Ligand Performance Insights and Molecular Properties

Range Of Lymphocytic

LF_dG

-8.96 -0.17

Library Of All Elements Present

Library

All

Range Of Molecular Weight

Molecular_Weight

111.10 379.30

Total Structures Present

18.91K

Count of Structure

Average Of Molecular Weight

240.67

Average of Molecular_Weight

Average Of Lymphocytic

-5.37

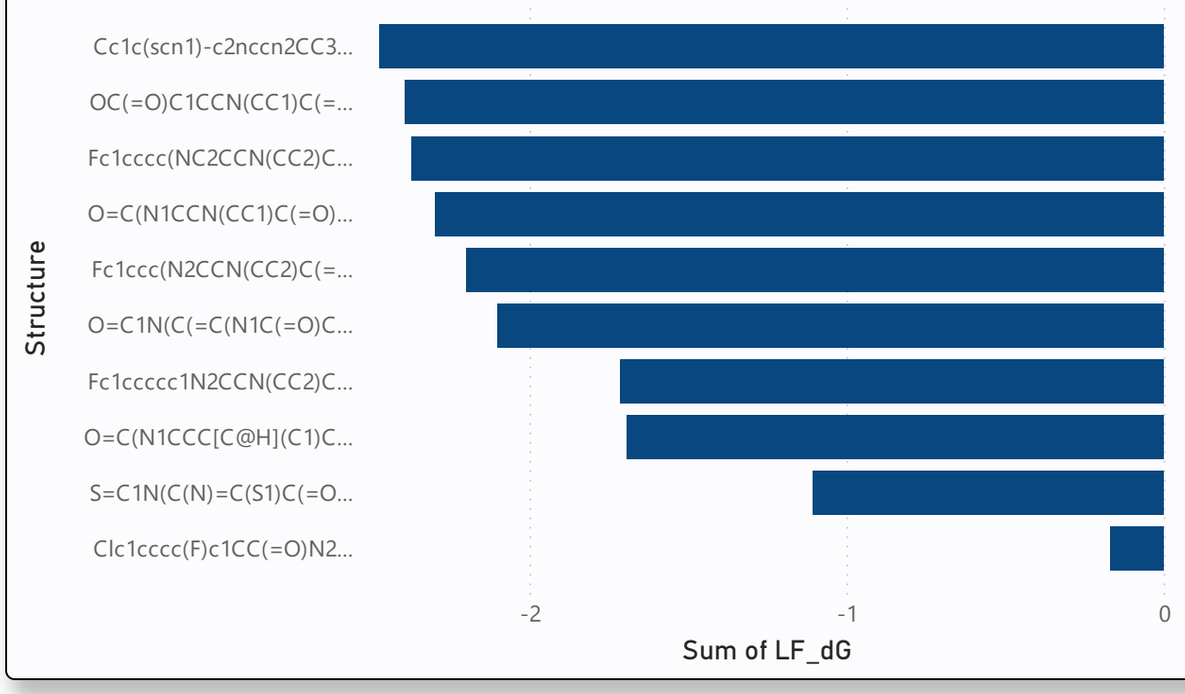
Average of LF_dG

Minimum of Lymphocytic

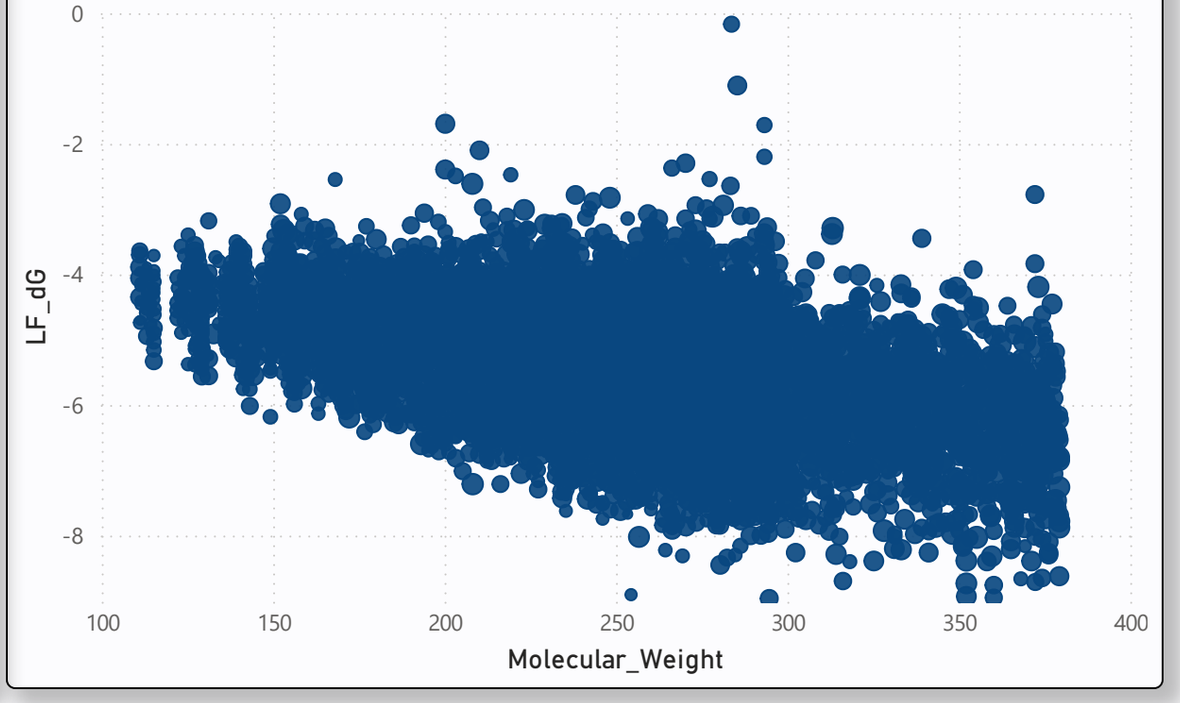
