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

{{chart}}

**Hydrogen bond propensity chart for {{identifier}}**

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

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Donor** | **Acceptor** | **Propensity** | **Lower bound** | **Upper bound** | **Observed Inter-?** |
| {%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)}} | {% if p.is\_observed %} **Yes** {% endif %} |
| {%tr endfor %} | | | | | |
|  | | | | | |

{% if intra\_flag %}

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

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Donor** | **Acceptor** | **Propensity** | **Lower bound** | **Upper bound** |
| {%tr for p in propensities if not 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 %} | | | | |
|  | | | | |

{% else %}

No intramolecular hydrogen bonds predicted

{% endif %}

**Hydrogen bond coordination likelihood**

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

Cells coloured green or red are the observed outcomes for each atom. Green is the optimal outcome, red is sub-optimal.

**Molecular Structure and Hydrogen Bond Donor/Acceptor Definitions**

{{diagram}}

**Chemical diagram for {{identifier}}**

|  |
| --- |
| **Hydrogen Bond Donor Atoms** |
| {%tr for item in don %} |
| {{item[:-2]}} |
| {%tr endfor %} |

|  |
| --- |
| **Hydrogen Bond Acceptor Atoms** |
| {%tr for item in acc %} |
| {{item[:-2]}} |
| {%tr endfor %} |

**Functional Group Definitions for CSD Substructure Searches**

|  |  |
| --- | --- |
| **Search Fragments** | |
| {%tr for key, value in fg\_diagrams|dictsort %} | |
| {{key}} | {{value}} |
| {%tr endfor %} | |

Key:

Tn = atom makes n bonds

a = atom is acyclic

c = atom is cyclic

ⓐ= bond is acyclic

© = bond is cyclic

Hn = n bonded H atoms

v = any bond order

**Search Results**

|  |  |
| --- | --- |
| **Functional Group** | **Number of Hits Selected** |
| {%tr for g in functional\_groups %} | |
| {{g.identifier}} | {{ data.nitems(g)}} ({{data.advice\_comment(g)}}) |
| {%tr endfor %} | |

**Number of hits selected per functional group**

Total hits selected for training dataset: {{len\_data}} ({{data.advice\_comment()}})

**Hydrogen Bond Analysis of Training Dataset**

|  |  |  |  |
| --- | --- | --- | --- |
| **Category** | **Label** | **# True** | **# False** |
| {%tr for d in donors %} | | | |
| Donor | {{d.functional\_group\_identifier}} (matches {{d.label}}) | {{d.npositive}} | {{d.nnegative}} |
| {%tr endfor %} | | | |
| {%tr for a in acceptors %} | | | |
| Acceptor | {{a.functional\_group\_identifier}} (matches {{a.label}}) | {{a.npositive}} | {{a.nnegative}} |
| {%tr endfor %} | | | |

**Hydrogen bond donor and acceptor outcomes.**

**Regression Analysis**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Coefficients** | **Estimate** | **Std. error** | **z-value** | **Pr(>|z|)** | **Significance code** | **Lower bound** | **Upper Bound** |
| {%tr for c in coefficients %} | | | | | | | |
| {{c.identifier}} | **{{c.estimate|round(3)}}** | {%if c.standard\_error %}{{c.standard\_error|round(3)}}  {%else %}N/A  {%endif %} | {%if c.z\_value %}{{c.z\_value|round(3)}}  {%else %}N/A  {%endif %} | {%if c.p\_value %}{{c.p\_value|round(3)}}  {%else %}N/A  {%endif %} | {{c.significance\_code}} | {%if c.confidence\_interval[0] %}{{c. confidence\_interval [0]|round(3)}}  {%else %}N/A  {%endif %} | {%if c.confidence\_interval[1] %}{{c. confidence\_interval [1]|round(3)}}  {%else %}N/A  {%endif %} |
| {%tr endfor %} | | | | | | | |

**Model coefficients**

**Goodness of fit**

Area under ROC curve: {{model.area\_under\_roc\_curve|round(3)}} – {{model.advice\_comment}} discrimination