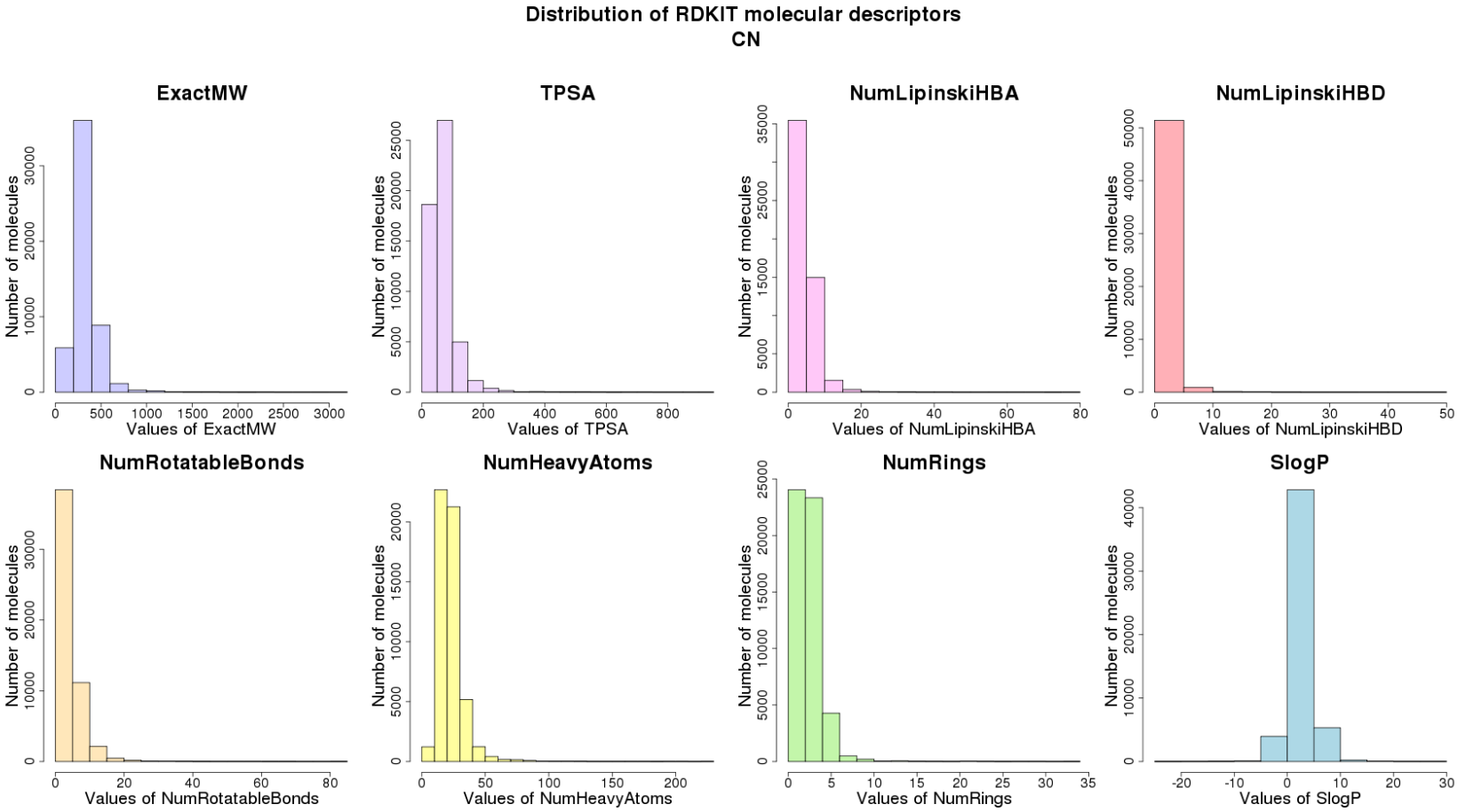
