

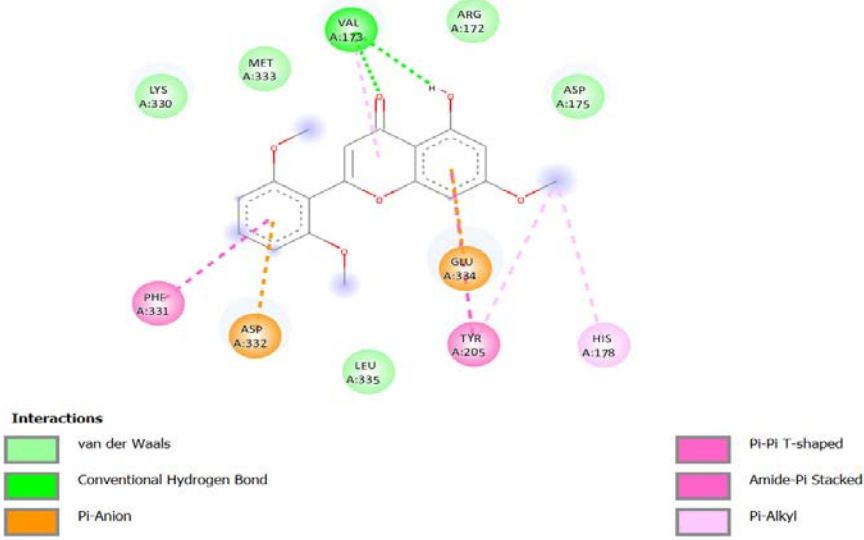
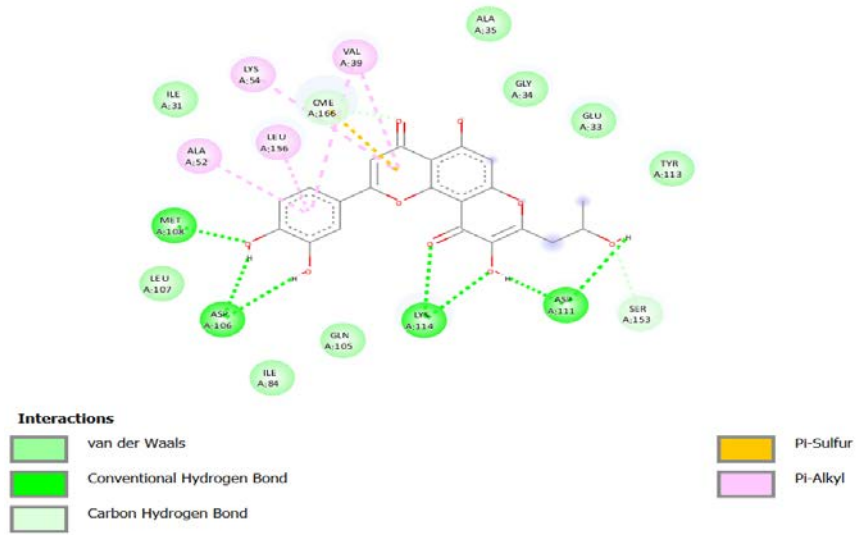
Competitive inhibition of catechol from *Andrographis paniculata* in the complex of ERK2 in lung metastasis

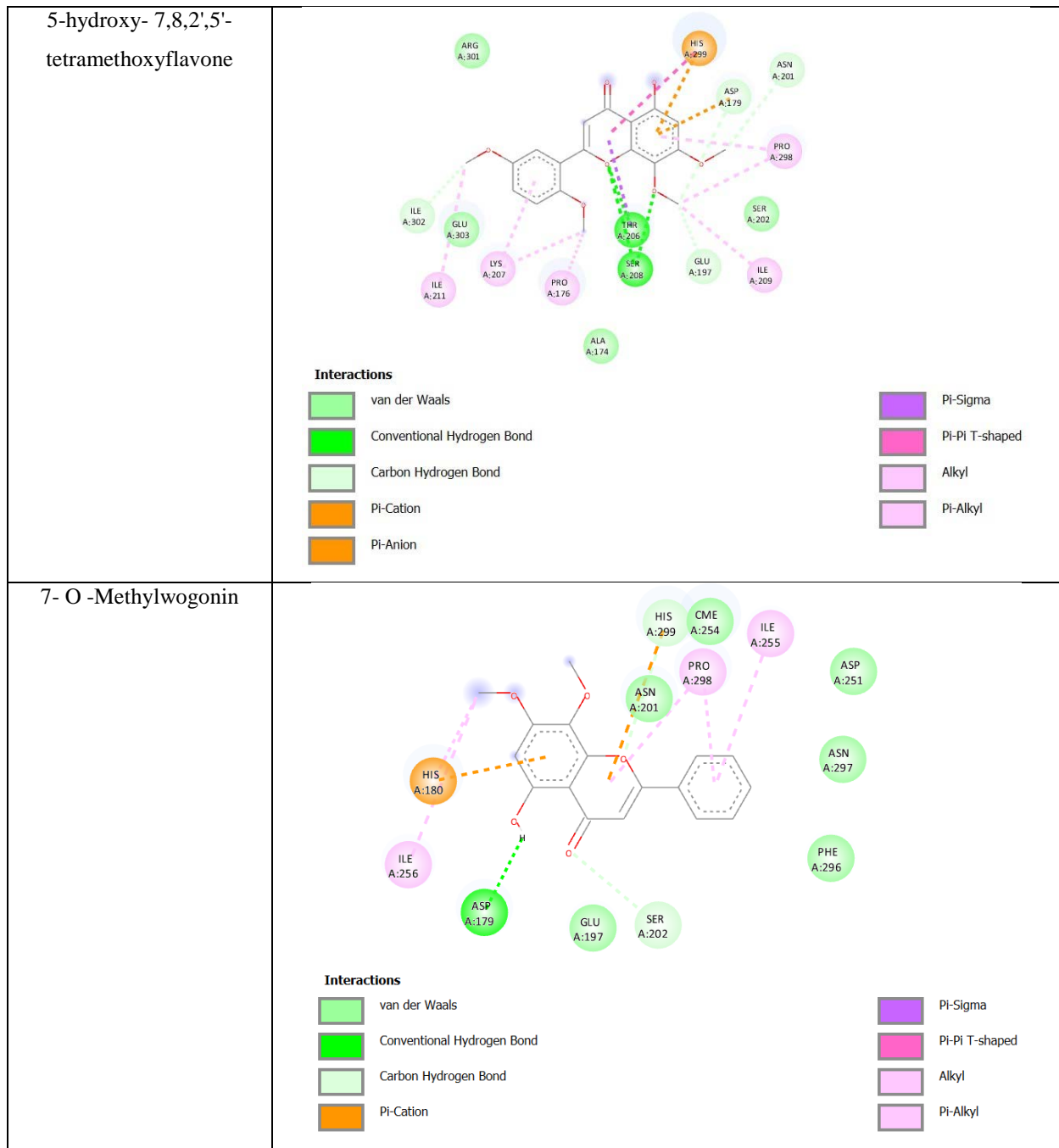
Surya Pratap Gurjar, Arpita Roy, Aaryan Gupta

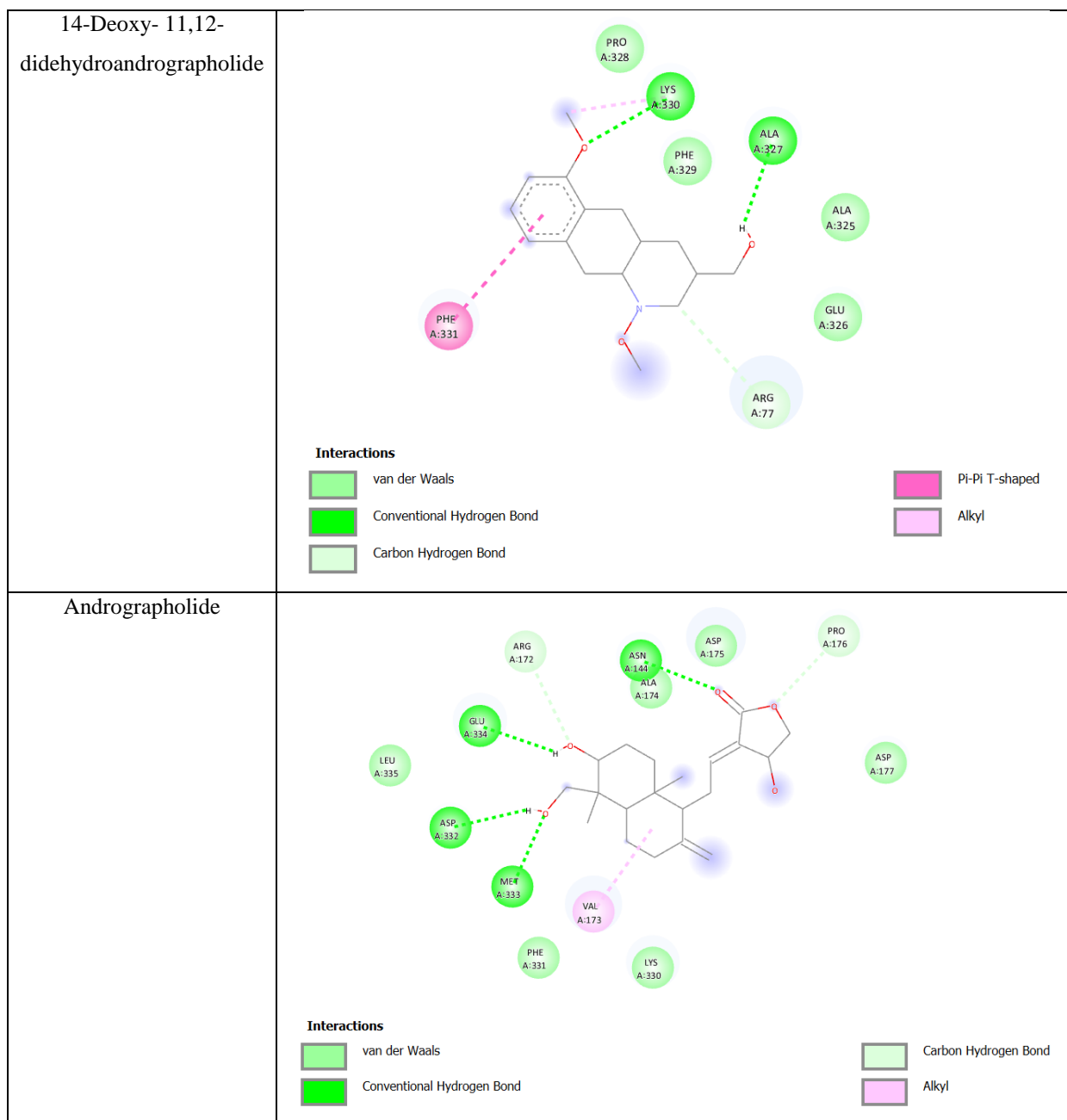
Department of Biotechnology, School of Engineering and Technology, Sharda University, Greater Noida, India

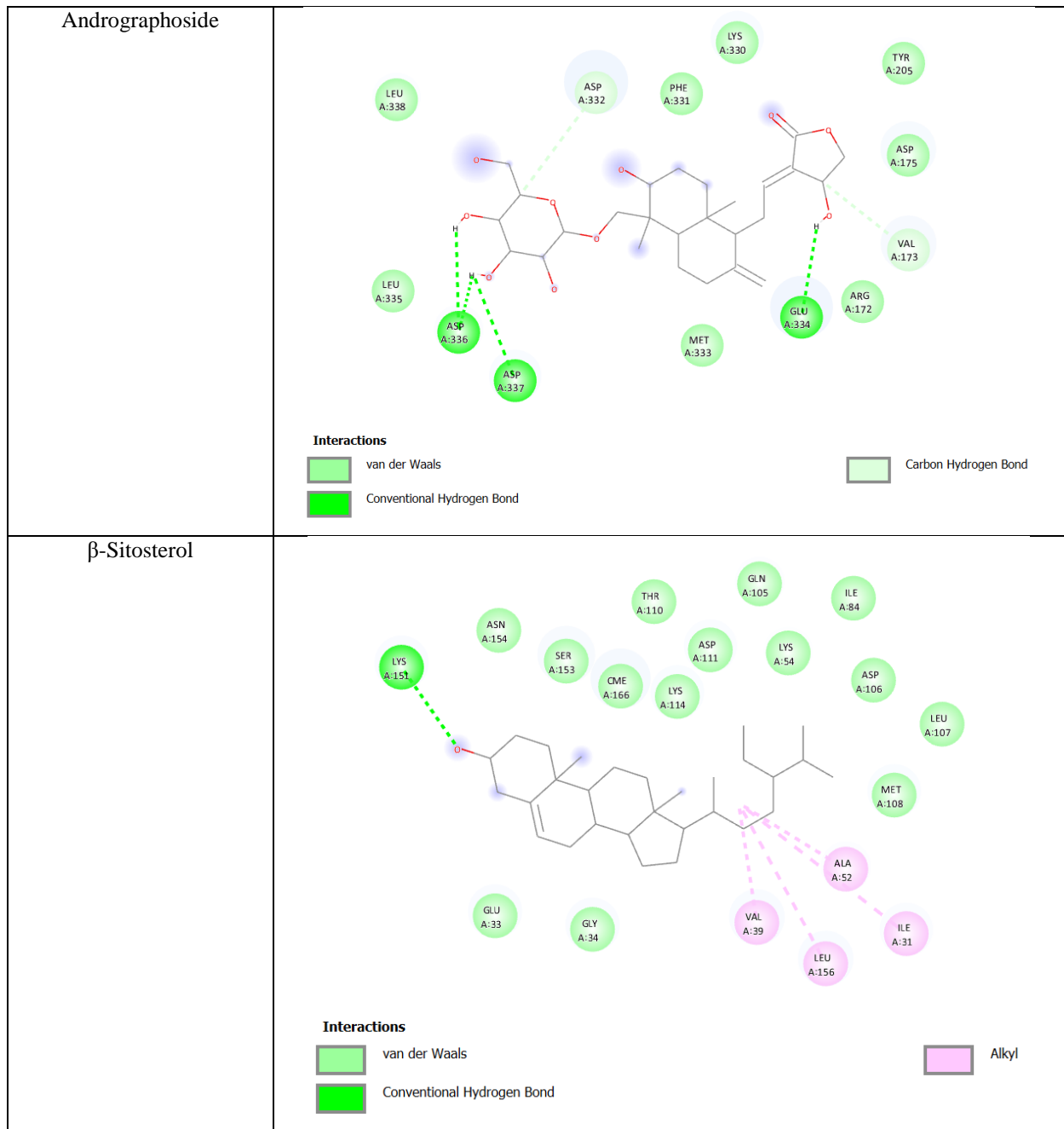
