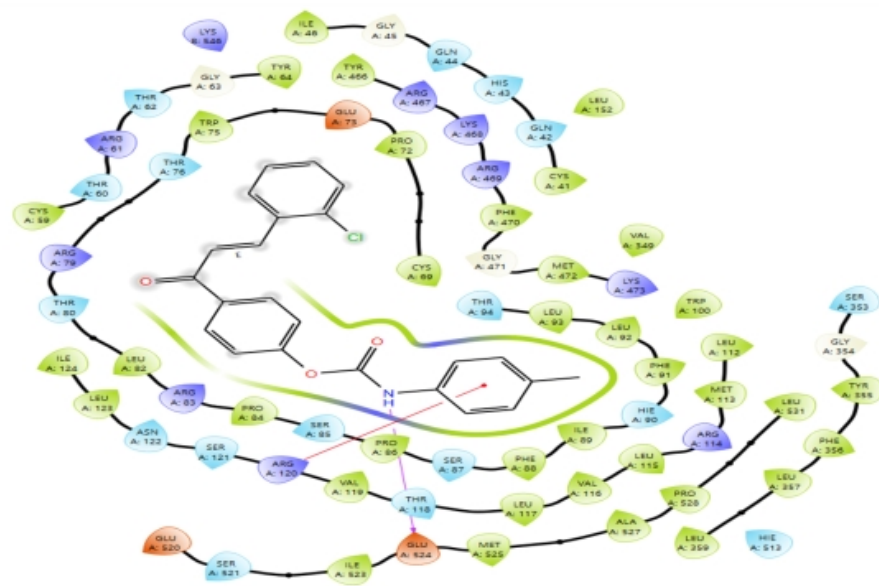
- | | | | |
|--|--|--|--|
|  Charged (negative) |  Polar |  Distance |  Pi-cation |
|  Charged (positive) |  Unspecified residue |  H-bond |  Salt bridge |
|  Glycine |  Water |  Halogen bond |  Solvent exposure |
|  Hydrophobic |  Hydration site |  Metal coordination | |
|  Metal |  Hydration site (displaced) |  Pi-Pi stacking | |

AS1-9

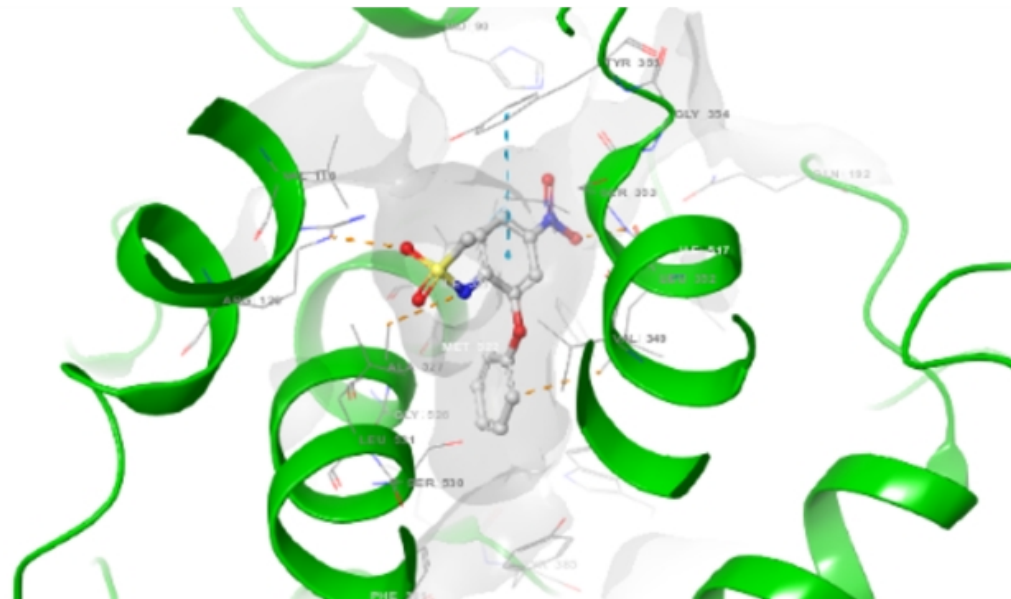
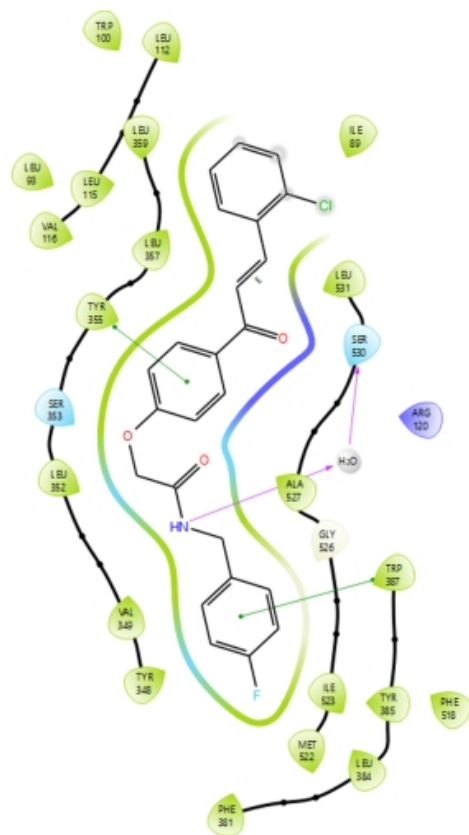


- | | | | |
|--------------------|----------------------------|--------------------|------------------|
| Charged (negative) | Polar | Distance | Pi-cation |
| Charged (positive) | Unspecified residue | H-bond | Salt bridge |
| Glycine | Water | Halogen bond | Solvent exposure |
| Hydrophobic | Hydration site | Metal coordination | |
| Metal | Hydration site (displaced) | Pi-Pi stacking | |

