Supplementary Fig 1: PatchDock Analysis
### Molecular Docking Algorithms Based on Shape Complementarity Principles

#### Table 1: Results of the Molecular Docking

| Solution No | Score 1 | Score 2 | Score 3 | Transformations | Plot File of the Complex |
|-------------|---------|---------|---------|-----------------|--------------------------|
| 1           | 23880   | 413.70  | 54.79   | -3.37           | 1.51.2.52.42.56.91.11.16 |
| 2           | 21500   | 109.40  | 54.79   | -2.34           | 1.51.2.52.42.56.91.11.16 |
| 3           | 20100   | 48.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 4           | 19900   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 5           | 19700   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 6           | 19500   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 7           | 19300   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 8           | 19200   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 9           | 19100   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 10          | 19000   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |

**NEXT** E-mail view

### Molecular Docking Algorithms Based on Shape Complementarity Principles

#### Table 2: Additional Results

| Solution No | Score 1 | Score 2 | Score 3 | Transformations | Plot File of the Complex |
|-------------|---------|---------|---------|-----------------|--------------------------|
| 11          | 18900   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 12          | 18800   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 13          | 18700   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 14          | 18600   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 15          | 18500   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 16          | 18400   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 17          | 18300   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 18          | 18200   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 19          | 18100   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
| 20          | 18000   | 41.50   | 54.79   | -1.34           | 1.51.2.52.42.56.91.11.16 |