Supplementary Information File

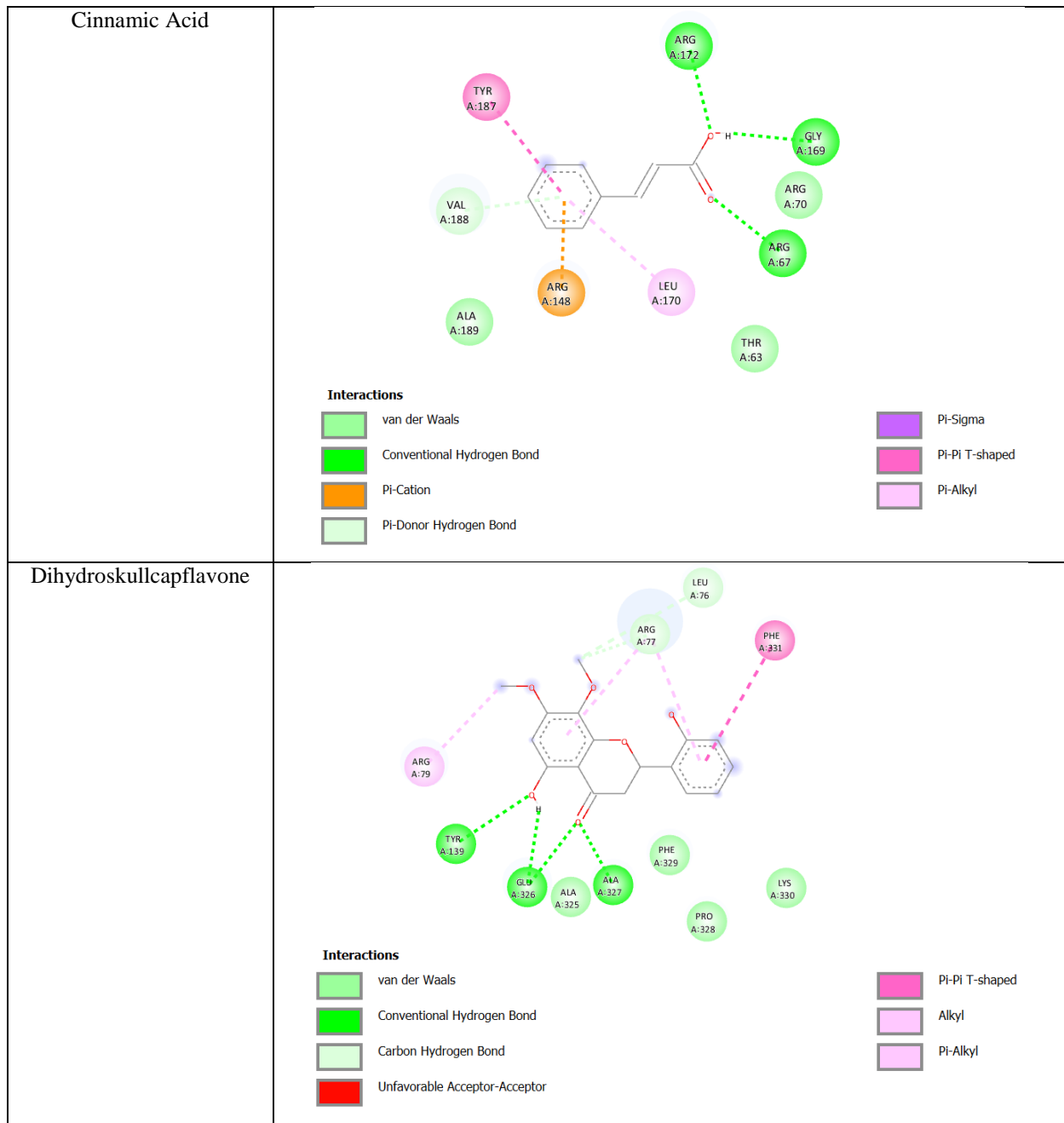
Table 4: Various 2D Ligand interactions generated by compounds of *Andrographis paniculata* with Complex of ERK2 with catechol (PDB: 4ZXT) at the catalytically active site

Ligands	2D Ligand Interactions with 4ZXT
5-Hydroxy- 7,2',6'-trimethoxyflavone	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Pi-Anion Pi-Pi T-shaped Amide-Pi Stacked Pi-Alkyl