AS1-10



AS1-11



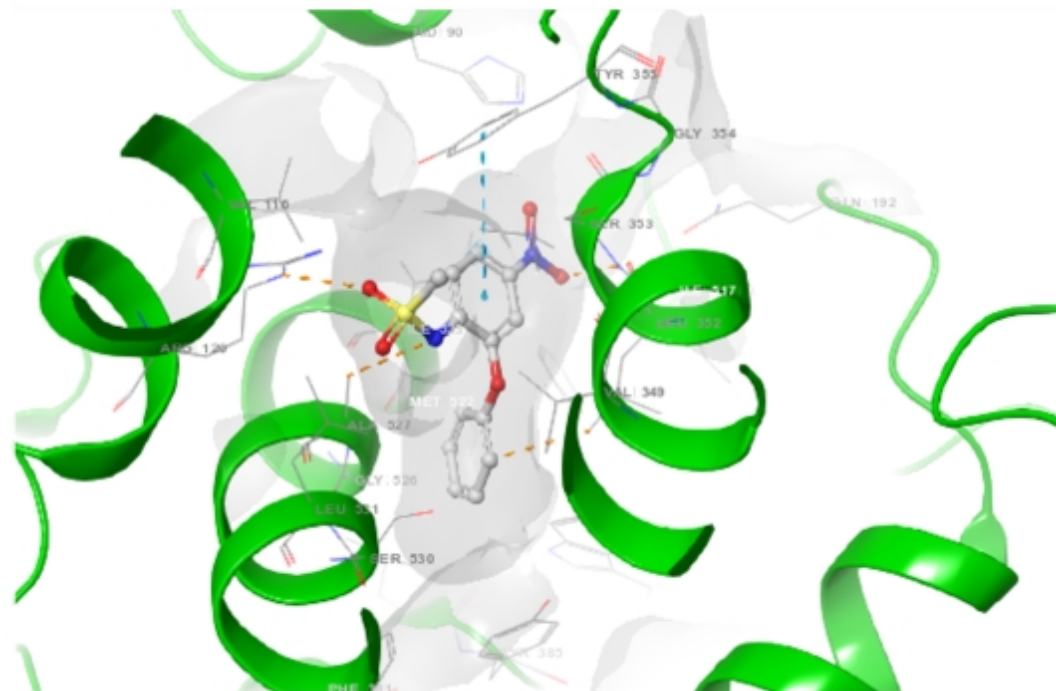
- Charged (negative)
- Charged (positive)
- Glycine
- Hydrophobic
- Metal

- Polar
- Unspecified residue
- Water
- Hydration site
- ✗ Hydration site (displaced)

- Distance
- H-bond
- Halogen bond
- Metal coordination
- Pi-Pi stacking

- Pi-cation
- Salt bridge
- Solvent exposure

Charged (negative) Polar

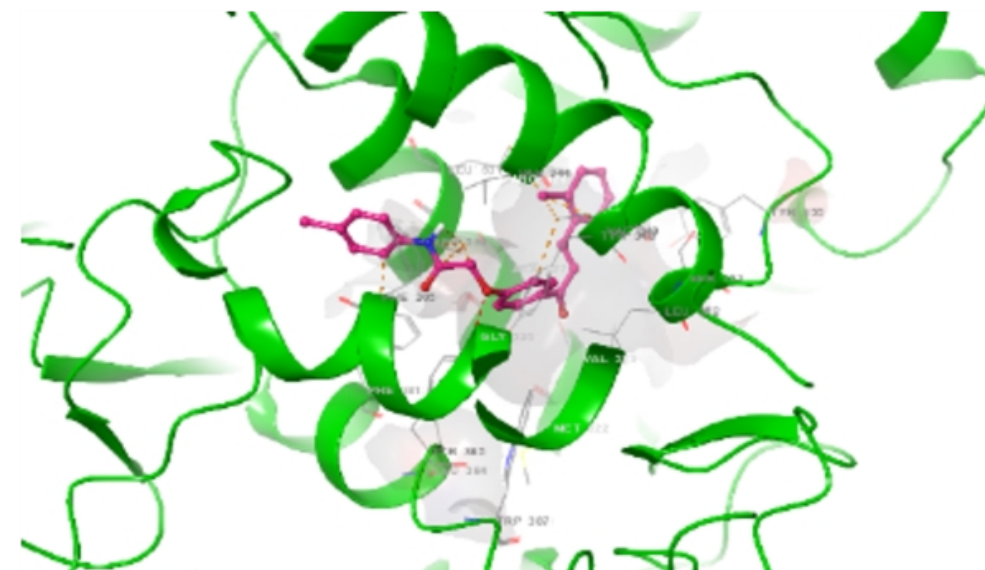
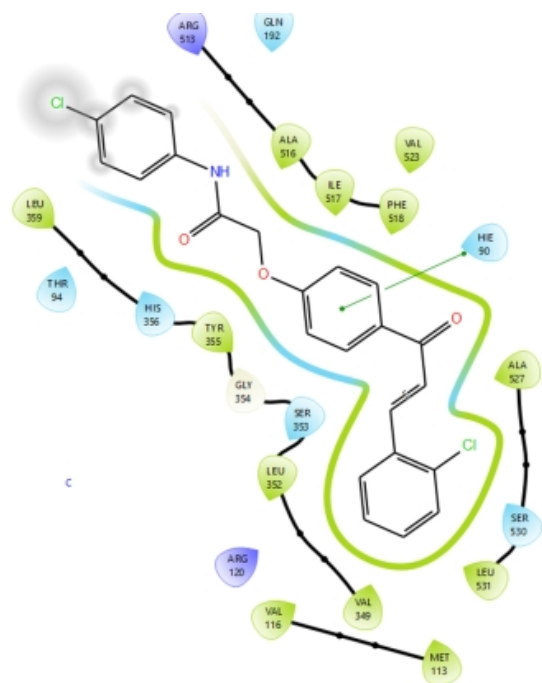


-  Distance
 H-bond
 Halogen bond
 Metal coordination
 Pi-Pi stacking
 Pi-cation
 Salt bridge
 Solvent exposure

AS1 series docking tiff images

COX-2

AS1-1



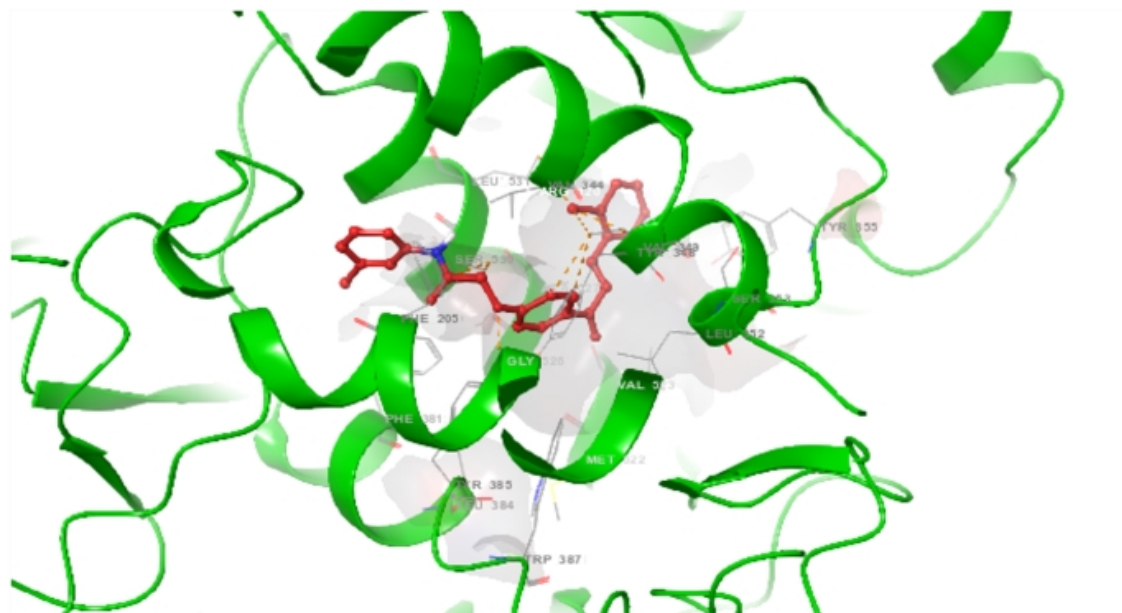
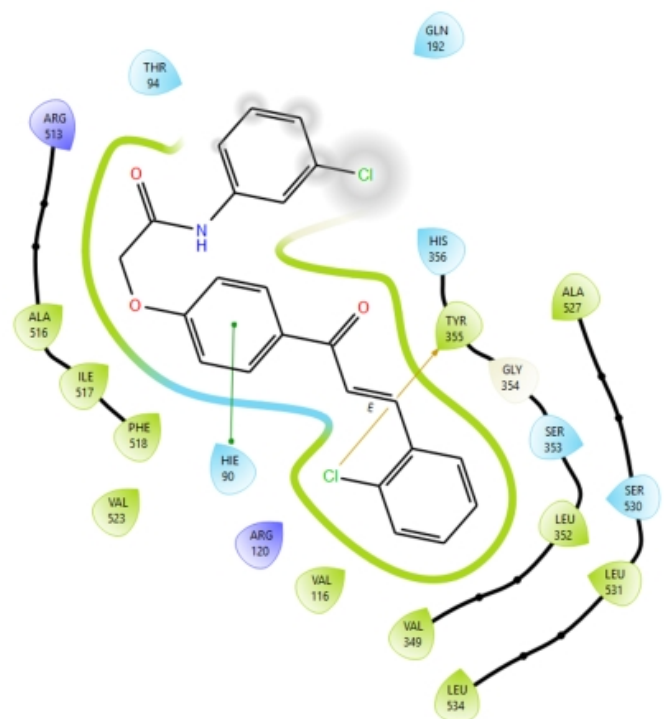
- Charged (negative)
- Charged (positive)
- Glycine
- Hydrophobic
- Metal

