### Supplementary material:

#### Table 1: Results of Drug-Receptor Interactions

| Compounds       | Docking pose | Docking Scores | Receptor-ligand Hydrogen bonds | Amino acid | Position | Atom in amino acid | Atom in Ligand | Bond length |
|-----------------|--------------|----------------|--------------------------------|------------|----------|-------------------|----------------|-------------|
| **Absolute energy** | **Libdock score/No. of Hot spots** | **Total no. of H bonds/No. of contacts** | | | | | | | |
| Allixin         | 37.052       | 106.496/"4.59,8.01,6.95,A,57,5-2.39,-7.81,10.95,P,59,90.81,7,21,10.15,A,67,15" | 1/6 | GLU | 192 | OE2 | H34 | 2.17653 |
| Anethole        | 27.785       | 90.911/"5.01,-6.41,15.55,A,88,1,8.01,-5.61,19.15,A,97,5,6.81,-3.81,18,35,A,96,9" | 0/11 | - | - | - | - | - |
| Capsaicin       | 35.705       | 141.365/"4.19,-13.01,5,35,A,48,7-1.79,-8.21,9,95,A,66,181,81,-6.41,7,35,A,60,22" | 2/5 | ASP | 189 | OD1 | H46 | 1.84857 |
| Linearol        | 57.072       | 101.382/"-4.59,-8.01,6,95,A,57,1-4.99,-14,01,4,35,A,38,80.21,-16,01,5,15,A,46,17" | 0/9 | - | - | - | - | - |
| Syringic acid   | 34.445       | 68.893/"1.81,-6.41,7,35,A,60,1-4.59,-8.01,6,95,A,57,11,0.41,-7.61,11,75,P,63,14" | 2/6 | ALA | 190 | O | H24 | 2.28496 |
| Zoladex         | 64.012       | 146.95/"-4.19,-13.01,5,35,A,48,3-4.59,-8.01,6,95,A,57,34,-1.79,-8.21,9,95,A,66,39" | 6/6 | ALA | 195 | HN | O33 | 1.69827 |
|                 |              |                |                                | GLY        | 193     | HN | O33 | 1.96936 |
|                 |              |                |                                | GLY        | 193     | HN | O7  | 1.64495 |
|                 |              |                |                                | ASN        | 143     | HD22 | O29 | 2.12107 |
|                 |              |                |                                | THR        | 147     | O   | H73 | 2.22932 |
|                 |              |                |                                | GLU        | 39      | OE1 | H59 | 1.87838 |