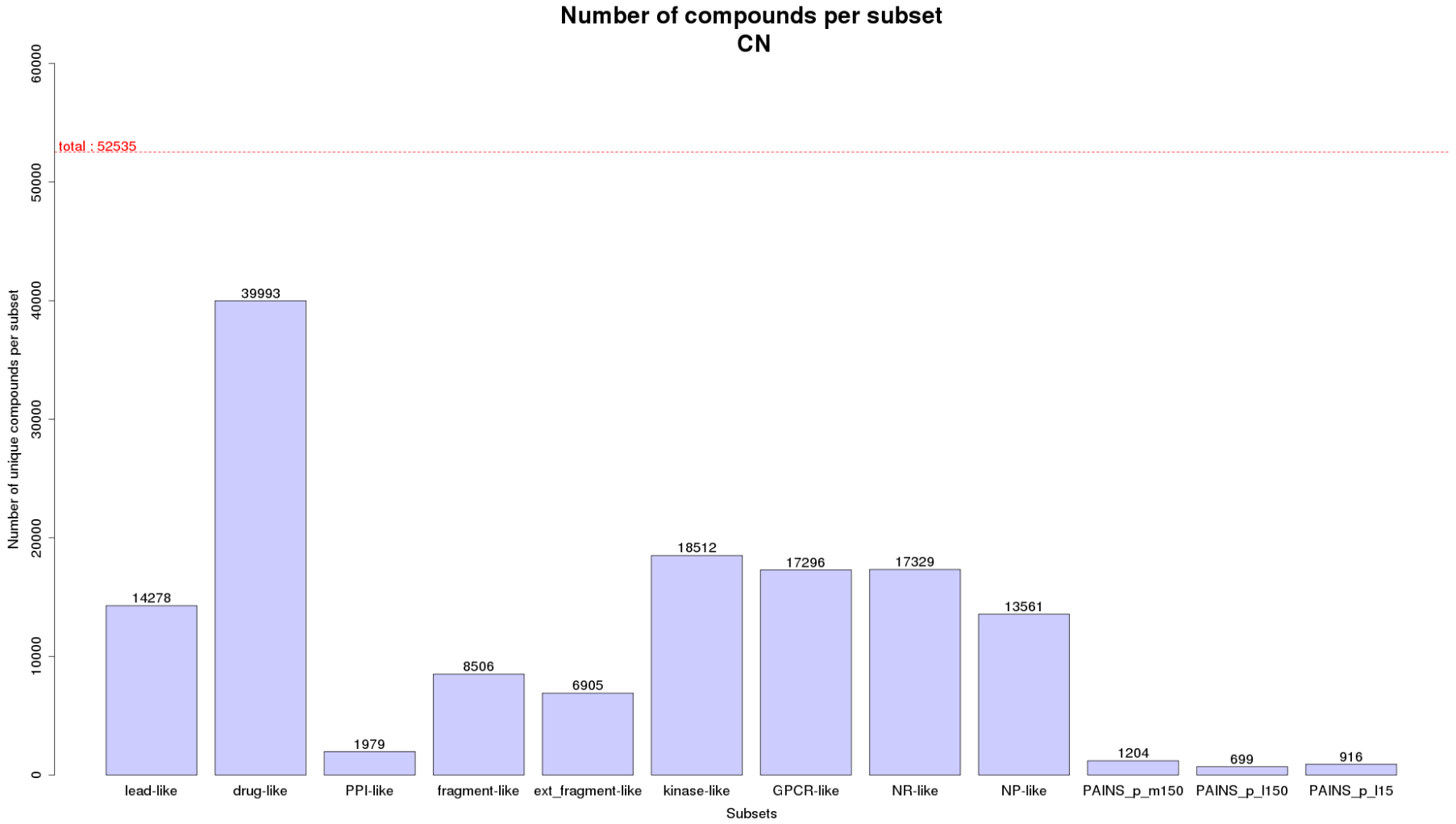
CN (55837 molecules)