- Polar
- Unspecified residue
- Water
- Hydration site
- ✗ Hydration site (displaced)

- ⋯ Distance
- H-bond
- Halogen bond
- Metal coordination
- Pi-Pi stacking

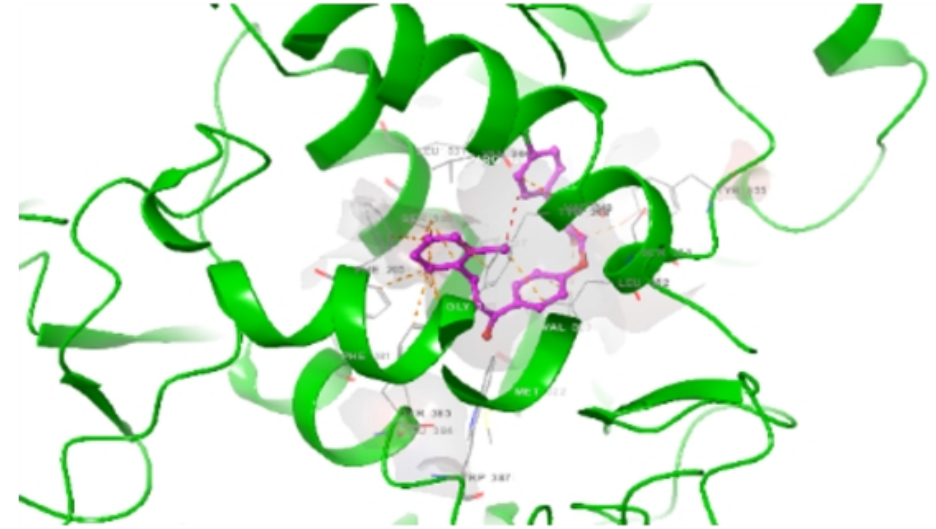
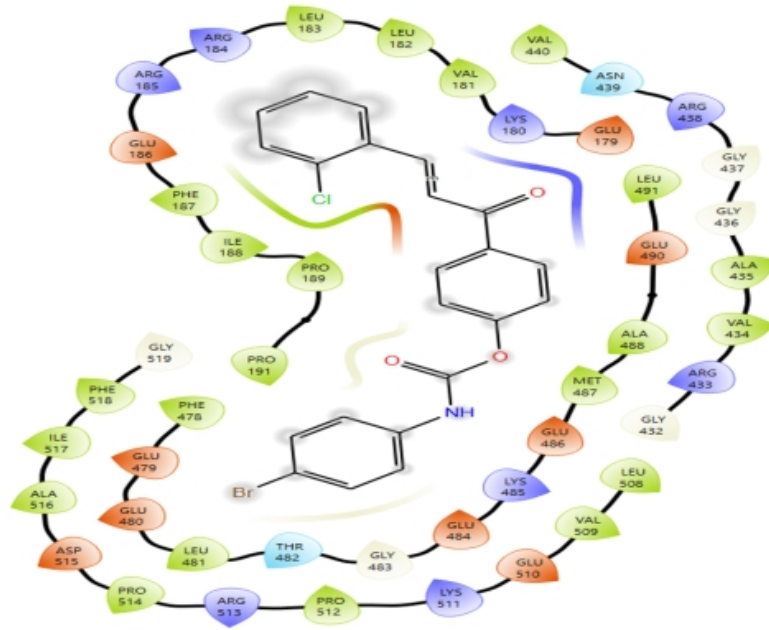
- Pi-cation
- Salt bridge
- Solvent exposure

AS1-2



- | | | | |
|--------------------|----------------------------|--------------------|------------------|
| Charged (negative) | Polar | Distance | Pi-cation |
| Charged (positive) | Unspecified residue | H-bond | Salt bridge |
| Glycine | Water | Halogen bond | Solvent exposure |
| Hydrophobic | Hydration site | Metal coordination | |
| Metal | Hydration site (displaced) | Pi-Pi stacking | |

