Supplementary material:

Table 1: The structure both of ligand molecules test and ligands comparison as antihistamin (1) native ligand 5EH (2) native ligand D7V (3) (E,R)-marmin (4) skimmianine (5) (S)-aegeline (6) auraptene (7) zeorine (8) dustanine (9) cetirizine (10) diphenhydramine (11) chlorpheniramine (12) histamine

| No | Molecule           | Structure | No | Molecule | Structure |
|----|--------------------|-----------|----|----------|-----------|
| 1  | native ligand 5EH  |           | 7  | zeorine  |           |
| 2  | native ligand D7V |           | 8  | dustanine|           |
| 3  | (E,R)-marmin       |           | 9  | cetirizine|           |
| 4  | skimmianine        |           | 10 | diphenhydramine |     |
| 5  | (S)-aegeline       |           | 11 | chlorpheniramine|   |
| 6  | auraptene          |           | 12 | histamine |           |