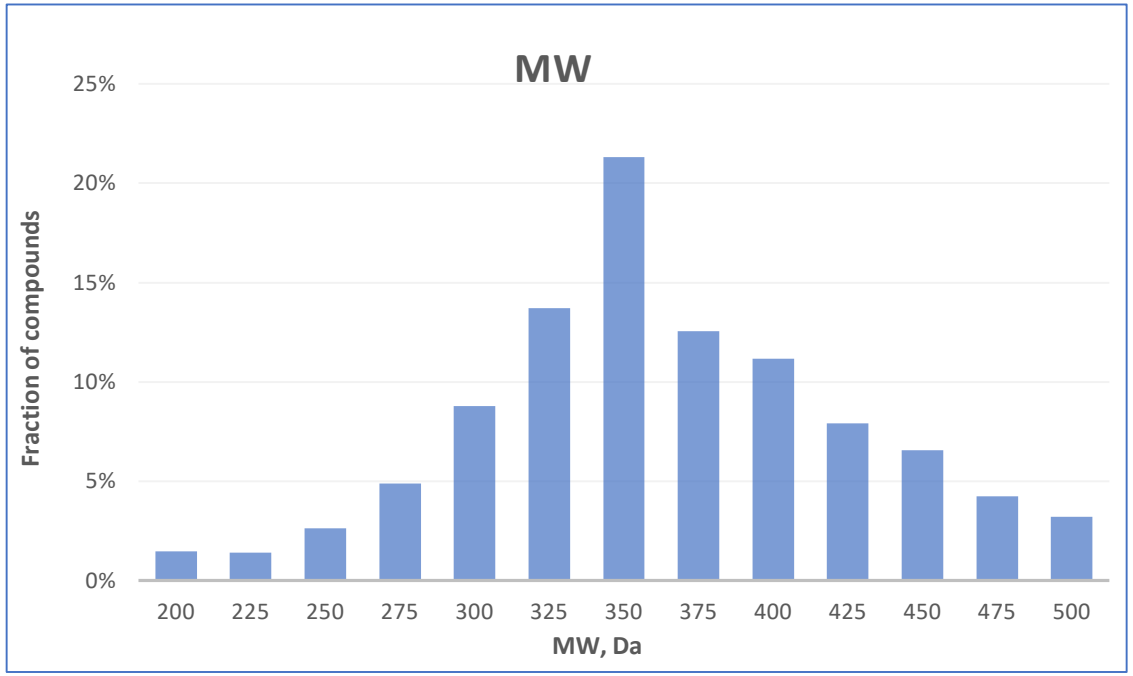
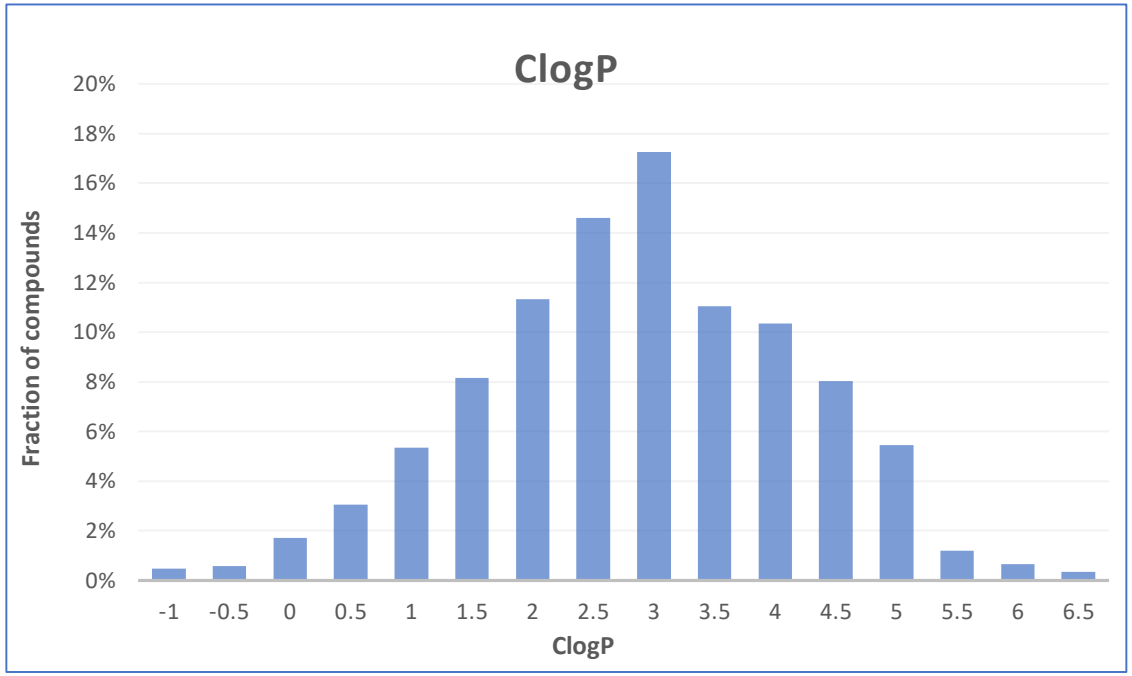
