### Additional File 2 – Transferred and obsolete identifiers and EC numbers per database

#### Genes

| Database       | Number of Entrez Gene IDs | Number of Ensembl Gene IDs |
|----------------|---------------------------|-----------------------------|
|                | transferred | obsolete |                | database | obsolete |                |
| EHMN           | 4          | 24       |                | EHMN     | 37       |                |
| H. sapiens Recon 1 | 10         | 5        |                | H. sapiens Recon 1 | x       |                |
| HumanCyc       | 38         | 5        |                | HumanCyc | 31       |                |
| KEGG           | 1          | 0        |                | KEGG     | 12       |                |
| Reactome       | 10         | 22       |                | Reactome | 35       |                |

#### EC numbers

| Database       | Number of EC numbers |                |
|----------------|----------------------|----------------|
|                | incomplete | transferred | obsolete |                |
| EHMN           | 41         | 4           | 1        |                |
| H. sapiens Recon 1 | 2         | 8           | 1        |                |
| HumanCyc       | 34         | 2           | 0        |                |
| KEGG           | 34         | 0           | 0        |                |
| Reactome       | 19         | 3           | 0        |                |

#### Metabolites

| Database       | Number of KEGG Compound | Number of KEGG Glycan | Number of CAS | Number of ChEBI | Number of PubChem Compound | Number of PubChem Substance IDs that do not map to a PubChem Compound ID | obsolete |
|----------------|-------------------------|-----------------------|---------------|-----------------|----------------------------|--------------------------------------------------------------------------|---------|
|                | incorrectly formatted   | transferred | obsolete | incorrectly formatted | obsolete | incorrectly formatted | transferred | obsolete |                |                |                         |                      |
| EHMN           | 0                       | 28          | 4        | 0                | 0            | 3                         | 0               |                | 35               | 0^b                |
| H. sapiens Recon 1 | 8^a                 | 14          | 21       | 50               | 2           | 7                         | x              | x               | x                | 1                  |
| HumanCyc       | 0                       | 9           | 0        | x                | x           | 2^a                       | 1              | 39              | x                | 106                |
| KEGG           | 0                       | 0           | 0        | 0                | 0            | 0                         | 0              | 0               | 259              | 0^b                |
| Reactome       | 0                       | 8           | 1        | x                | x           | x                         | 0              | 0               | 12               | 0^b                |

^a One could not be corrected and was therefore removed

^b As the CID-SID.gz file from PubChem was used to convert the PubChem Substance IDs to PubChem Compound IDs these are naturally up-to-date.

An 'x' indicates that the particular identifier is not available for this database.