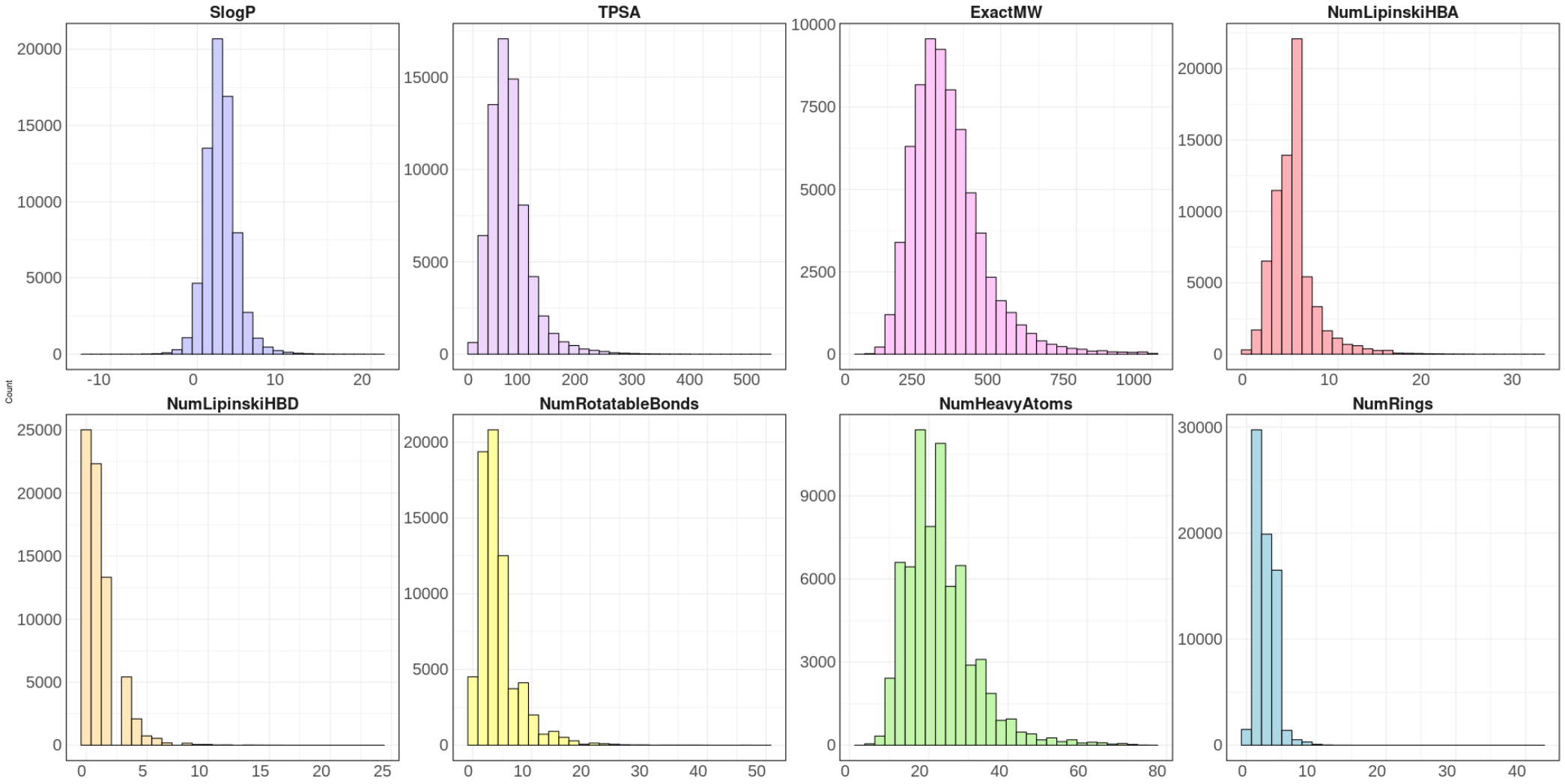
CN profiling
(24 octobre 2020)