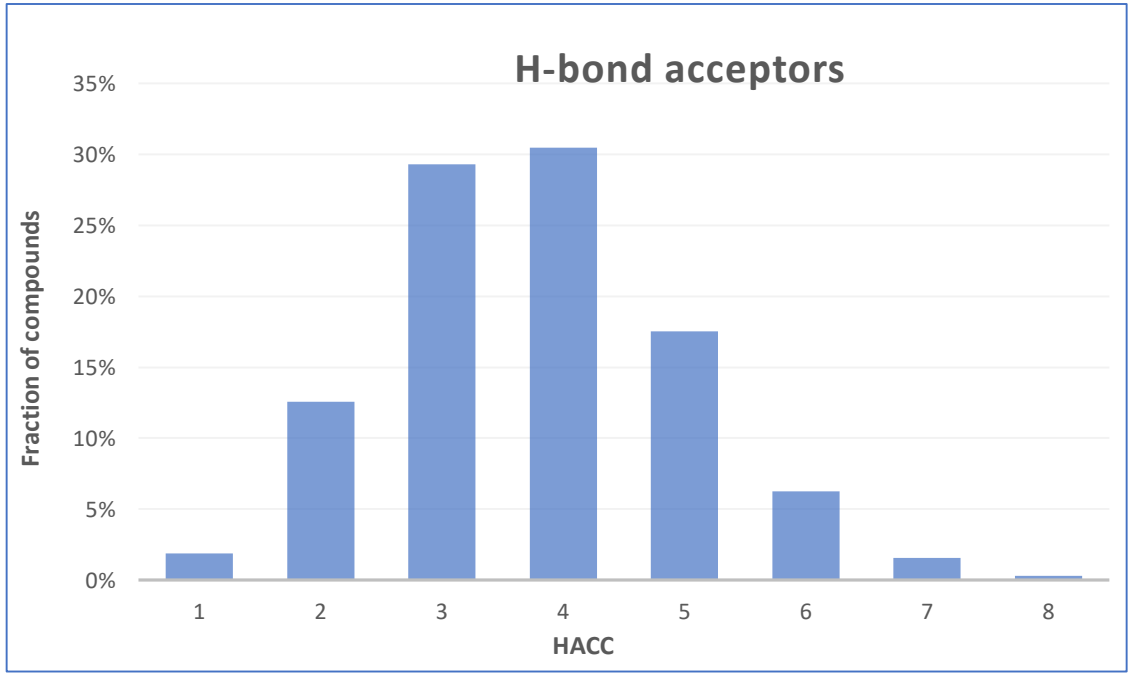