AS1-3



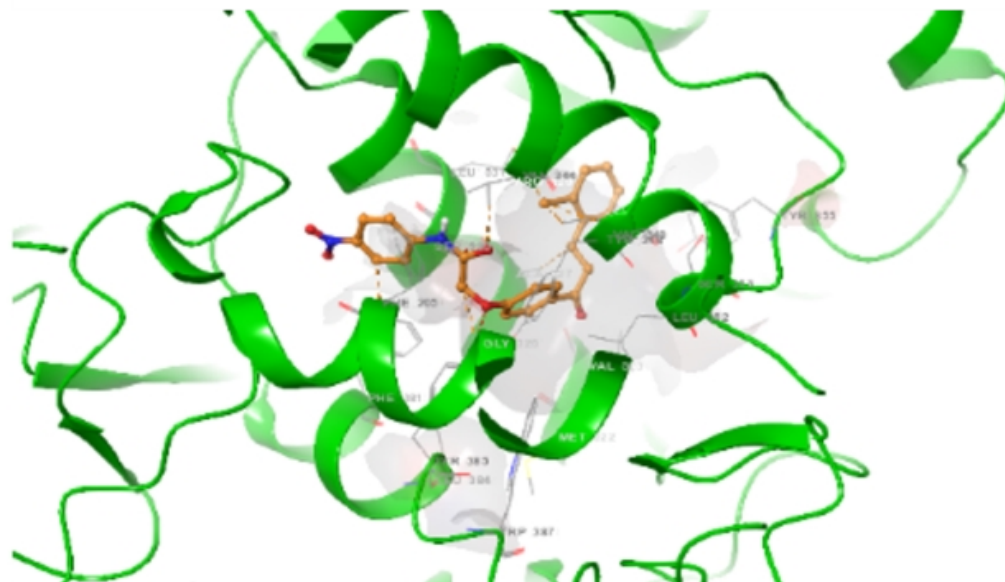
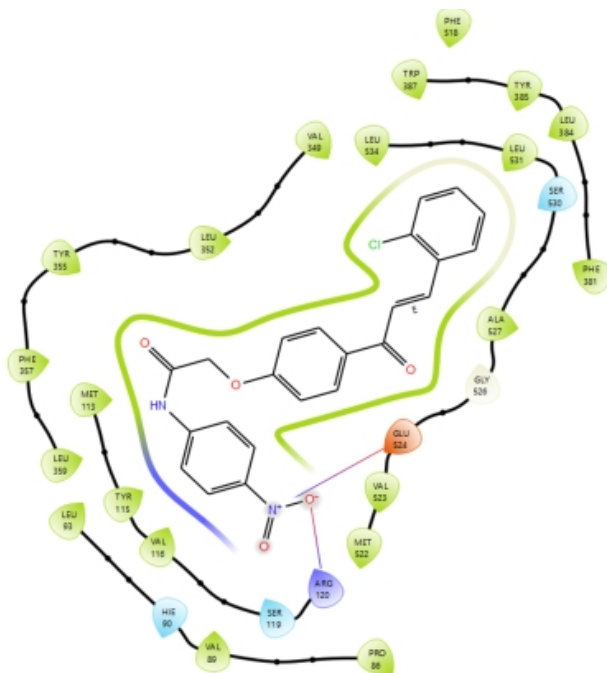
- Charged (negative)
- Charged (positive)
- Glycine
- Hydrophobic
- Metal

- Polar
- Unspecified residue
- Water
- Hydration site
- ✗ Hydration site (displaced)

- Distance
- H-bond
- Halogen bond
- Metal coordination
- Pi-Pi stacking

- Pi-cation
- Salt bridge
- Solvent exposure

AS1-4



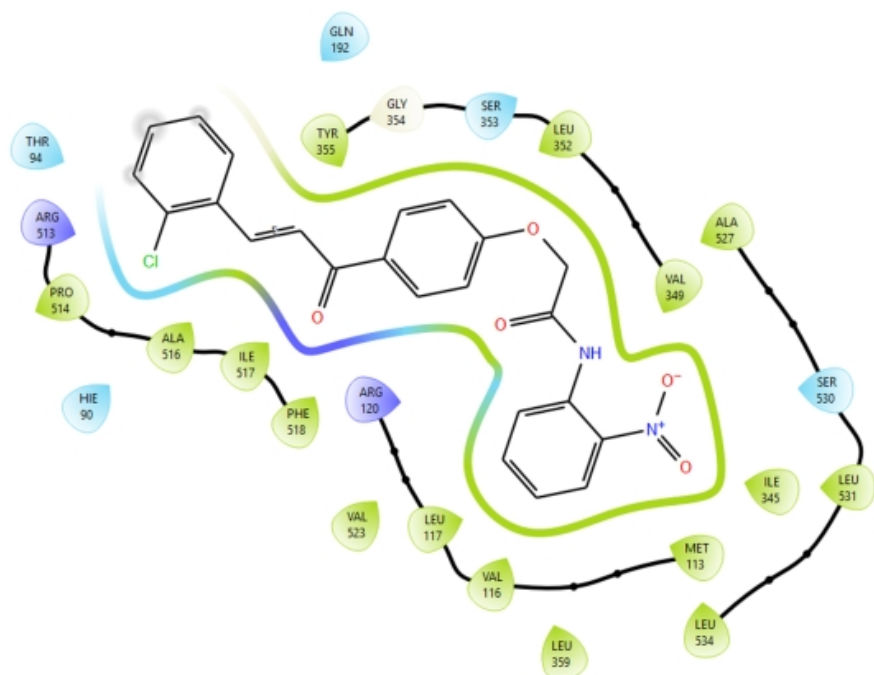
- Charged (negative)
- Charged (positive)
- Glycine
- Hydrophobic
- Metal

- Polar
- Unspecified residue
- Water
- Hydration site
- ✗ Hydration site (displaced)

