# Tests-InChI-105

# Pre-release

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| inchi-1 | Linux | 64bit | PubChem Compound (60,915175) |
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|  | Options | Result | Completed |
| std-01 |  | + | 2016-09-11 |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.std-02-105.out PUBCC\_20151028.std-02-105.log NUL -AuxNone -NoLabels -NEWPSOFF & |  |  |  |
| std-03 | -Snon | + | 2016-09-18 |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.std-04-105.out PUBCC\_20151028.std-04-105.log NUL -AuxNone -NoLabels -DoNotAddH & |  |  |  |
| ################ nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.std-05-105.out PUBCC\_20151028.std-05-105.log NUL -AuxNone -NoLabels -SNon -DoNotAddH & |  |  |  |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-01-105.out PUBCC\_20151028.non-std-01-105.log NUL -AuxNone -NoLabels -SUU -SLUUD & |  |  |  |
| non-std-02 | -SRel | + | 2016-09-19 |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-03-105.out PUBCC\_20151028.non-std-03-105.log NUL -AuxNone -NoLabels -SRac & |  |  |  |
| non-std-04 | -SUU -SLUUD -SUCF | + | 2016-09-18 |
| non-std-05 | -NEWPSOFF -Srel | + | 2016-09-17 |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-06-105.out PUBCC\_20151028.non-std-06-105.log NUL -AuxNone -NoLabels -NEWPSOFF -SRac & |  |  |  |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-07-105.out PUBCC\_20151028.non-std-07-105.log NUL -AuxNone -NoLabels -NEWPSOFF -SLUUD -SUCF & |  |  |  |
| non-std-08 | -FixedH | + | 2016-09-13 |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-09-105.out PUBCC\_20151028.non-std-09-105.log NUL -AuxNone -NoLabels -NEWPSOFF -FixedH & |  |  |  |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-10-105.out PUBCC\_20151028.non-std-10-105.log NUL -AuxNone -NoLabels -FixedH -SNon & |  |  |  |
| non-std-11 | -FixedH -SRel | + | 2016-09-18 |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-12-105.out PUBCC\_20151028.non-std-12-105.log NUL -AuxNone -NoLabels -RecMet & |  |  |  |
| non-std-13 | NoLabels -NEWPSOFF -RecMet | + | 2016-09-13 |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-14-105.out PUBCC\_20151028.non-std-14-105.log NUL -AuxNone -NoLabels -RecMet -SNon & |  |  |  |
| non-std-15 | -RecMet -SRel | + | 2016-09-18 |
| non-std-16 | -FixedH -RecMet | + | 2016-09-12 |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-17-105.out PUBCC\_20151028.non-std-17-105.log NUL -AuxNone -NoLabels -NEWPSOFF -FixedH -RecMet& |  |  |  |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-18-105.out PUBCC\_20151028.non-std-18-105.log NUL -AuxNone -NoLabels -FixedH -RecMet -SNon & |  |  |  |
| non-std-19 | -FixedH -RecMet -SRel -SDF:PUBCHEM\_COMPOUND\_CID | + | 2016-09-13 |
| non-std-20 | -KET | + | 2016-09-13 |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-21-105.out PUBCC\_20151028.non-std-21-105.log NUL -AuxNone -NoLabels -KET -SNon & |  |  |  |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-22-105.out PUBCC\_20151028.non-std-22-105.log NUL -AuxNone -NoLabels -KET -SRel & |  |  |  |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-23-105.out PUBCC\_20151028.non-std-23-105.log NUL -AuxNone -NoLabels -15T -Key & |  |  |  |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-24-105.out PUBCC\_20151028.non-std-24-105.log NUL -AuxNone -NoLabels -15T -SNon & |  |  |  |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-25-105.out PUBCC\_20151028.non-std-25-105.log NUL -AuxNone -NoLabels -15T -SRel & |  |  |  |
| non-std-26 | -KET -15T | + | 2016-09-13 |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-27-105.out PUBCC\_20151028.non-std-27-105.log NUL -AuxNone -NoLabels -NEWPSOFF -KET -15T -Key & |  |  |  |
| #nohup ./inchi-1 PUBCC\_20151028.sdf PUBCC\_20151028.non-std-28-105.out PUBCC\_20151028.non-std-28-105.log NUL -AuxNone -NoLabels -NEWPSOFF -KET -15T -SUU -SLUUD & |  |  |  |
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#### InChI round-trip test

The success rate for conversion of InChI to structures was measured using Rtrip option of test\_ixa program. In the round trip, InChIs generated from Molfile-format records were then used to restore structures and re-create InChIs from those structures, via corresponding API calls; original and final InChIs were then compared.

The results for PubChem Compound (60,915,175 molecules; checked in 64 bit Linux environmemt) are as follow:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| InChI options\* | Conversion failures | Conversion mismatches | Total problems, % | Success rate, % |
|  |  |  |  |  |
| Standard | 10 | 39596 | 0.07 | 99.93 |
| Non-standard |  |  |  |  |
| FixedH | 22 | 42165 | 0.07 | 99.93 |
| FixedH RecMet | 22 | 47896 | 0.08 | 99.92 |