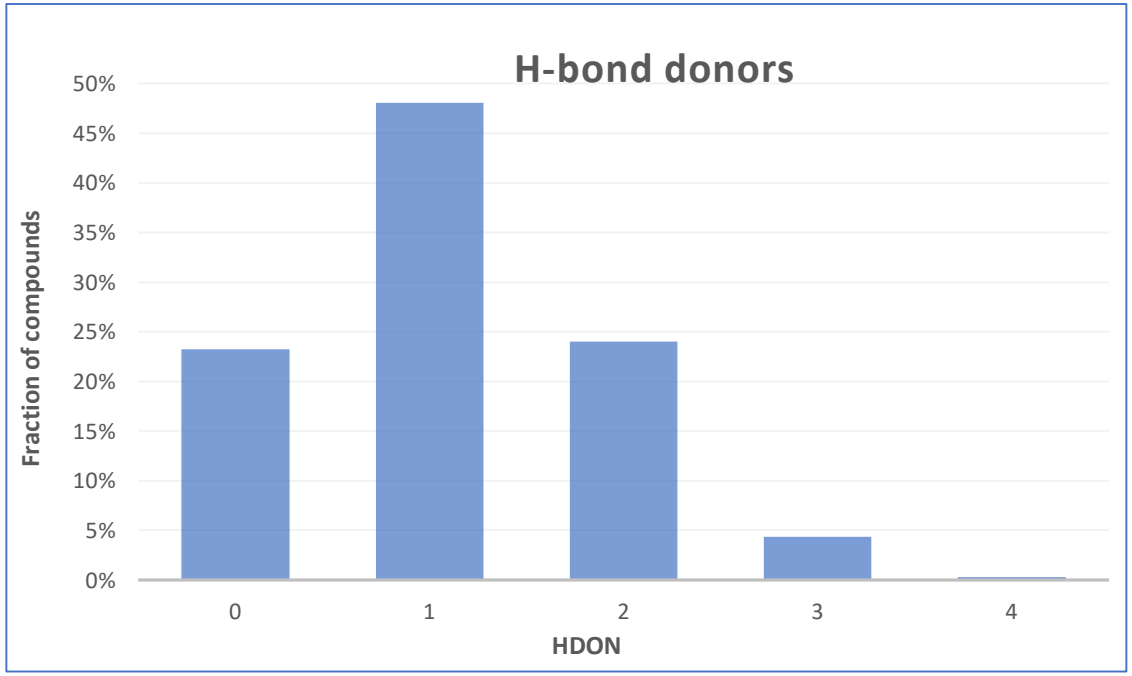
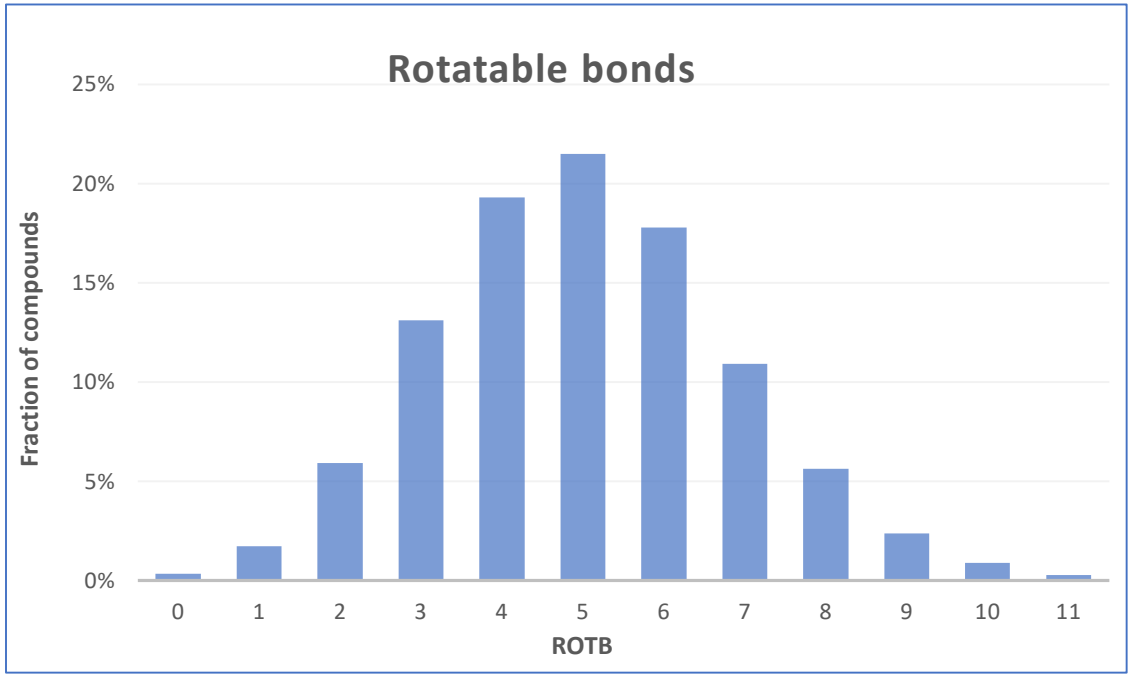