5-hydroxy- 7,8,2',3'-tetramethoxyflavone	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Sulfur Pi-Alkyl









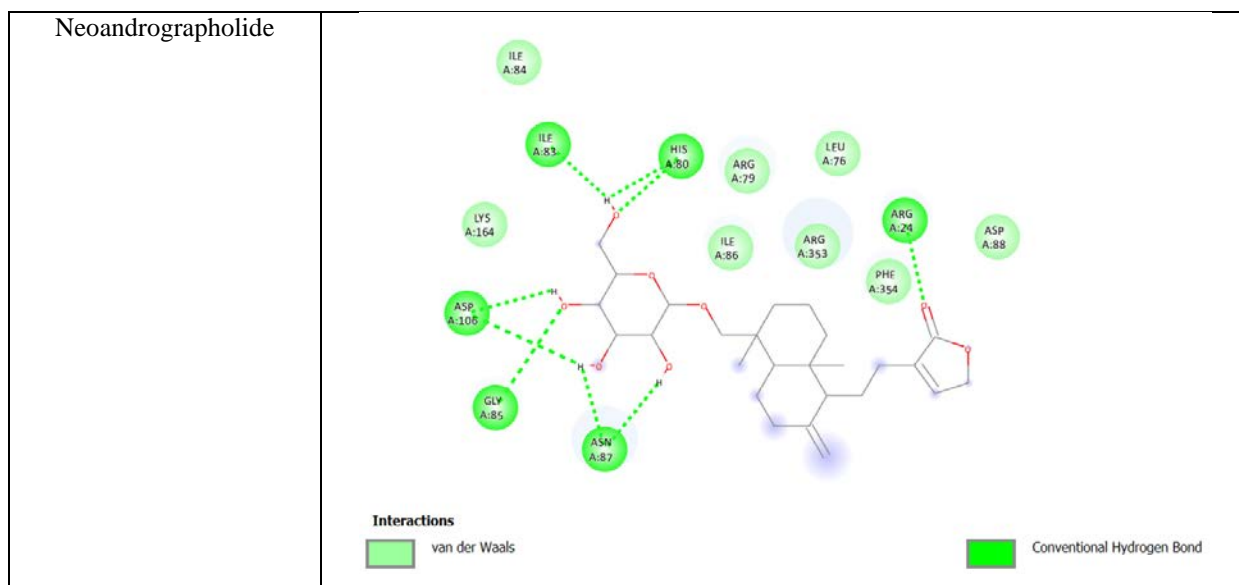
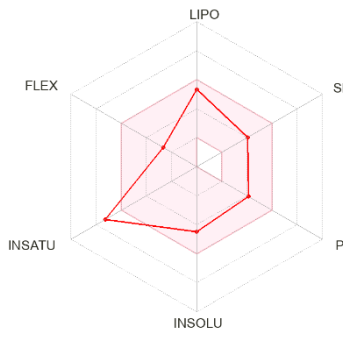
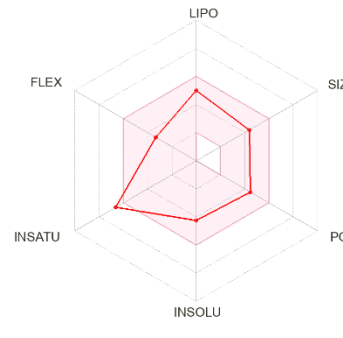
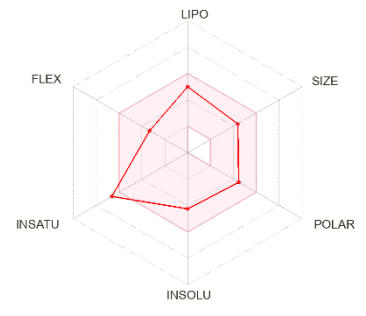
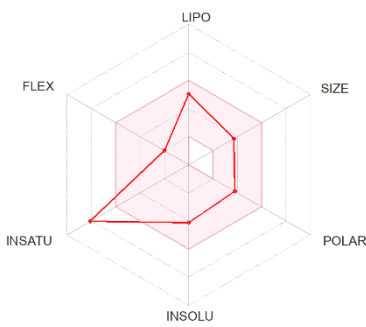
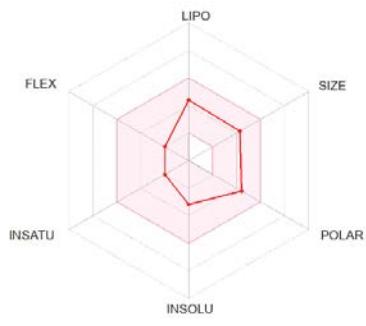
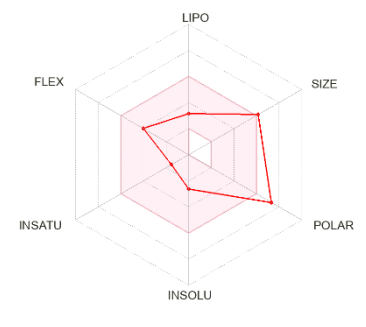


Table 5: Bioavailability Radar analysis of screened compounds using SwissADME

Compounds	Bioavailability Radar