-8.96

Min of LF_dG

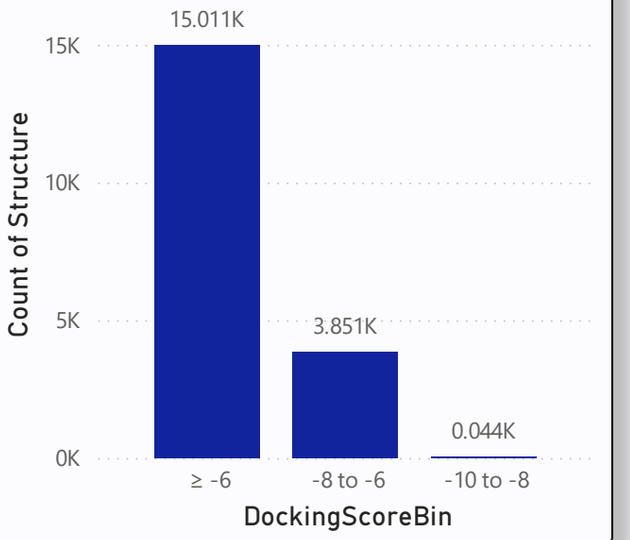
Top 10 Ligands with Best Docking Score



TPSA vs Molecular Weight vs LF_dG



Count of Structure by Range

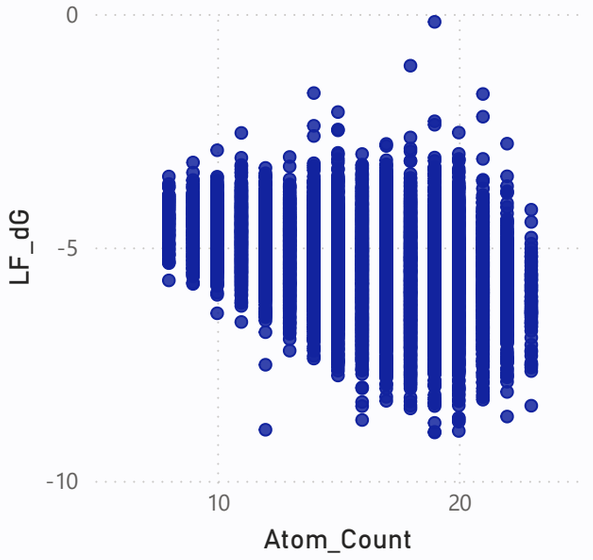


Score Binning, Atom Count & Property Breakdown

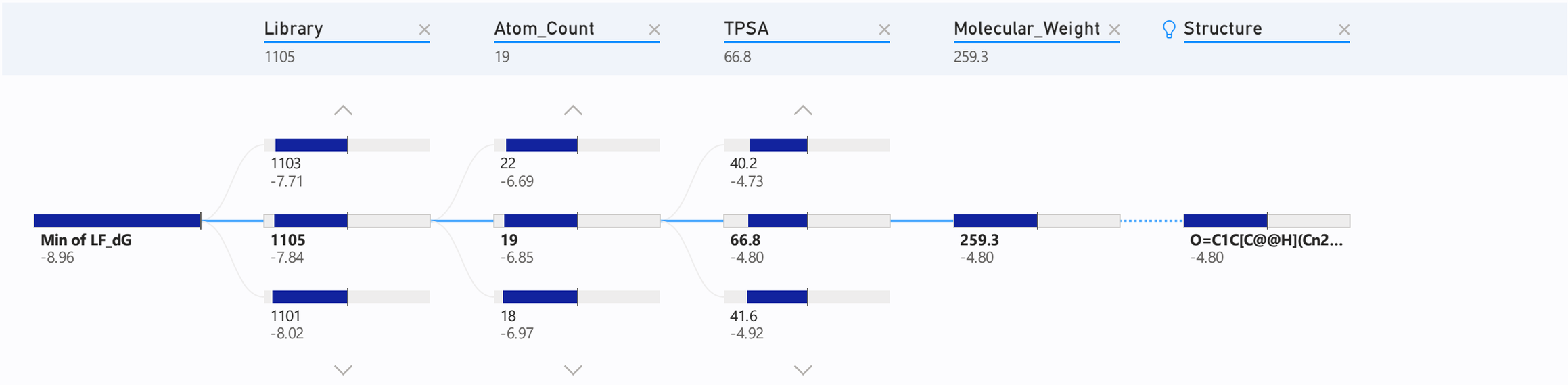
Narrative Summary of All Visuals

- At 15,011, ≥ -6 had the highest Count of Structure and was 34,015.91% higher than -10 to -8, which had the lowest Count of Structure at 44.