- Distance
- H-bond
- Halogen bond
- Metal coordination
- Pi-Pi stacking

- Pi-cation
- Salt bridge
- Solvent exposure

AS1-5

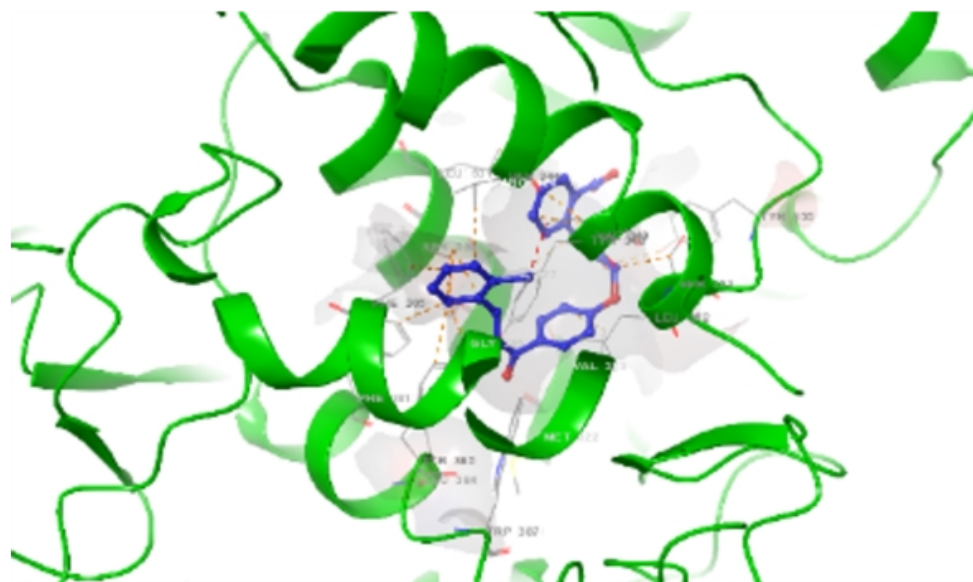


- Charged (negative)
- Charged (positive)
- Glycine
- Hydrophobic
- Metal

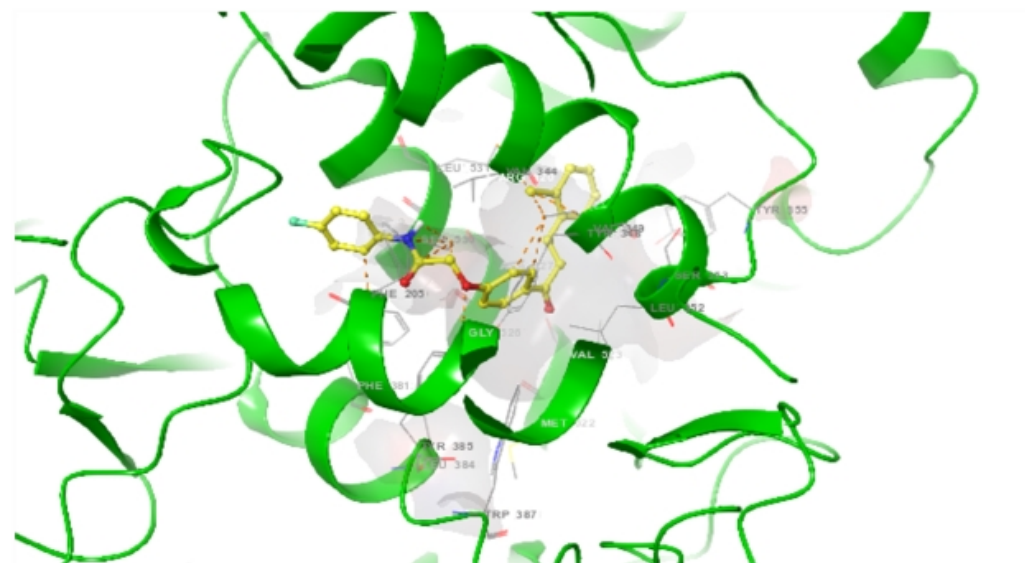
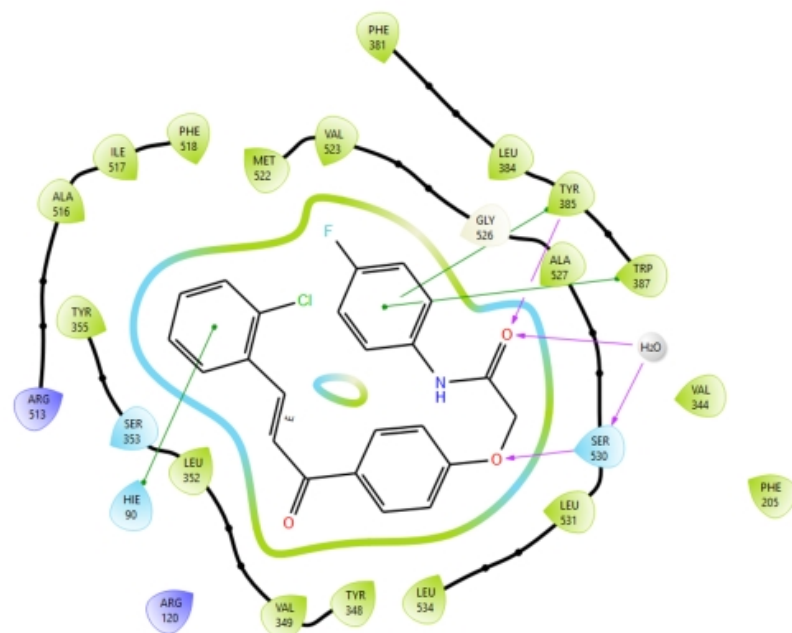
- Polar
- Unspecified residue
- Water
- Hydration site
- ✗ Hydration site (displaced)

- Distance
- H-bond
- Halogen bond
- Metal coordination
- Pi-Pi stacking

- Pi-cation
- Salt bridge
- Solvent exposure

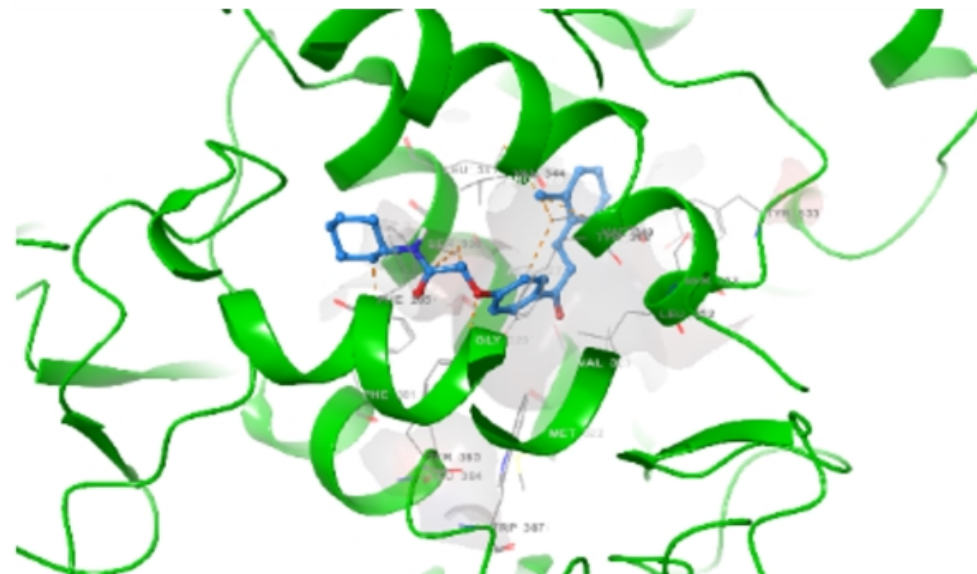
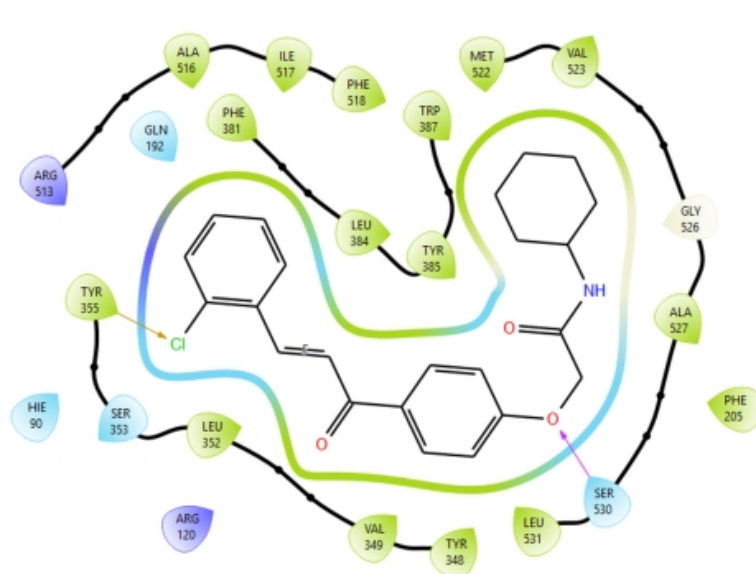