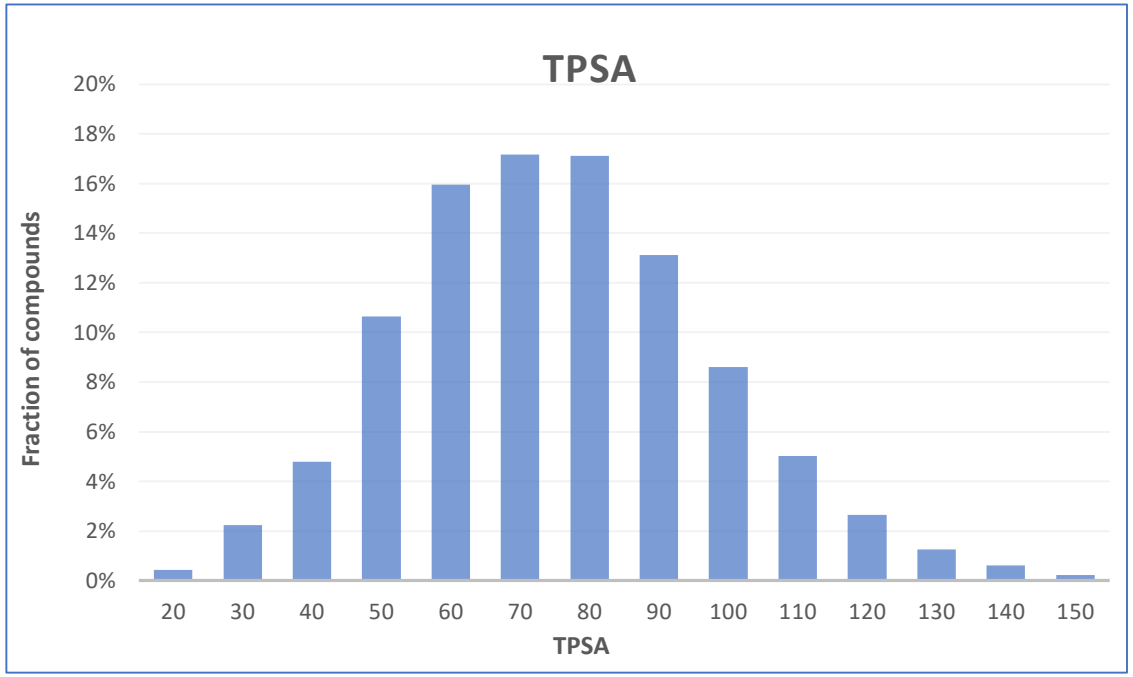

