# NPC\_PD2 Compound-file metadata

Here we describe the columns in the compound CSV file released in Feb. 2015 in the first public release of the NCATS-NPC Lilly-OIDD-PD2 phenotypic assay dataset. This release is comprised of three datafiles, for (1) compounds, (2) assays, and (3) measured bioactivity, and associated metadata.

|  |  |  |
| --- | --- | --- |
| **column** | **source** | **description** |
| OIDD:Serial No. | OIDD | ? |
| **OIDD:NCATS\_Name** | **OIDD** | **NCGC\_ID** |
| OIDD:OIDD\_ID of Untitled 5 | OIDD | ? |
| OIDD:Trivial Name | OIDD |  |
| OIDD:Drug DB name | OIDD |  |
| OIDD:Drug DB CAS | OIDD | CAS RegNo |
| OIDD:Name | OIDD |  |
| OIDD:Old NCGC | OIDD |  |
| OIDD:NPC Browser Name | OIDD |  |
| **NCATS:Sample ID** | **NCATS** | **NCGC\_ID** |
| **NCATS:PubChem SID** | **NCATS** | **Substance ID** |
| NCATS:Synonym | NCATS |  |
| SMILES | PubChem | Structure associated with SID. May be stereo, may be salt. |
| **PUBCHEM\_SUBSTANCE\_ID** | **PubChem** | **Substance ID** |
| PUBCHEM\_EXT\_DATASOURCE\_REGID | PubChem | NCGC\_ID |
| PUBCHEM\_SUBSTANCE\_SYNONYM | PubChem |  |
| PUBCHEM\_XREF\_EXT\_ID | PubChem |  |
| PUBCHEM\_CID\_ASSOCIATIONS | PubChem | Compound ID |