The project **report 1** contains **16** samples and **148** compounds. **8** columns of samples informations and **12** columns of compound information are included in the project. A summary of sample information and compound information are given in Table 23 and Table 24.

| sample info | number of unique | mean (SD) | levels | type | number of missing |
| --- | --- | --- | --- | --- | --- |
| species | 1 | - | Mice | character | 0 |
| treatment | 1 | - | Non Swimmi... | character | 0 |
| organ | 1 | - | Heart | character | 0 |
| mx sample id | 1 | 415186 (0) | 415186 | numeric | 0 |
| fake\_two\_group | 2 | - | A, B | character | 0 |
| id | 16 | - | M102, M103... | character | 0 |
| two\_groups | 2 | - | Control MH... | character | 0 |
| label | 16 | - | M102, M102... | character | 0 |

Table 23: sample info

| compound info | number of unique | mean (SD) | levels | type | number of missing |
| --- | --- | --- | --- | --- | --- |
| CompoundID | 148 | - | CPD001, CP... | character | 0 |
| Order | 148 | 74.5 (42.8680144941035) | 1, 2, 3 | numeric | 0 |
| Compound Name | 148 | - | xylose, xy... | character | 0 |
| Assay | 1 | - | GCTOF | character | 0 |
| MIUnit | 1 | - | Peak heigh... | character | 0 |
| HMDBID | 118 | - | HMDB00098,... | character | 31 |
| LipidMAPS | 31 | - | NA, LMPR01... | character | 118 |
| KEGGID | 139 | - | C00181, C0... | character | 10 |
| PubChemID | 148 | 1931208.89189189 (9105898.48373919) | 135191, 69... | numeric | 0 |
| InChiKey | 148 | - | SRBFZHDQGS... | character | 0 |
| SMILES | 148 | - | C1[C@H]([C... | character | 0 |
| label | 148 | - | xylose, xy... | character | 0 |

Table 24: compound info