5-Hydroxy- 7,2',6'-trimethoxyflavone	
5-hydroxy- 7,8,2',3'-tetramethoxyflavone	

<p>5-hydroxy- 7,8,2',5'-tetramethoxyflavone</p>	 <p>A radar chart with six axes: LIPO (top), SIZE (top-right), POLAR (right), INSOLU (bottom), INSATU (bottom-left), and FLEX (left). The chart shows a red line connecting the data points for each axis, with a light red shaded area representing the overall profile. The values are relatively balanced across all axes.</p>
<p>7- O -Methylwogonin</p>	 <p>A radar chart with six axes: LIPO (top), SIZE (top-right), POLAR (right), INSOLU (bottom), INSATU (bottom-left), and FLEX (left). The chart shows a red line connecting the data points, with a light red shaded area. The INSATU axis shows a notably higher value compared to the other axes.</p>
<p>14-Deoxy- 11,12-didehydroandrographolide</p>	 <p>A radar chart with six axes: LIPO (top), SIZE (top-right), POLAR (right), INSOLU (bottom), INSATU (bottom-left), and FLEX (left). The chart shows a red line connecting the data points, with a light red shaded area. The values are relatively balanced across all axes.</p>
<p>Andrographolide</p>	 <p>A radar chart with six axes: LIPO (top), SIZE (top-right), POLAR (right), INSOLU (bottom), INSATU (bottom-left), and FLEX (left). The chart shows a red line connecting the data points, with a light red shaded area. The POLAR axis shows a notably higher value compared to the other axes.</p>