AS1-6



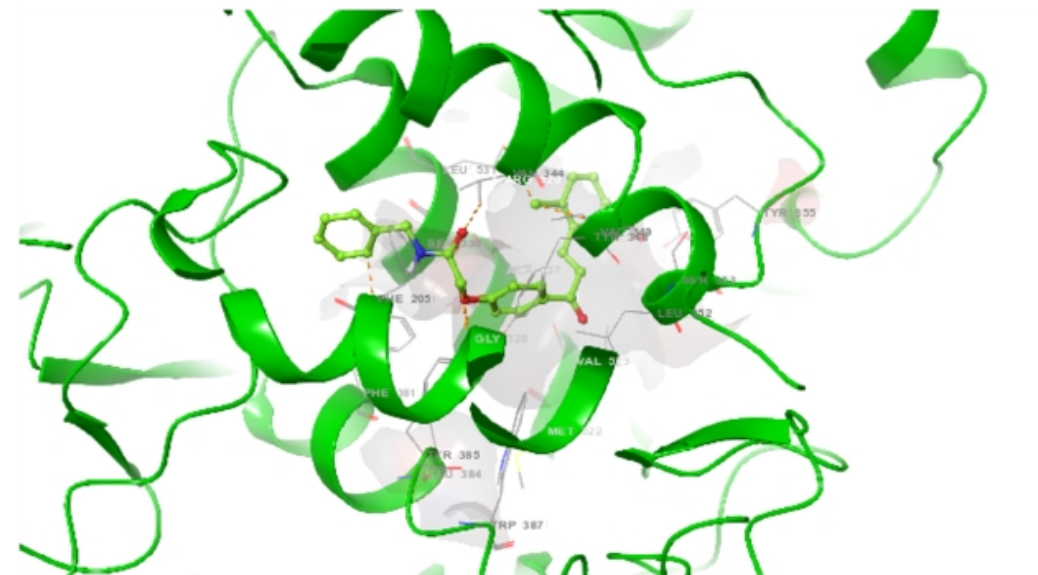
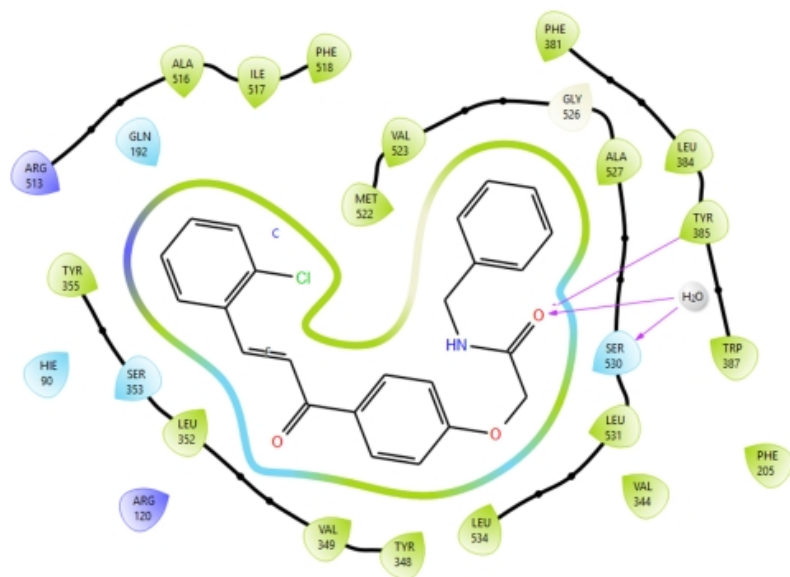
- | | | | |
|--|---|--|--|
| ● Charged (negative) | ● Polar | --- Distance | —●— Pi-cation |
| ● Charged (positive) | ● Unspecified residue | —●— H-bond | —●— Salt bridge |
| ● Glycine | ● Water | —●— Halogen bond | ○ Solvent exposure |
| ● Hydrophobic | ○ Hydration site | —●— Metal coordination | |
| ● Metal | ✗ Hydration site (displaced) | —●— Pi-Pi stacking | |

AS1-7



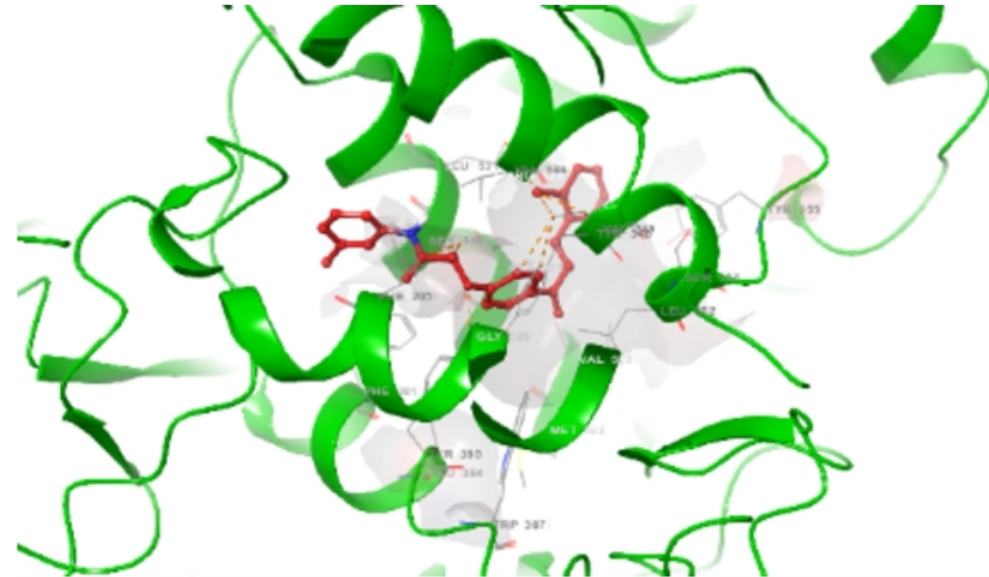
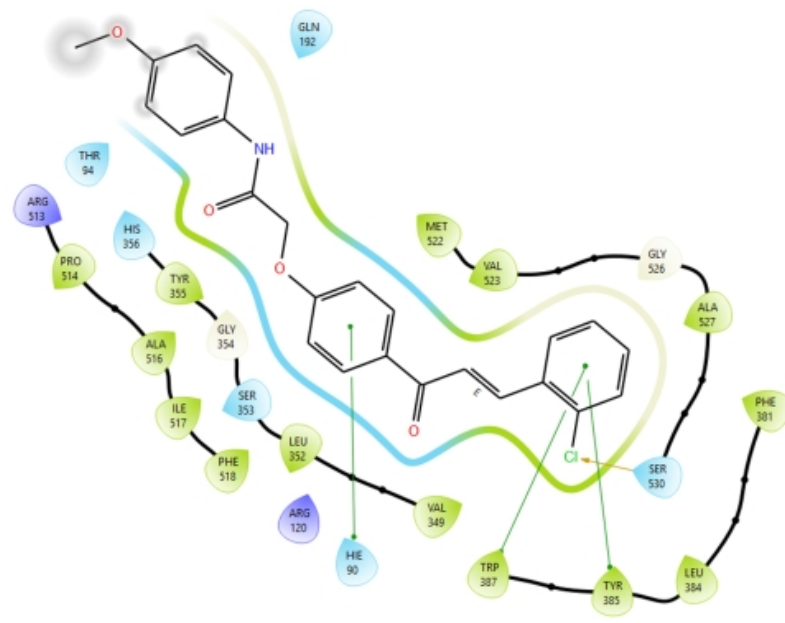
- | | | | |
|--------------------|----------------------------|--------------------|------------------|
| Charged (negative) | Polar | Distance | Pi-cation |
| Charged (positive) | Unspecified residue | H-bond | Salt bridge |
| Glycine | Water | Halogen bond | Solvent exposure |
| Hydrophobic | Hydration site | Metal coordination | |
| Metal | Hydration site (displaced) | Pi-Pi stacking | |

