

Antioxidant, cytotoxic, and anti-venom activity of *Alstonia parvifolia* Merr. Bark

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SUPPLEMENTARY DATA

Table 2. Top three clusters of HPT conformations docked to candidate targets in *Naja sp.* venom.

| Species | PLA ₂ homologues | No. of conformations | Highest binding energy (kcal/mol) |
|-------------------------|--------------------------------|-------------------------|--------------------------------------|
| <i>Naja sagittifera</i> | 1LN8 | | |
| | cluster 1 | 57 | -8.74 |
| | cluster 2 | 105 | -7.78 |
| | cluster 3 | 23 | -7.45 |
| | 1S6B | | |
| | cluster 1 | 169 | -9.77 |
| | cluster 2 | 12 | -9.53 |
| | cluster 3 | 9 | -8.49 |
| | <i>Naja naja</i> | 1PSH | |
| cluster 1 | | 54 | -9.66 |
| cluster 2 | | 34 | -9.33 |
| cluster 3 | | 49 | -9.33 |
| 1A3F | | | |
| cluster 1 | | 136 | -9.39 |
| cluster 2 | 5 | -7.83 | |
| cluster 3 | 10 | -7.38 | |