- ≥ -6 had the highest Count of Structure at 15,011, followed by -8 to -6 at 3,851 and -10 to -8 at 44.
- ≥ -6 accounted for 79.40% of Count of Structure.
- -10 to -8 had 44 Count of Structure, -8 to -6 had 3,851, and ≥ -6 had 15,011.

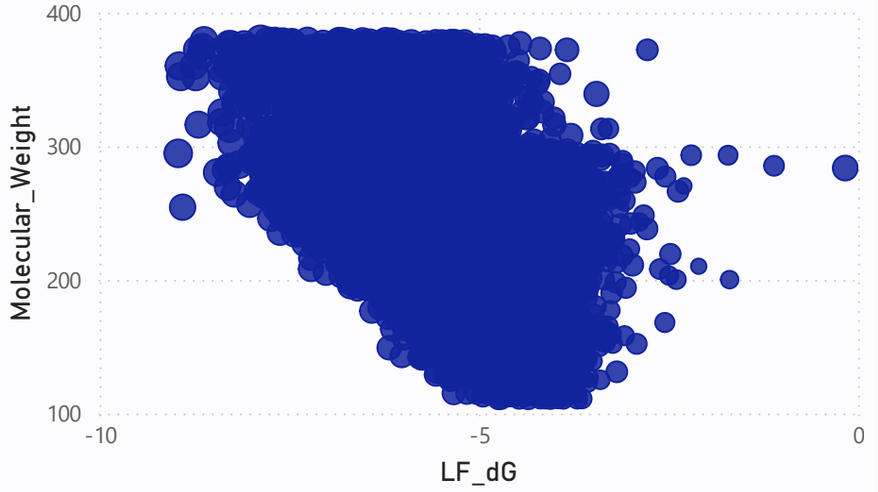
Atom Count VS Lymphocytic



Decomposition Tree b/w Library, Atom Count, TPSA, Molecular Weight and Structure



Sum of LF VSscore by LF_dG and Molecular_Weight



Halogen Analysis:

Bromine in Ligand, Chlorine in Ligand, Fluorine in Ligand Structures

Number Of Elements Containing Bromine

2407

Count of LF_dG with Bromine

Number Of Elements Containing Chlorine

1440

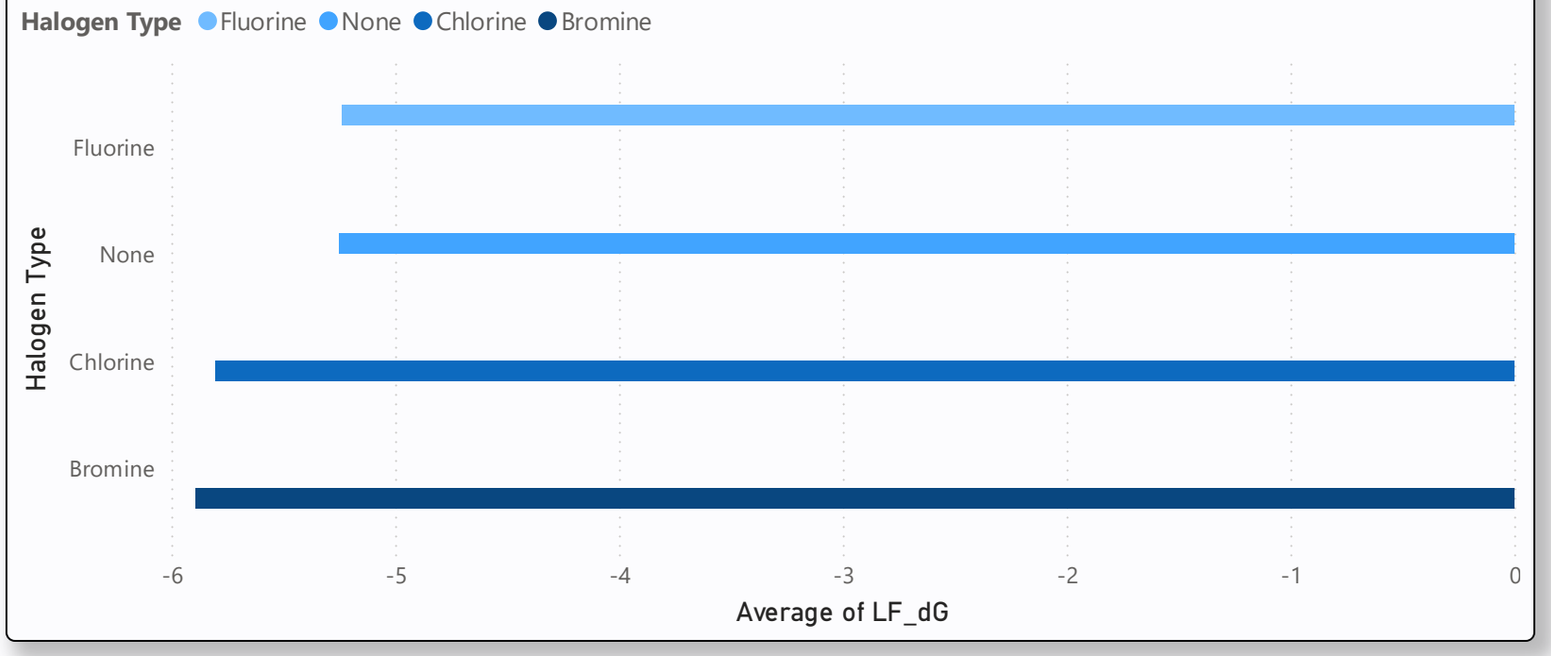
Count of LF_dG with Chlorine

Number Of Elements Containing Fluorine

3407

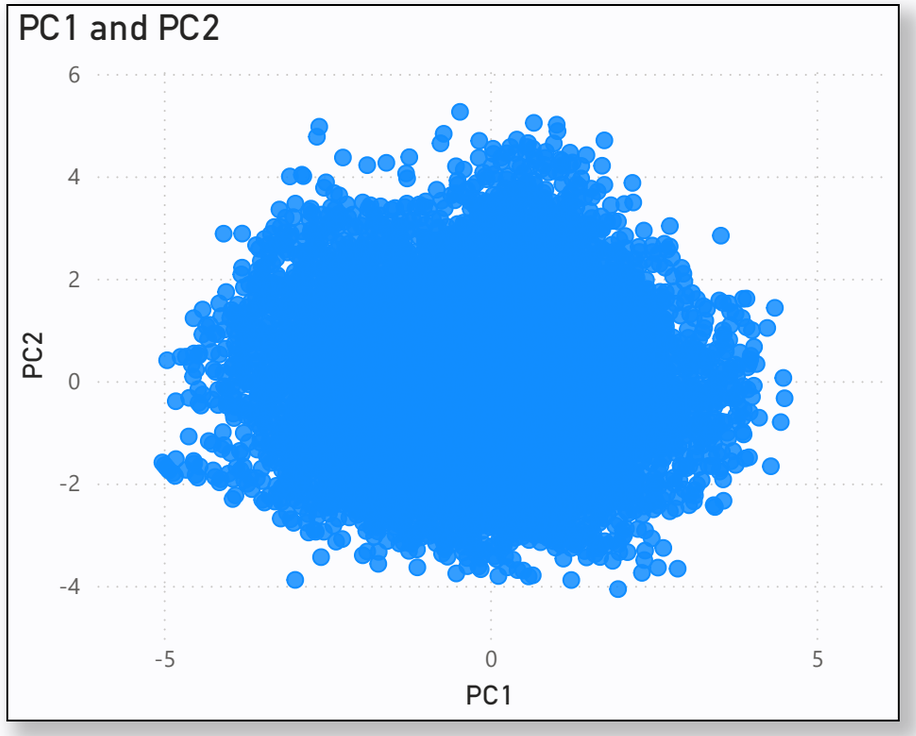
Count of LF_dG with Fluorine

Average of LF_dG by Halogen Type and Halogen Type



Best Binding Ligands: Binding Energy, Molecular Weight, TPSA, and Lipophilicity Overview

SMILES	Binding Energy (kcal/mol)	Molecular_Weight	TPSA	Lipophilicity	Library
Sc1nnc2c(n(c3ccc(F)cc32)C)n1	-5.41	234.30	43.60	2.20	ExpressPick
Sc1nnc2c([nH]c3ccc(F)cc23)n1	-5.63	220.20	54.50	2.20	ExpressPick
Sc1nnc(n1CC)CNC(=O)c2ccccc2F	-6.88	280.30	59.80	1.90	ExpressPick
Sc1nnc(n1-c2ccccc2F)-c3ccncc3	-6.31	272.30	43.60	3.00	ExpressPick
Sc1nc(cc(n1)C(F)F)-c2ccccc2	-5.56	238.30	25.80	3.40	ExpressPick
SC1=Nc2ccccc2C(=O)N1c3ccc(F)cc3	-6.63	272.30	32.70	3.70	ExpressPick
