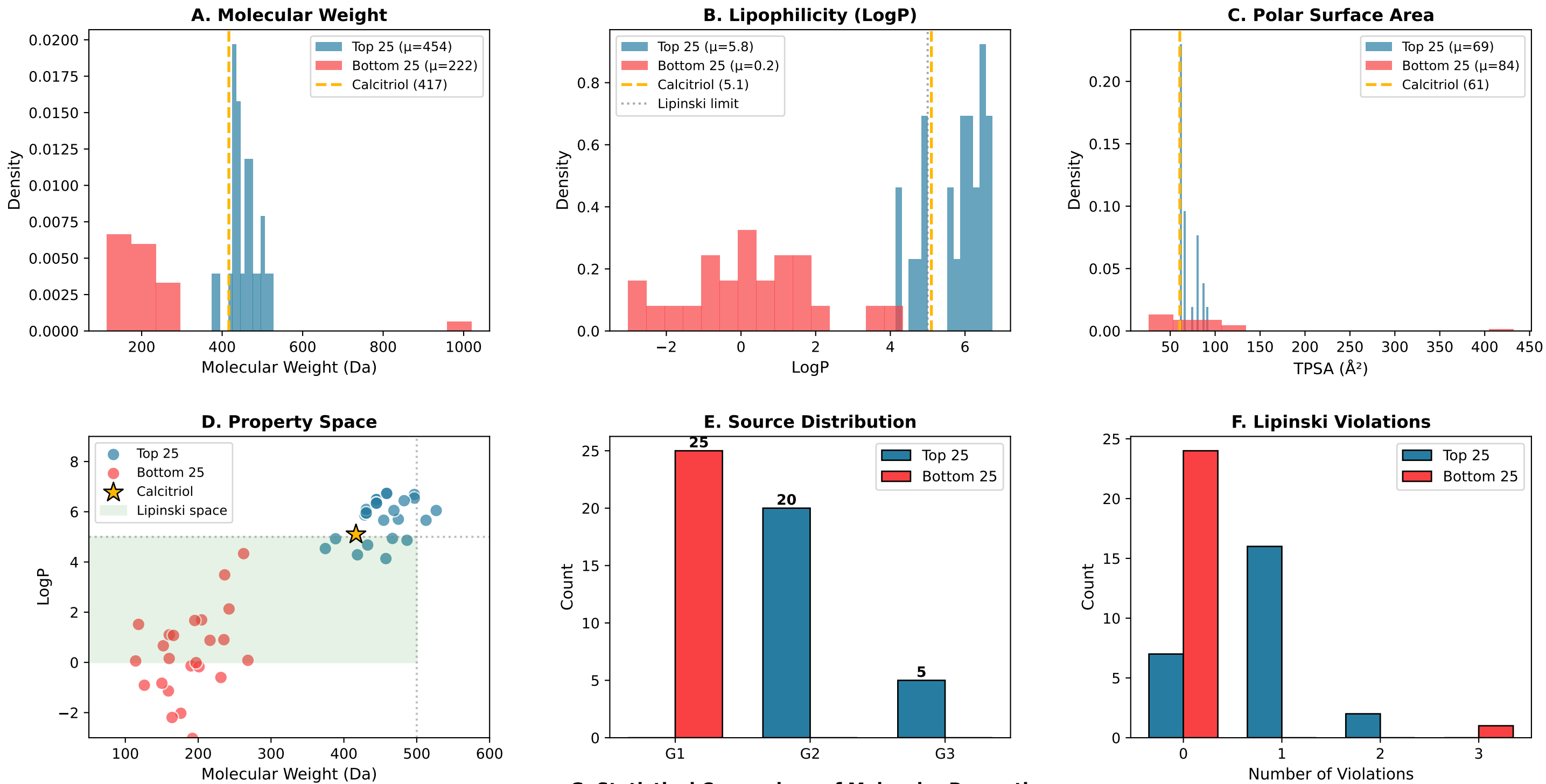


Molecular Property Analysis: Top vs Bottom G-Structures



G. Statistical Comparison of Molecular Properties
(* $p<0.05$, ** $p<0.01$, *** $p<0.001$)

Property	Top 25 (mean \pm std)	Bottom 25 (mean \pm std)	Calcitriol	p-value
MW	454.2 \pm 35.4	221.6 \pm 171.5	416.64	2.59e-08 ***
LogP	5.8 \pm 0.8	0.2 \pm 1.8	5.1	7.52e-19 ***
TPSA	69.1 \pm 10.5	84.3 \pm 77.6	60.69	3.37e-01
HBD	2.9 \pm 0.6	2.6 \pm 2.9	3	5.92e-01
HBA	3.6 \pm 0.7	3.9 \pm 2.6	3	6.58e-01
RotBonds	7.0 \pm 1.9	3.9 \pm 4.3	6	2.18e-03 **
Rings	3.2 \pm 0.6	0.9 \pm 0.5	-	1.02e-19 ***
HeavyAtoms	32.8 \pm 2.6	15.6 \pm 12.1	-	9.50e-09 ***