**Hydrogen Bond Propensity Analysis for {{identifier}}**

**Predicted intermolecular hydrogen bond propensities of {{identifier}}**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Donor** | **Acceptor** | **Propensity** | **Lower bound** | **Upper bound** |
| {%tr for p in propensities if p.is\_intermolecular %} | | | | |
| {{p.donor\_label}} | {{p.acceptor\_label}} | **{{p.propensity|round(3)}}** | {{p.bounds[0]|round(3)}} | {{p.bounds[1]|round(3)}} |
| {%tr endfor %} | | | | |
|  | | | | |

**Hydrogen bond coordination likelihood**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Atom (D/A)** | **0** | **1** | | **2** |  |
| {%tr for d in donors %} | | |  | | |
| {{d.label}} of {{d.functional\_group\_identifier}} (d) | {{dscores[d.label][0]}} | {{dscores[d.label][1]}} | | {{dscores[d.label][2]}} |  |
| {%tr endfor %} | | |  | | |
| {%tr for a in acceptors %} | | |  | | |
| {{a.label}} of {{a.functional\_group\_identifier}} (a) | {{ascores[a.label][0]}} | {{ascores[a.label][1]}} | | {{ascores[a.label][2]}} |  |
| {%tr endfor %} | | |  | | |
|  |  |  | |  |  |