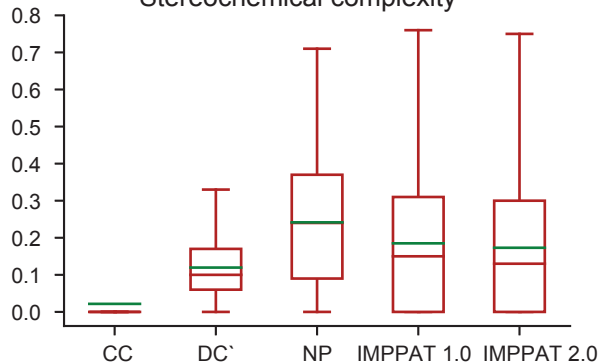
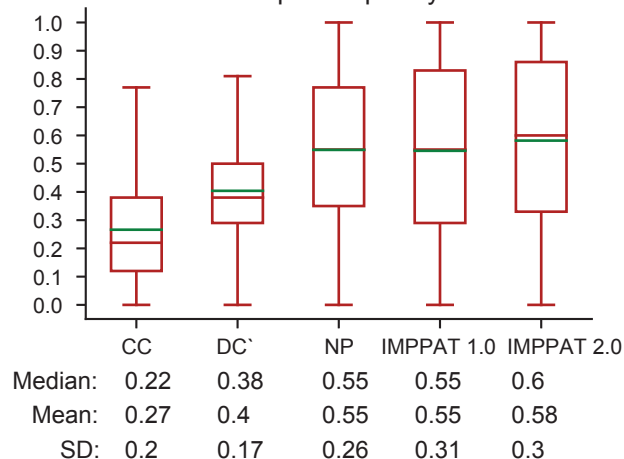


**A****Stereochemical complexity****B****Shape complexity****C**

	Molecular weight (g/mol)			Log P			Topological Polar surface Area (TPSA) Å <sup>2</sup>		
	Median	Mean	SD	Median	Mean	SD	Median	Mean	SD
CC	311.34	314.19	74.62	3.30	3.21	1.50	55.98	58.33	26.06
DC`	495.54	509.50	158.65	3.97	3.98	2.14	94.56	97.08	40.68
NP	386.53	457.22	231.65	1.94	1.64	2.35	105.20	136.56	93.56
IMPPAT	334.24	377.23	259.43	2.46	2.38	3.43	69.96	98.02	109.42
IMPPAT 2.0	317.30	363.09	225.00	2.81	2.87	3.02	58.88	85.36	93.75

	Hydrogen bond donors			Hydrogen bond acceptors			Rotatable bonds		
	Median	Mean	SD	Median	Mean	SD	Median	Mean	SD
CC	1	0.94	0.89	4	4.01	1.79	3	3.62	2.02
DC`	1	1.59	1.16	6	6.09	2.53	8	8.09	4.55
NP	3	4.06	3.59	6	8.29	5.87	5	5.91	4.60
IMPPAT 1.0	2	2.84	4.00	4	5.89	6.09	3	5.03	6.77
IMPPAT 2.0	1	2.38	3.46	4	5.36	5.72	3	5.07	5.95