SC1=NC(=C([C@H](N1)c2ccc(F)cc2)C(OC)=O)C	-7.84	280.30	50.70	2.50	ExpressPick
s1cnnc1N2CCc3c(c(n[nH]3)C4CC4)CC2	-6.43	261.30	57.70	1.70	1204
s1cnnc1N2CC3(C2)COc4ccccc4C3	-6.40	259.30	38.30	2.00	1216
s1cncc1CNC2CC2	-5.37	154.20	24.90	1.40	ExpressPick
s1cncc1CN2CC3(C2)COc4ccccc4C3	-7.48	272.40	25.40	2.60	1216
s1cncc1-c2nccn2Cc3cscn3	-5.47	248.30	43.60	2.50	1105
s1cncc1-c2nccn2Cc3cnccc3	-4.46	242.30	43.60	2.40	1105
s1cncc1-c2nccn2Cc3cnc4ccccn43	-6.14	281.30	48.00	2.70	1105
s1cncc1-c2nccn2CC3CCOCC3	-5.55	249.30	39.90	2.40	1105
s1cncc1-c2nccn2Cc3ccco3	-5.35	231.30	43.80	2.10	1105
s1cncc1-c2nccn2Cc3ccccc3	-5.89	241.30	30.70	3.10	1105
s1cncc1-c2nccn2CC3CCC3	-5.50	219.30	30.70	2.80	1105
s1cncc1-c2nccn2C3CCC3	-5.11	205.30	30.70	2.70	1105
s1cncc1-c2nccn2C3CC3	-4.81	191.30	30.70	2.30	1105
s1cncc1-c2nccn2C[C@@H]3C[C@@H]4CC[C@H]3O4	-5.96	261.30	39.90	2.60	1105
s1cncc1-c2nccn2[C@@H]3C=CCCC3	-6.06	231.30	30.70	3.10	1105



16.45

Average of Atom_Count