- P Bonnet
- S Bourg

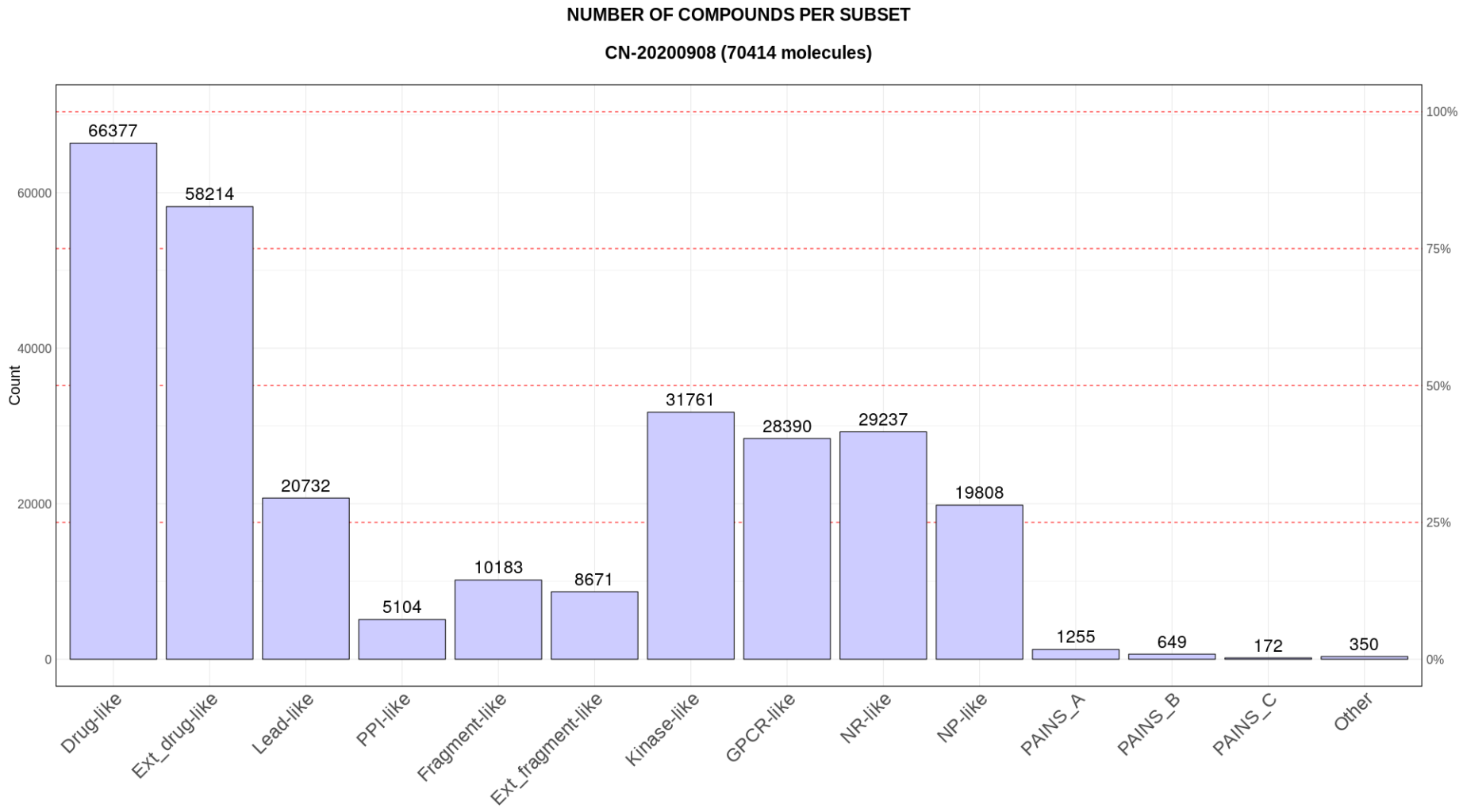
CN

DISTRIBUTION OF RDKIT MOLECULAR DESCRIPTORS

CN-20200908



CN



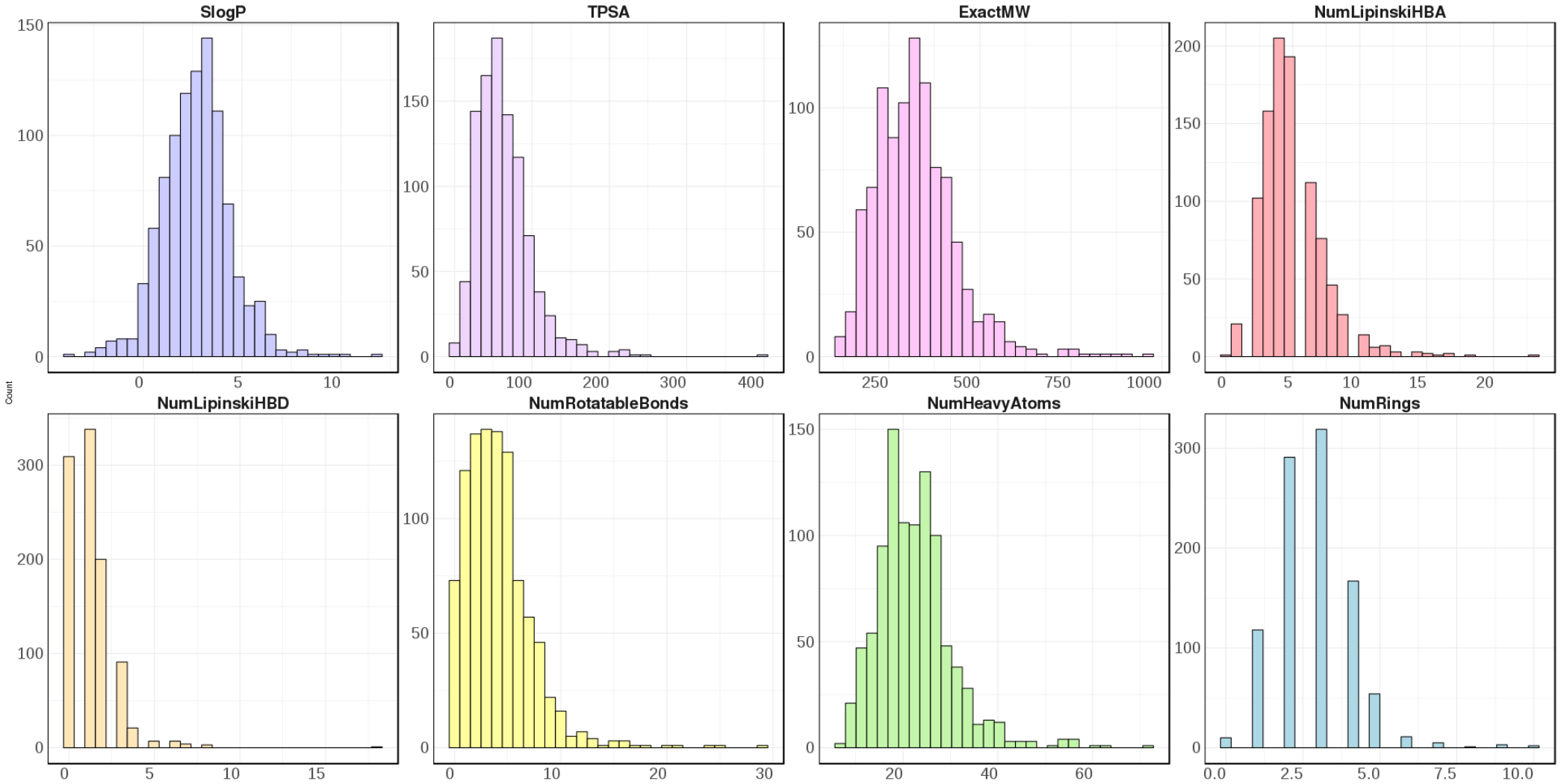
Few molecules removed during the preparation :

solvent: 64
more than 2 unspecified stereocenters: 3813
MW > 1.000 Da: 675
Too many rotatable bonds: 1
inorganic molecules: 1818
duplicated entry: 1091
isotope: 4