AS1-8



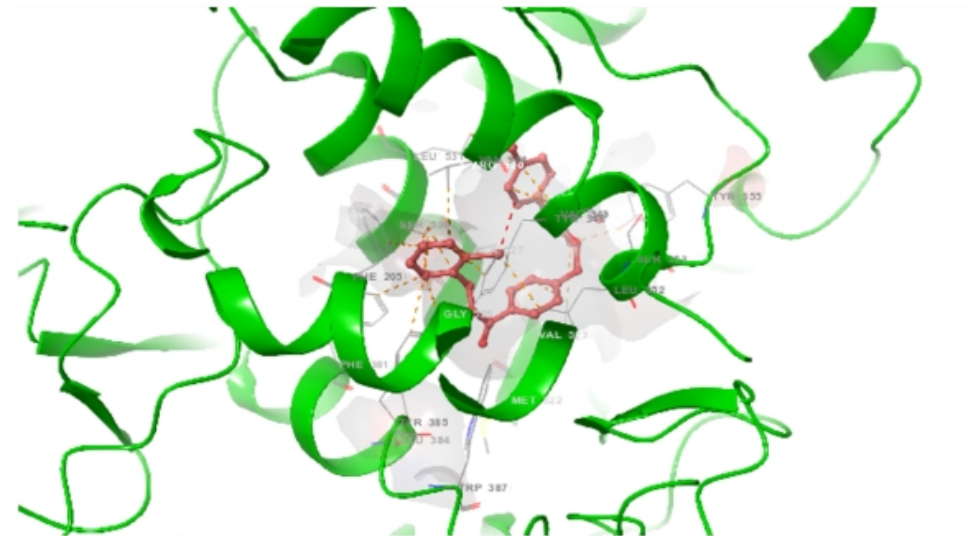
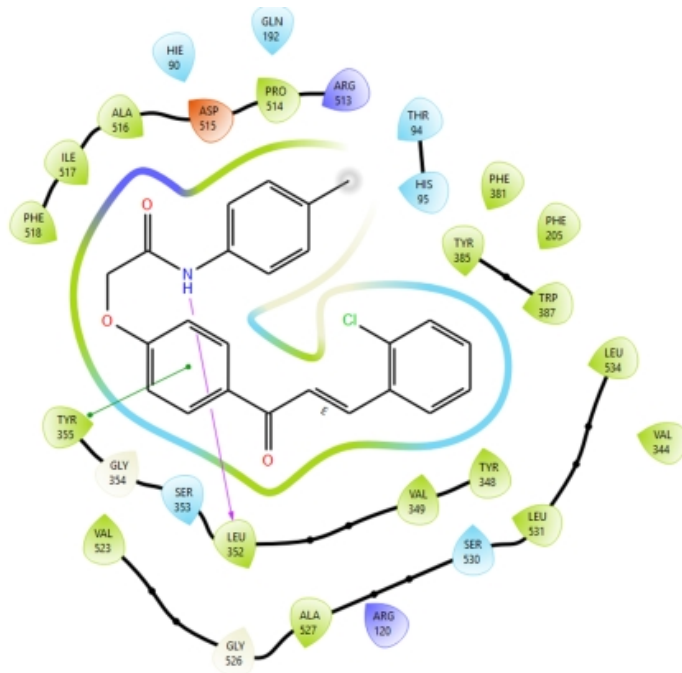
- | | | | |
|--|--|--|--|
|  Charged (negative) |  Polar |  Distance |  Pi-cation |
|  Charged (positive) |  Unspecified residue |  H-bond |  Salt bridge |
|  Glycine |  Water |  Halogen bond |  Solvent exposure |
|  Hydrophobic |  Hydration site |  Metal coordination | |
|  Metal |  Hydration site (displaced) |  Pi-Pi stacking | |

AS1-9



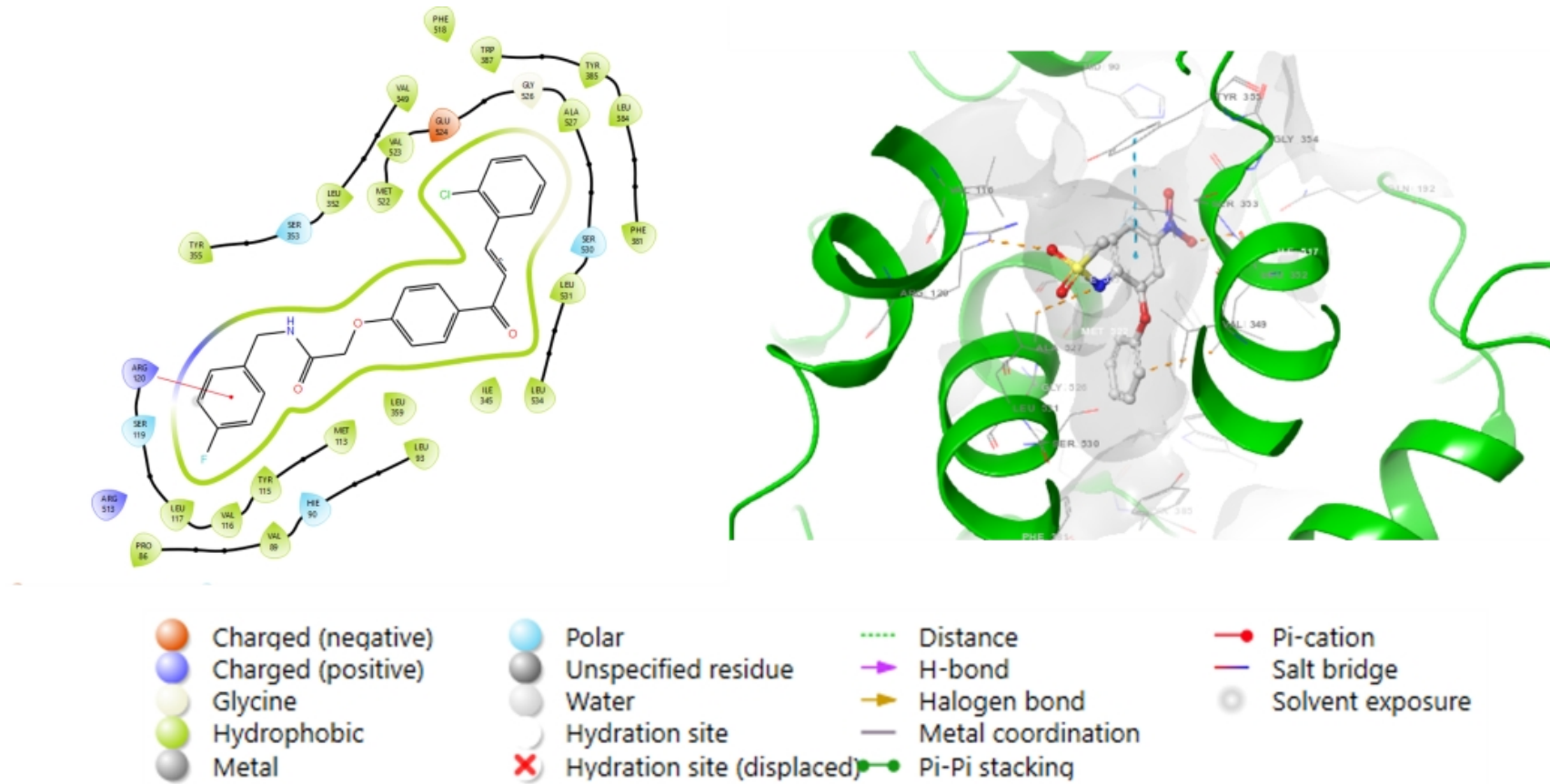
- | | | | |
|--|---|--|--|
| ● Charged (negative) | ● Polar | --- Distance | —●— Pi-cation |
| ● Charged (positive) | ● Unspecified residue | → H-bond | — Salt bridge |
| ● Glycine | ● Water | → Halogen bond | ○ Solvent exposure |
| ● Hydrophobic | ○ Hydration site | — Metal coordination | |
| ● Metal | ✗ Hydration site (displaced) | —●— Pi-Pi stacking | |

