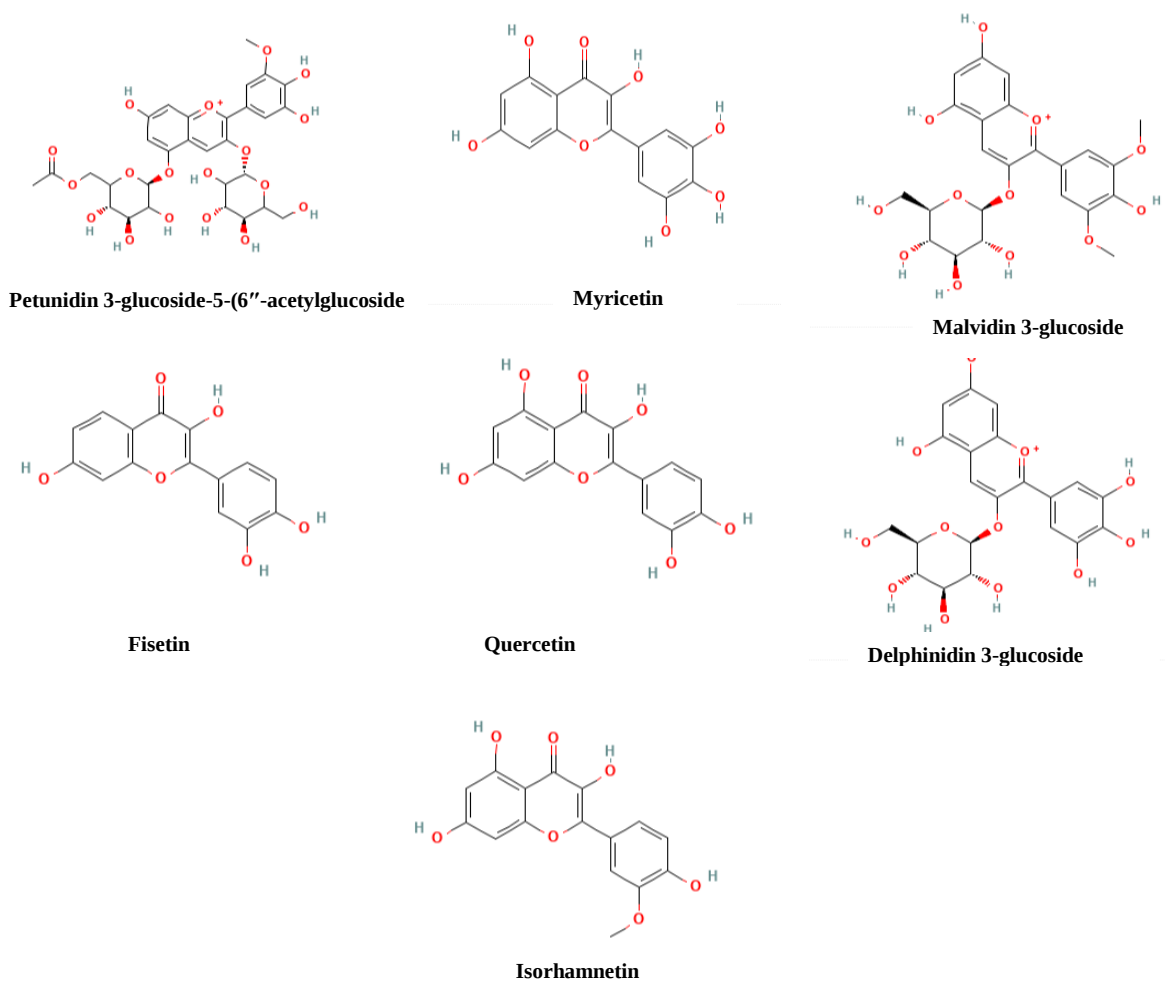


## Supplementary Material

### Computational Investigation of Compounds of *Allium cepa* as Potential Inhibitors of Transforming Growth Factor-beta Signaling in Cancer

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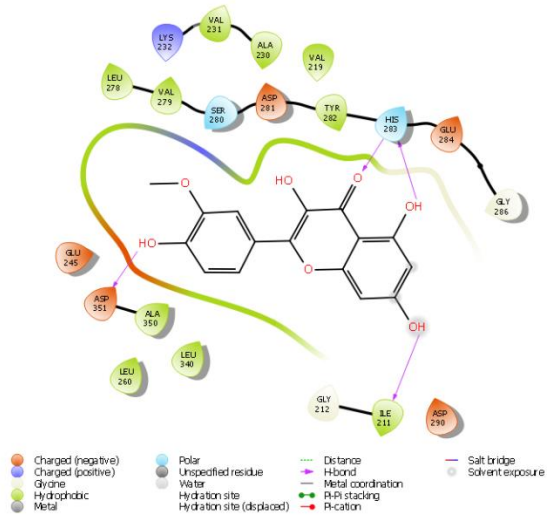