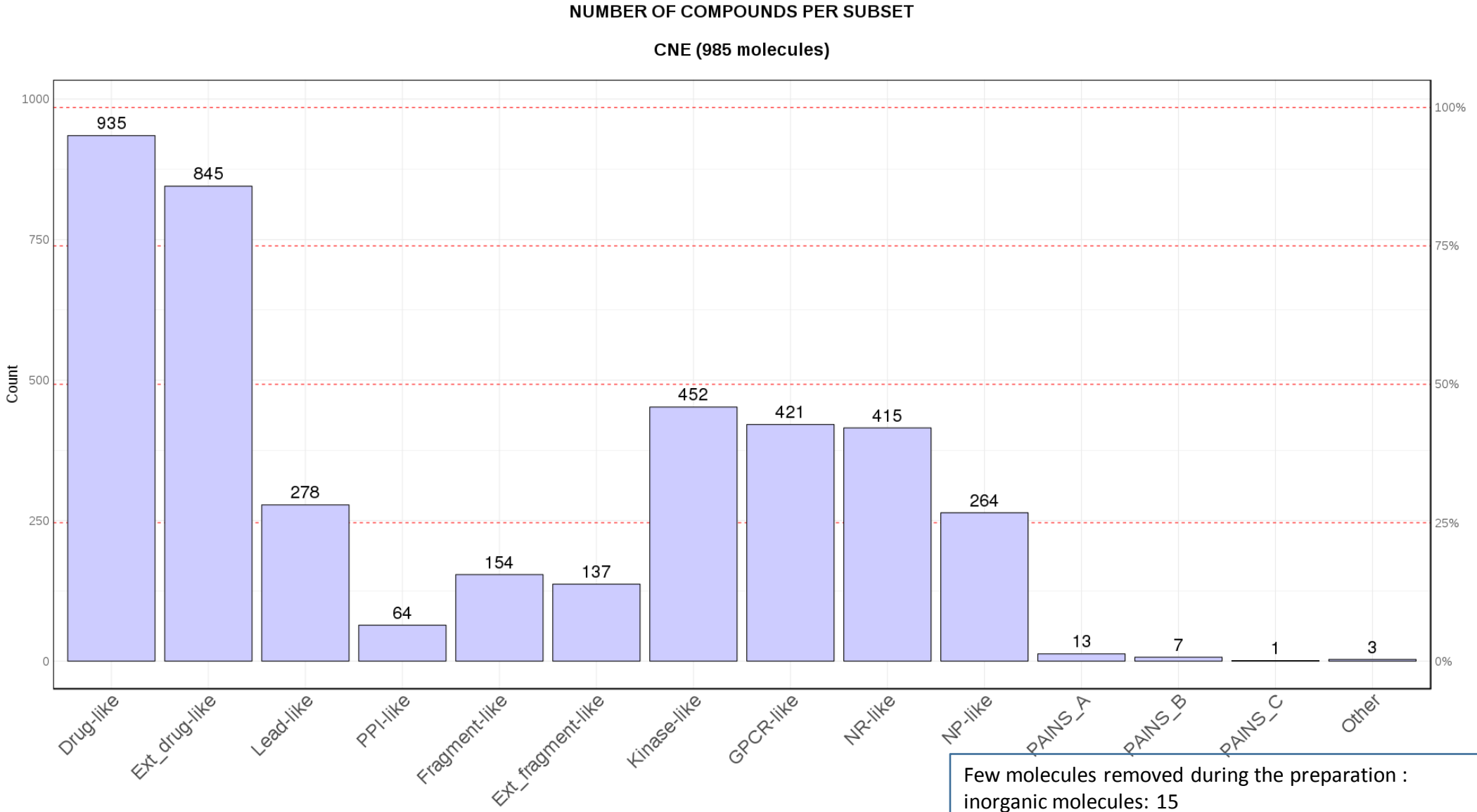
CNE

DISTRIBUTION OF RDKIT MOLECULAR DESCRIPTORS

CNE

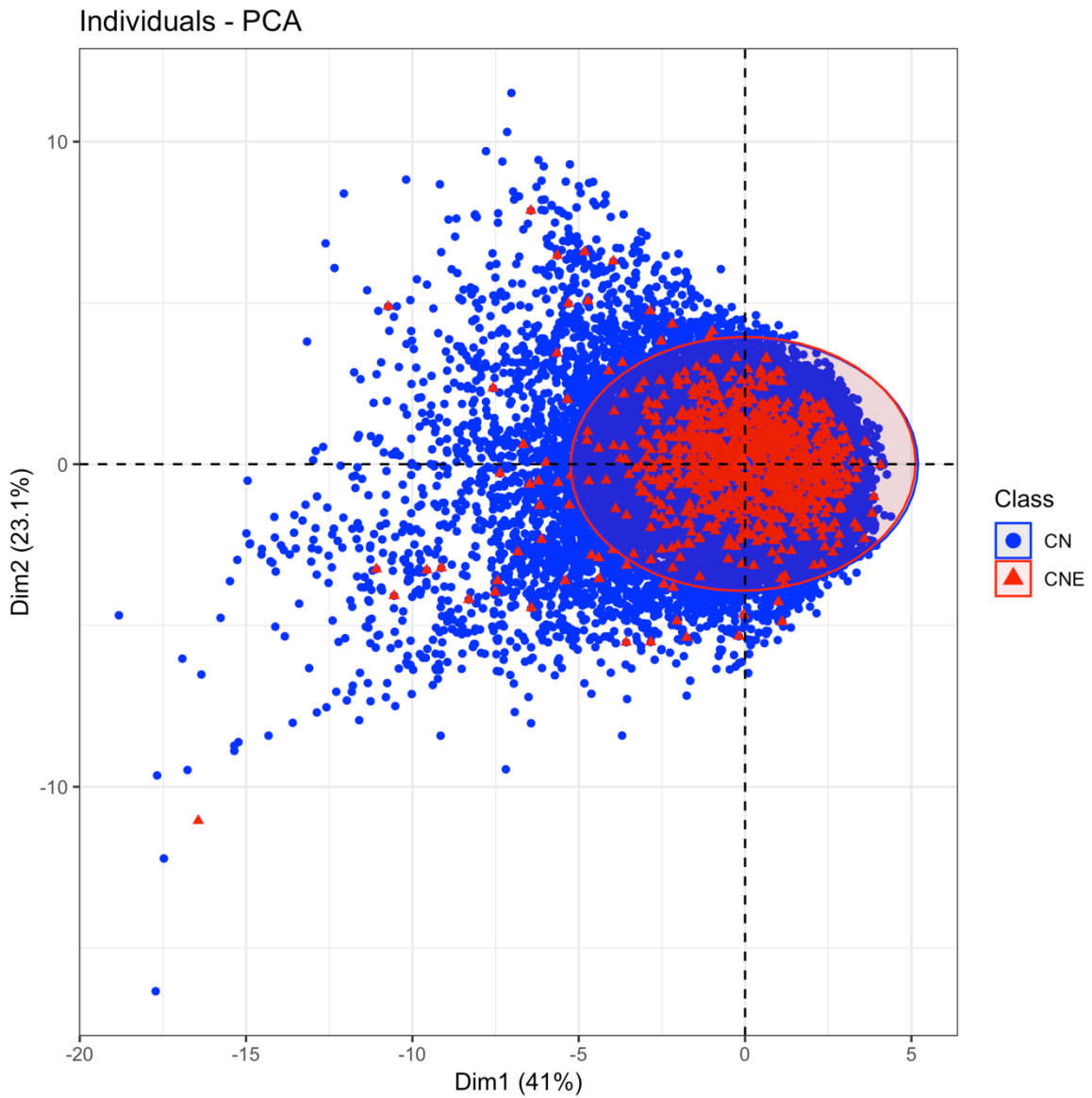


CNE



Few molecules removed during the preparation :
inorganic molecules: 15
more than 2 unspecified stereocenters: 35
MW > 1.000 Da: 5

PCA


Individuals - PCA
10
0
-10
Dim2 (23.1%)
-20
-15
-10
-5
0
5
Dim1 (41%)
Class
CN
CNE

- Molecular descriptors were computed using RDKit (http://www.rdkit.org/) Lead-like, drug-like, PPI-like and fragment-like molecules were evaluated based on published descriptor thresholds.
  - Lipinski, C. A. J. Pharm. Tox. Methods 44, 235–249 (2000)
  - Teague, S. J. Ang. Chem. Int. Ed. 38, 3743–3748 (1999)
  - Hamon, V. J R Soc Interface 11, 20130860–20130860 (2013)
  - Congreve, M. Drug Discov. Today 8, 876–877 (2003)

- Pains were computed by performing substructure search
  - Baell J.B. et al. J. Med. Chem. 53, 2719-2740 (2010)

- NR-like (nuclear receptor), NP-like (natural products), GPCR-like and Kinase-like molecules were calculated by similarity search of corresponding published or in-house databases
  - Gatica, E. A. et al. J. Chem. Inf. Model. 52, 1–6 (2011)
  - Lagarde, N. et al. J. Med. Chem. 57, 3117–3125(2014)

- PCA calculations were performed with R libraries: factoextra, ade4, ggplot2.

- For more information, please contact Prof. Pascal Bonnet: pascal.bonnet@univ-orleans.fr