

Appendix 1

Table 1. Summary results from ClusPro2.0

| Cluster | Members | Weighted Score (kcal/mol) |
|---------|---------|---------------------------|
| 0 | 128 | -199,1 |
| 1 | 191 | -213,5 |
| 2 | 110 | -209,8 |
| 3 | 21 | -215,6 |
| 4 | 37 | -225,8 |
| 5 | 22 | -224,2 |
| 6 | 22 | -207 |
| 7 | 21 | -196,4 |
| 8 | 20 | -211,5 |
| 9 | 12 | -206,5 |
| 10 | 12 | -203,8 |
| 11 | 10 | -208,6 |
| 12 | 10 | -203,2 |
| 13 | 10 | -196,1 |