AS1-10

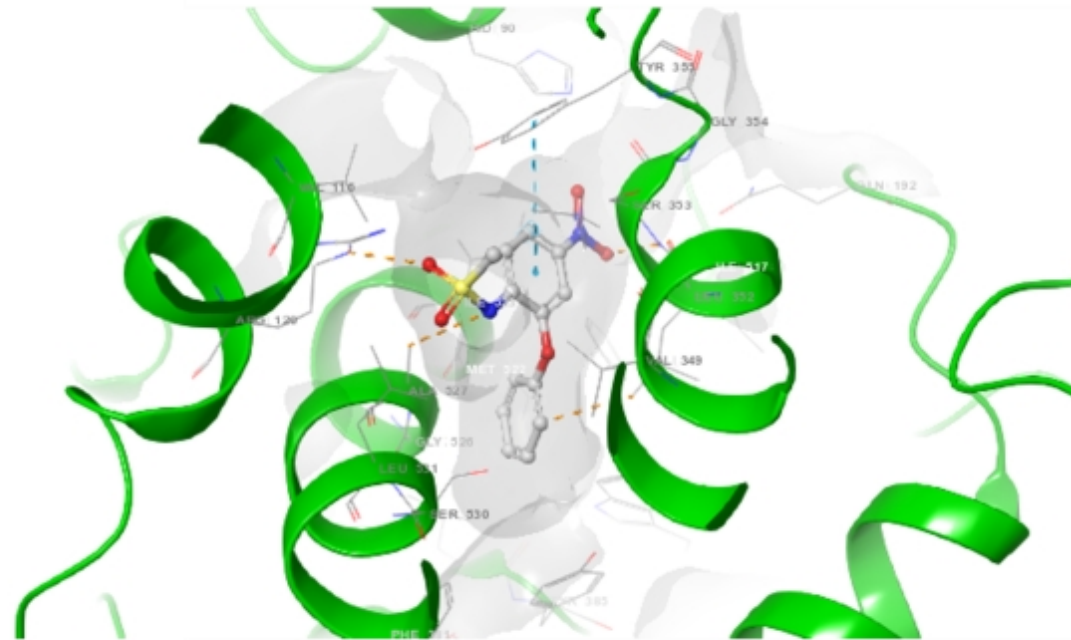
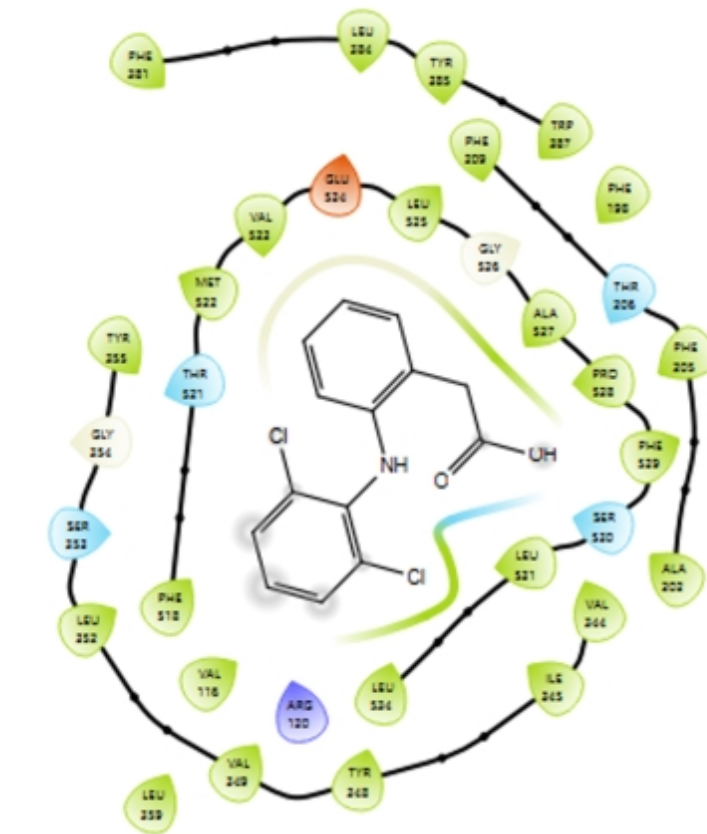


- | | | | |
|--|---|--|--|
| ● Charged (negative) | ● Polar | --- Distance | —●— Pi-cation |
| ● Charged (positive) | ● Unspecified residue | —●— H-bond | —●— Salt bridge |
| ● Glycine | ○ Water | —●— Halogen bond | ○ Solvent exposure |
| ● Hydrophobic | ○ Hydration site | —●— Metal coordination | |
| ● Metal | ✗ Hydration site (displaced) | —●— Pi-Pi stacking | |

AS1-11



Diclofenac sodium



- | | | | |
|--|--|--|--|
|  Charged (negative) |  Polar |  Distance |  Pi-cation |
|  Charged (positive) |  Unspecified residue |  H-bond |  Salt bridge |
|  Glycine |  Water |  Halogen bond |  Solvent exposure |
|  Hydrophobic |  Hydration site |  Metal coordination | |
|  Metal |  Hydration site (displaced) |  Pi-Pi stacking | |