MW
Fraction of compounds
25%
20%
15%
10%
5%
0%
200
225
250
275
300
325
350
375
400
425
450
475
500
MW, Da

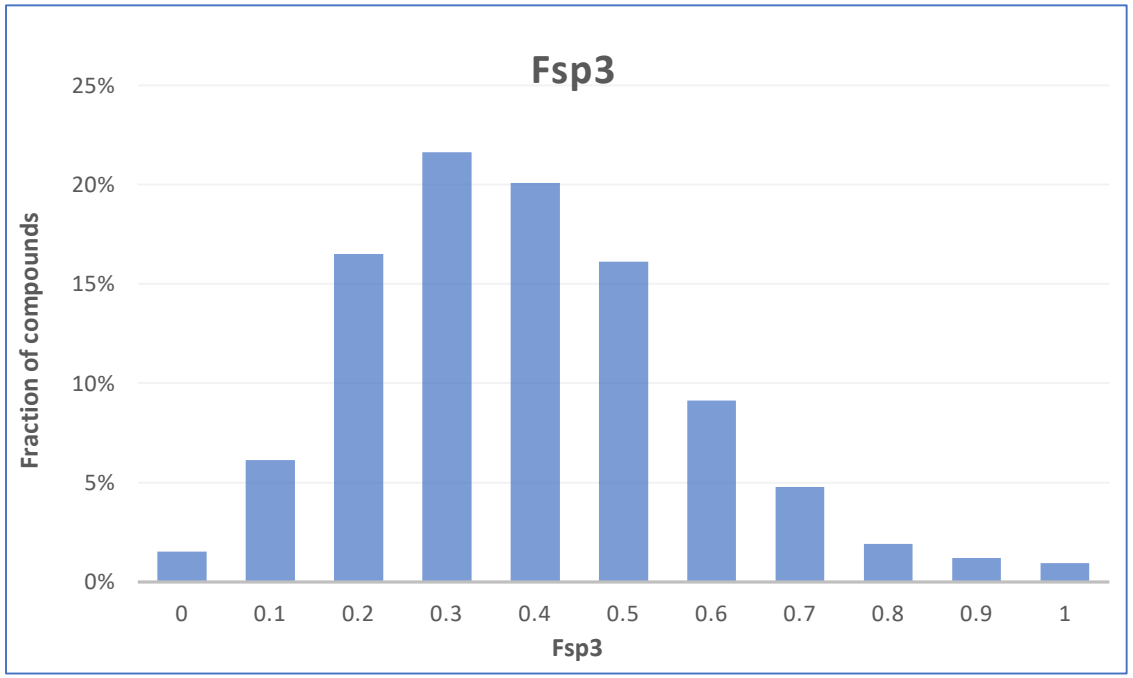

ClogP
Fraction of compounds
20%
18%
16%
14%
12%
10%
8%
6%
4%
2%
0%
-1
-0.5
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
ClogP

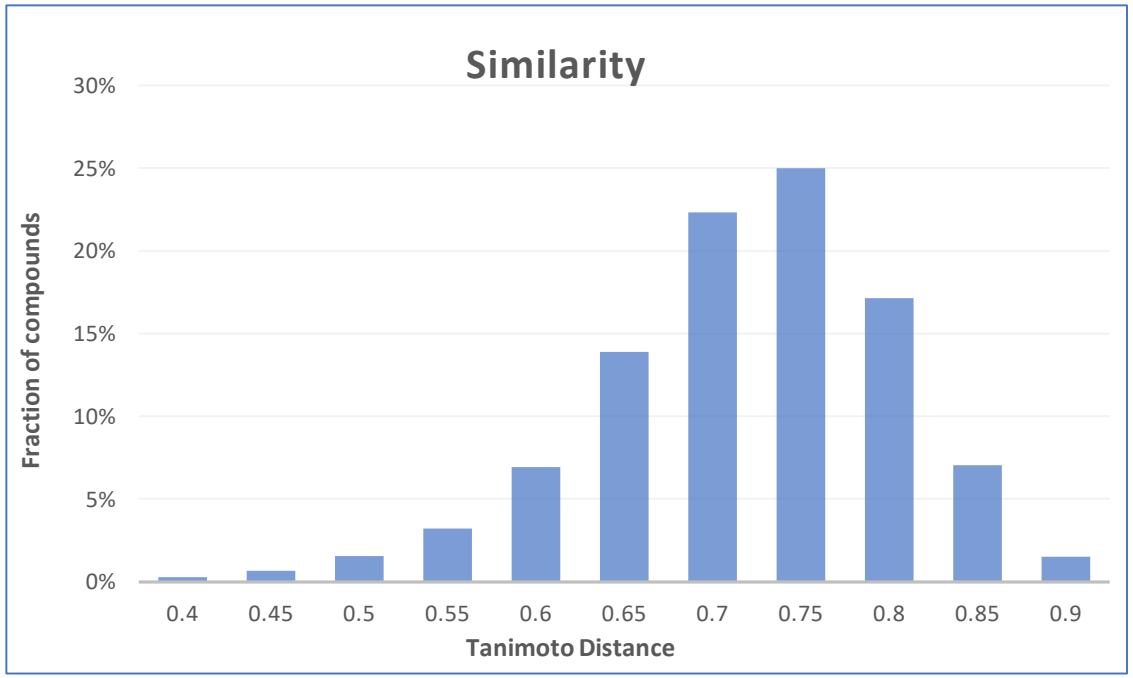

H-bond acceptors
Fraction of compounds
35%
30%
25%
20%
15%
10%
5%
0%
1
2
3
4
5
6
7
8
HACC


H-bond donors
Fraction of compounds
50%
45%
40%
35%
30%
25%
20%
15%
10%
5%
0%
0
1
2
3
4
HDON


Rotatable bonds
Fraction of compounds
25%
20%
15%
10%
5%
0%
0 1 2 3 4 5 6 7 8 9 10 11
ROTB


TPSA
Fraction of compounds
20%
18%
16%
14%
12%
10%
8%
6%
4%
2%
0%
20 30 40 50 60 70 80 90 100 110 120 130 140 150
TPSA


Fsp3
Fraction of compounds
25%
20%
15%
10%
5%
0%
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
Fsp3


Similarity
Fraction of compounds
30%
25%
20%
15%
10%
5%
0%
0.4 0.45 0.5 0.55 0.6 0.65 0.7 0.75 0.8 0.85 0.9
Tanimoto Distance