Performed by José-Manuel Gally, ICOA

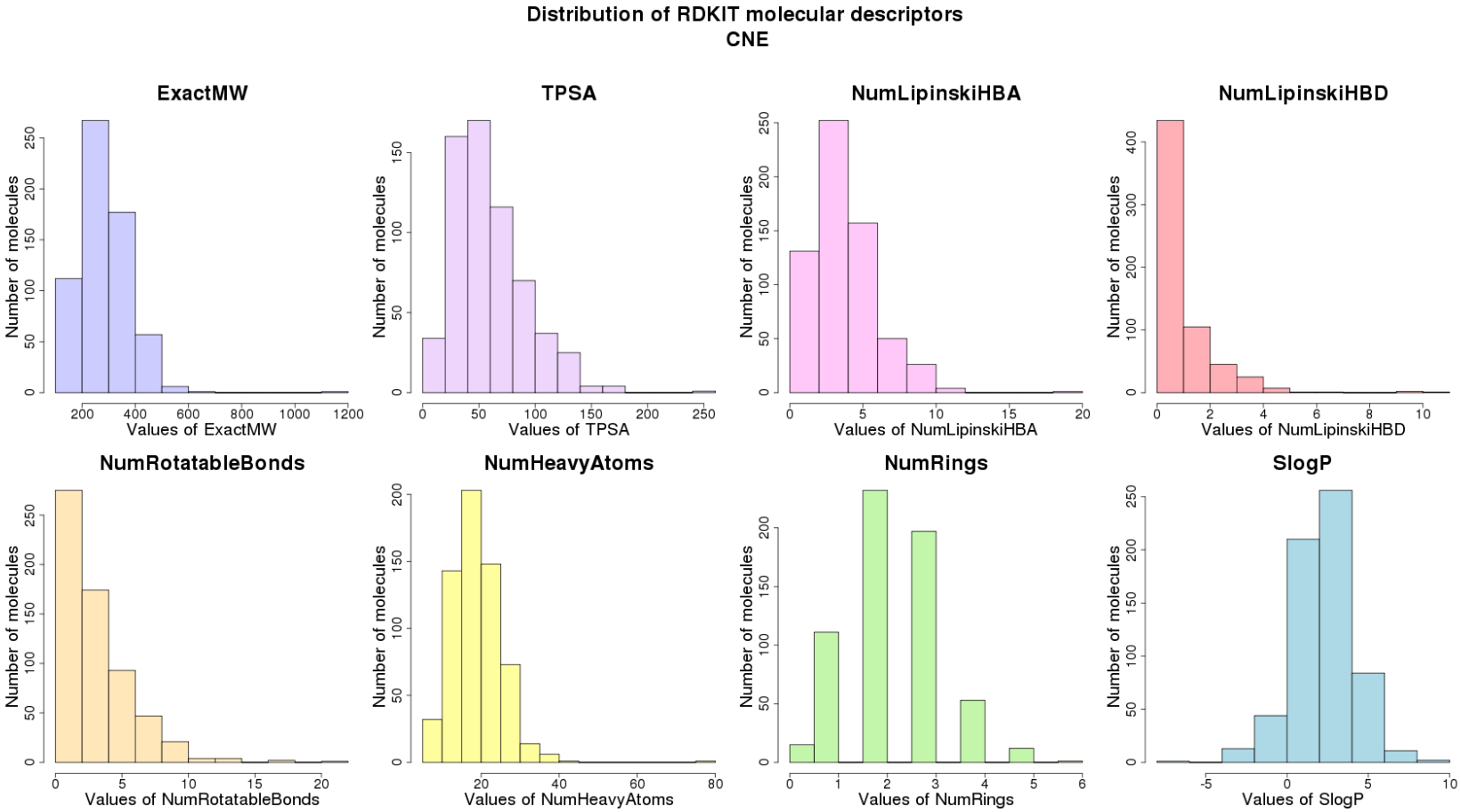
CN (55837 molecules)



Few molecules removed during the preparation of the molecules because they contain mixtures, bad atom types, inorganic atoms, etc.