**Fig. 1** The chemical structures of top scoring compounds.

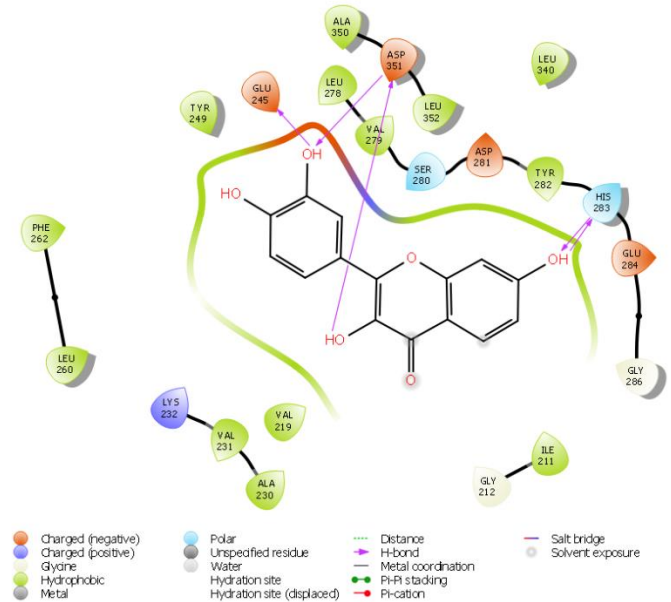
**Table S1** The 2D amino acid interaction of the top scoring compounds with TGFBR I.

| COMPOUNDS                                     | TGFBR I                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
|-----------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Petunidin 3-glucoside-5-(6''-acetylglucoside) | <p> <span style="color: red;">●</span> Charged (negative)<br/> <span style="color: blue;">●</span> Charged (positive)<br/> <span style="color: green;">●</span> Glycine<br/> <span style="color: yellow;">●</span> Hydrophobic<br/> <span style="color: grey;">●</span> Metal         </p> <p> <span style="color: blue;">○</span> Polar<br/> <span style="color: grey;">○</span> Unspecified residue<br/> <span style="color: grey;">○</span> Water<br/> <span style="color: grey;">○</span> Hydration site<br/> <span style="color: grey;">○</span> Hydration site (displaced)         </p> <p> <span style="color: red;">---</span> Distance<br/> <span style="color: blue;">---</span> H-bond<br/> <span style="color: green;">---</span> Metal coordination<br/> <span style="color: yellow;">---</span> Pi-Pi stacking<br/> <span style="color: red;">---</span> Pi-cation         </p> <p> <span style="color: red;">---</span> Salt bridge<br/> <span style="color: grey;">○</span> Solvent exposure         </p> |
| Myricetin                                     | <p> <span style="color: red;">●</span> Charged (negative)<br/> <span style="color: blue;">●</span> Charged (positive)<br/> <span style="color: green;">●</span> Glycine<br/> <span style="color: yellow;">●</span> Hydrophobic<br/> <span style="color: grey;">●</span> Metal         </p> <p> <span style="color: blue;">○</span> Polar<br/> <span style="color: grey;">○</span> Unspecified residue<br/> <span style="color: grey;">○</span> Water<br/> <span style="color: grey;">○</span> Hydration site<br/> <span style="color: grey;">○</span> Hydration site (displaced)         </p> <p> <span style="color: red;">---</span> Distance<br/> <span style="color: blue;">---</span> H-bond<br/> <span style="color: green;">---</span> Metal coordination<br/> <span style="color: yellow;">---</span> Pi-Pi stacking<br/> <span style="color: red;">---</span> Pi-cation         </p> <p> <span style="color: red;">---</span> Salt bridge<br/> <span style="color: grey;">○</span> Solvent exposure         </p> |
| Malvidin-3-glucoside                          | <p> <span style="color: red;">●</span> Charged (negative)<br/> <span style="color: blue;">●</span> Charged (positive)<br/> <span style="color: green;">●</span> Glycine<br/> <span style="color: yellow;">●</span> Hydrophobic<br/> <span style="color: grey;">●</span> Metal         </p> <p> <span style="color: blue;">○</span> Polar<br/> <span style="color: grey;">○</span> Unspecified residue<br/> <span style="color: grey;">○</span> Water<br/> <span style="color: grey;">○</span> Hydration site<br/> <span style="color: grey;">○</span> Hydration site (displaced)         </p> <p> <span style="color: red;">---</span> Distance<br/> <span style="color: blue;">---</span> H-bond<br/> <span style="color: green;">---</span> Metal coordination<br/> <span style="color: yellow;">---</span> Pi-Pi stacking<br/> <span style="color: red;">---</span> Pi-cation         </p> <p> <span style="color: red;">---</span> Salt bridge<br/> <span style="color: grey;">○</span> Solvent exposure         </p> |

**Isorhamnetin**



**Fisetin**



**Table S2** The 2D amino acid interaction of the top scoring compounds with TGFBR II.

| COMPOUNDS | TGFBR II                                                                                                                                                                                                                                                                                                           |
|-----------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Myricetin | <p>Charged (negative)<br/>Charged (positive)<br/>Glycine<br/>Hydrophobic<br/>Metal</p> <p>Polar<br/>Unspecified residue<br/>Water<br/>Hydration site<br/>Hydration site (displaced)</p> <p>Distance<br/>H-bond<br/>Metal coordination<br/>Pi-Pi stacking<br/>Pi-cation</p> <p>Salt bridge<br/>Solvent exposure</p> |
| Quercetin | <p>Charged (negative)<br/>Charged (positive)<br/>Glycine<br/>Hydrophobic<br/>Metal</p> <p>Polar<br/>Unspecified residue<br/>Water<br/>Hydration site<br/>Hydration site (displaced)</p> <p>Distance<br/>H-bond<br/>Metal coordination<br/>Pi-Pi stacking<br/>Pi-cation</p> <p>Salt bridge<br/>Solvent exposure</p> |

**Legend:**

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