

Table: Residues and bond lengths of 10 bioactive compounds of *A. paniculata* docked with CTX-M-15

| S. No     | Compound             | Residues | Bond length   |
|-----------|----------------------|----------|---|
| <b>1</b>  | Onysilin             | ASN107   | 3.1 A <sup>0</sup>  |
|           |                      | ASN135   | 3.1 A <sup>0</sup>  |
| <b>2</b>  | Neoandrographolide   | ARG257   | 3.3 A <sup>0</sup>  |
|           |                      | ALA273   | 1.9 A <sup>0</sup>  |
|           |                      | ALA273   | 3.3 A <sup>0</sup>  |
|           |                      | PRO170   | 1.9 A <sup>0</sup>  |
| <b>3</b>  | Luteolin             | ASN135   | 2.4 A <sup>0</sup>  |
|           |                      | ASN107   | 3.3 A <sup>0</sup>  |
|           |                      | ARG257   | 2.3 A <sup>0</sup>  |
|           |                      | SER133   | 3 A <sup>0</sup>  |
| <b>4</b>  | Bisandrographolide A | GLY244   | 3.5 A <sup>0</sup>  |
|           |                      | ARG257   | 3.3 A <sup>0</sup>  |
| <b>5</b>  | Apigenin             | ASN107   | 3.3 A <sup>0</sup>  |
|           |                      | ASN135   | 3.2 A <sup>0</sup>  |
| <b>6</b>  | Andrographolactone   | SER240   | 2.5 A <sup>0</sup>  |
| <b>7</b>  | Andrographiside      | ARG257   | 3.5 A <sup>0</sup>  |
|           |                      | ASN135   | 2.2 A <sup>0</sup>  |
|           |                      | TYR132   | 2.3 A <sup>0</sup>  |
| <b>8</b>  | Andrographidine C    | SER240   | 3.4A <sup>0</sup> , 2.8A <sup>0</sup> , 2.5A <sup>0</sup> |
|           |                      | SER73    | 3.1A <sup>0</sup> , 3.5A <sup>0</sup>                     |
|           |                      | THR238   | 2A <sup>0</sup> , 3A <sup>0</sup>                         |
|           |                      | TYR108   | 2.8A <sup>0</sup>   |
| <b>9</b>  | Andrographidine A    | ASN107   | 3.5A <sup>0</sup>   |
|           |                      | ARG257   | 2.7A <sup>0</sup> , 2.9A <sup>0</sup>                     |
| <b>10</b> | Andrograpanin        | ARG257   | 2.6 A <sup>0</sup>  |