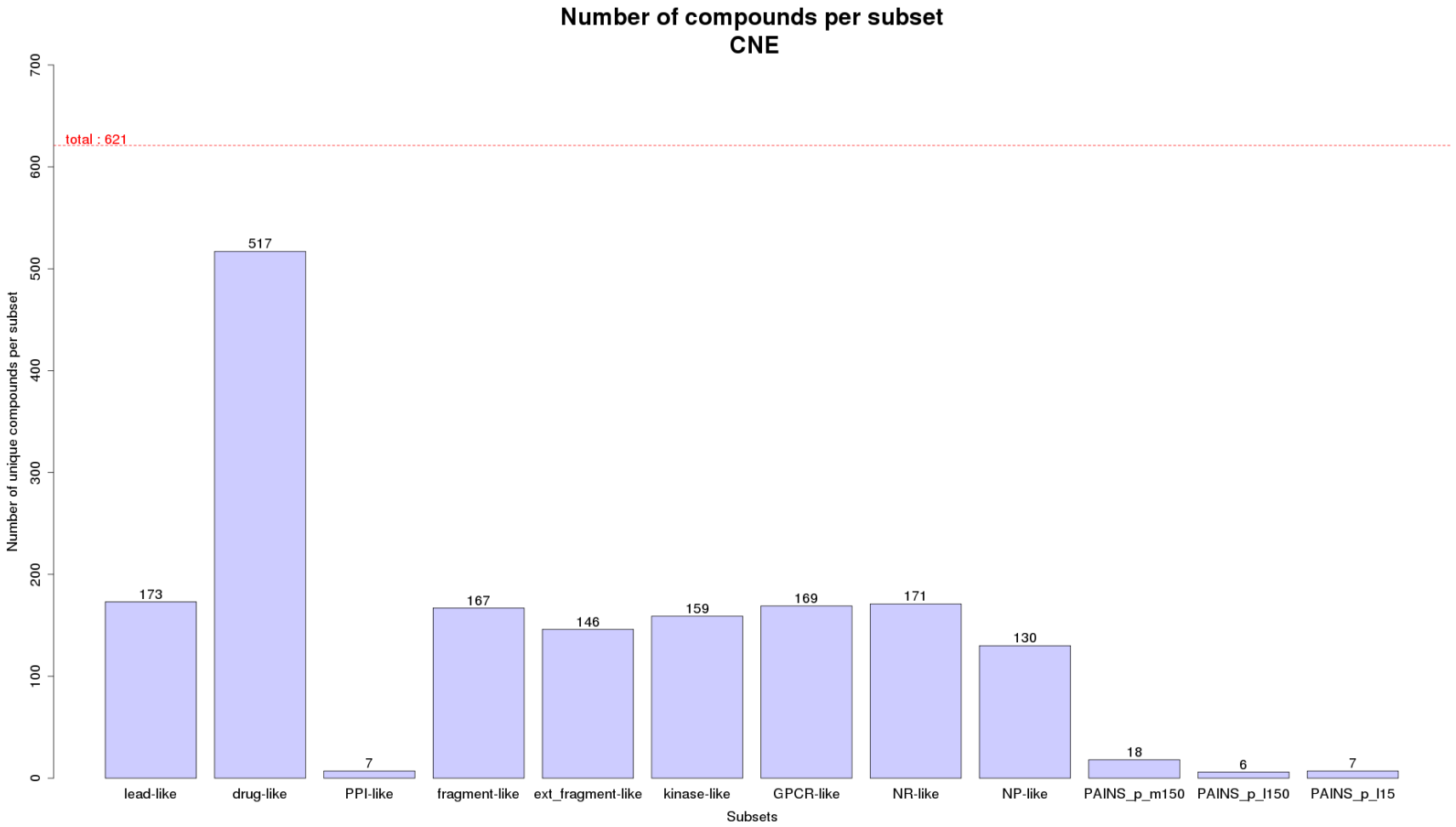
Performed by José-Manuel Gally, ICOA

CNE 640 molecules

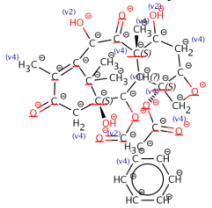


Performed by José-Manuel Gally, ICOA

CNE 640 molecules



Few molecules removed during the preparation of the molecules because they contain mixtures, bad atom types, inorganic atoms, etc.



Performed by José-Manuel Gally, ICOA

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 (GaticaE. A. *et al.* J. Chem. Inf. Model. 52, 1–6 (2011); Lagarde, N. *et al.* J. Med. Chem. 57, 3117–3125(2014))

Calculations were performed by José-Manuel Gally, PhDstudent in the Structural Bioinformatics and Chemoinformatics group of the ICOA, University of Orléans, France.

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