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

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | | {{identifier}}  ({{obs\_pairs}} pairs) | | | {{chart}} | | | | | | | | | |
| Number of intermolecular H-bond pairs | | | | | | | | | | | | | | |
| {% if mpair\_flag %}<={% endif %}{{colour\_pairs[0]}} | | | {{colour\_pairs[1]}} | {{colour\_pairs[2]}} | | {{colour\_pairs[3]}} | {{colour\_pairs[4]}} | {{colour\_pairs[5]}} | {{colour\_pairs[6]}} | {{colour\_pairs[7]}} | {{colour\_pairs[8]}} | {{colour\_pairs[9]}} | {% if mpair\_flag %}>={% endif %}{{colour\_pairs[10]}} |
| ({{count\_pairs[0]}}) | | | ({{count\_pairs[1]}}) | ({{count\_pairs[2]}}) | | ({{count\_pairs[3]}}) | ({{count\_pairs[4]}}) | ({{count\_pairs[5]}}) | ({{count\_pairs[6]}}) | ({{count\_pairs[7]}}) | ({{count\_pairs[8]}}) | ({{count\_pairs[9]}}) | ({{count\_pairs[10]}}) |
|  | | | | | | | | | | | | | |
|  | Min. donor co-ordination likelihood……...……………………………………………………………………………. | | | | | | | | | | | | {{min\_donor\_coordination}} |
|  |  | | | | | | | | | | | | |
|  | Min. acceptor co-ordination likelihood………………………………………………………………………………… | | | | | | | | | | | | {{ min\_acceptor\_coordination}} |

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

Observed hydrogen bond network in {{identifier}} with {{obs\_pairs}} intermolecular H-bond pair(s), mean propensity of {{'%0.2f' % observed\_groups.hbond\_score}} and mean co-ordination of {{'%0.2f' % mean\_coordination}}.{% if intra\_obs %} An additional {{intra\_count}} intramolecular H-bond pair(s) occur.{% endif %}

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

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Donor** | **Acceptor** | **Propensity** | **Lower bound** | **Upper bound** | **#Hbonds** | **Donor ranking** | **Acc. ranking** | **Observed Inter-?** |
| {%tr for p in propensities if p.is\_intermolecular %} | | | | | | | | |
| {{p.donor\_label}}{% if p.donor.atom.formal\_charge > 0 %} (+{{p.donor.atom.formal\_charge}}){% elif p.donor.atom.formal\_charge < 0 %} ({{p.donor.atom.formal\_charge }}){% endif %} of {{p.donor.functional\_group\_identifier}} | {{p.acceptor\_label}}{% if p. acceptor.atom.formal\_charge > 0 %} (+{{p. acceptor.atom.formal\_charge}}){% elif p. acceptor.atom.formal\_charge < 0 %} ({{p. acceptor.atom.formal\_charge }}){% endif %} of {{p.acceptor.functional\_group\_identifier}} | **{{p.propensity|round(3)}}** | {{p.bounds[0]|round(3)}} | {{p.bounds[1]|round(3)}} | {{p.hbond\_count}} | {{p.donor\_rank}} | {{p.acceptor\_rank}} | {% if p.is\_observed %}**Yes**{% endif %}{% if p.is\_donor\_bifurcated and p.is\_acceptor\_bifurcated%} (dB+aB){% elif p.is\_donor\_bifurcated %} (dB){% elif p.is\_acceptor\_bifurcated %} (aB){% endif %} |
| {%tr endfor %} | | | | | | | | |
| \* Formal charge indicated in brackets if +/-, dB = donor bifurcated, aB = acceptor bifurcated | | | | | | | | |

{% if intra\_flag %}

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Donor** | **Acceptor** | **Propensity** | **Observed Intra-?** |
| {%tr for p in propensities if not p.is\_intermolecular %} | | | |
| {{p.donor\_label}}{% if p.donor.atom.formal\_charge > 0 %} (+{{p.donor.atom.formal\_charge}}){% elif p.donor.atom.formal\_charge < 0 %} ({{p.donor.atom.formal\_charge }}){% endif %} of {{p.donor.functional\_group\_identifier}} | {{p.acceptor\_label}}{% if p. acceptor.atom.formal\_charge > 0 %} (+{{p. acceptor.atom.formal\_charge}}){% elif p. acceptor.atom.formal\_charge < 0 %} ({{p. acceptor.atom.formal\_charge }}){% endif %} of {{p.acceptor.functional\_group\_identifier}} | **{{p.propensity|round(3)}}** | {% if p.is\_observed %}**Yes**{% endif %} |
| {%tr endfor %} | | | |
| \* Formal charge indicated in brackets if +/- | | |  |

{% else %}

No intramolecular hydrogen bonds predicted

{% endif %}

**Hydrogen bond co-ordination likelihood**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Atom (D/A)** | **=0** | **{%r if coord\_cols[1] %}=1{%r endif %}** | **{%r if coord\_cols[2] %}=2{%r endif %}** | **{%r if coord\_cols[3] %}=3{%r endif %}** | **{%r if coord\_cols[4] %}=4{%r endif %}** | **{%r if coord\_cols[5] %}=5{%r endif %}** | **{%r if coord\_cols[6] %}=6{%r endif %}** |
| {%tr for d in donors %} | | | | | | |  |
| {{d.label}}{% if d.atom.formal\_charge > 0 %} (+{{d.atom.formal\_charge}}){% elif d.atom.formal\_charge < 0 %} ({{d.atom.formal\_charge }}){% endif %} of {{d.functional\_group\_identifier}} (d) | {% 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]}} | {% cellbg dbg[d.label][3] %}{{dscores[d.label][3]}} | {% cellbg dbg[d.label][4] %}{{dscores[d.label][4]}} | {% cellbg dbg[d.label][5] %}{{dscores[d.label][5]}} | {% cellbg dbg[d.label][6] %}{{dscores[d.label][6]}} |
| {%tr endfor %} | | | | | | | |
| {%tr for a in acceptors %} | | | | | | | |
| {{a.label}}{% if a.atom.formal\_charge > 0 %} (+{{a.atom.formal\_charge}}){% elif a.atom.formal\_charge < 0 %} ({{a.atom.formal\_charge }}){% endif %} of {{a.functional\_group\_identifier}} (a) | {% 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]}} | {% cellbg abg[a.label][3] %}{{ascores[a.label][3]}} | {% cellbg abg[a.label][4] %}{{ascores[a.label][4]}} | {% cellbg abg[a.label][5] %}{{ascores[a.label][5]}} | {% cellbg abg[a.label][6] %}{{ascores[a.label][6]}} |
| {%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**

|  |
| --- |
| {%tr for c in component\_diagrams %} |
| {{c}} |
| {%tr endfor %} |

**Chemical diagram for each component in {{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**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Functional group definitions for CSD substructure searches** | | | | |
| Key: | Tn = atom makes n bonds | | | |
| a = atom is acyclic | c = atom is cyclic | | Hn = n bonded H atoms | |
| ⓐ = bond is acyclic | © = bond is cyclic | | v = any bond order | |
| {%tr for key, value in fg\_diagrams|dictsort %} | | | | |
| {{key}} | | {{value}} | | |
| {%tr endfor %} | | | | |
|  | |  | |  |

**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 %} | | | |

**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