A Stereochemical complexity

	CC	DC`	NP	IMPPAT 1.0	TCM-Mesh
Median:	0.0	0.1	0.24	0.15	0.2
Mean:	0.02	0.12	0.24	0.19	0.21
SD:	0.05	0.08	0.17	0.19	0.18

B Shape complexity

	CC	DC`	NP	IMPPAT 1.0	TCM-Mesh
Median:	0.22	0.38	0.55	0.54	0.56
Mean:	0.26	0.4	0.55	0.54	0.56
SD:	0.2	0.16	0.26	0.31	0.29
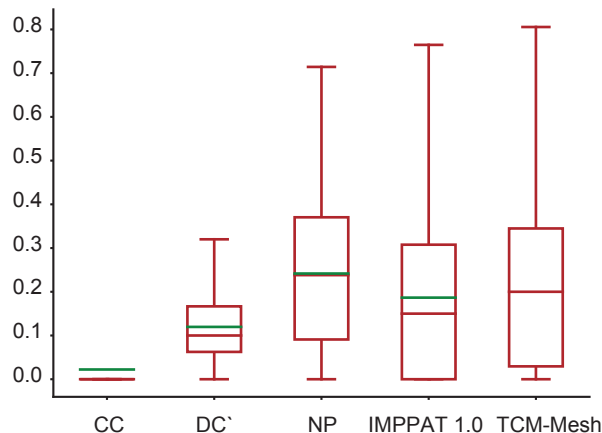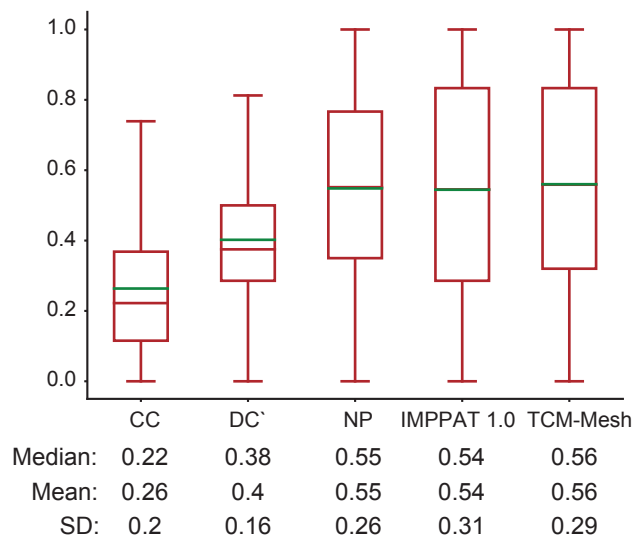
C

	Molecular weight (g/mol)			Log P			Toplogical Polar surface Area (TPSA) $Å^2$		
	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	334.34	377.56	259.25	2.46	2.38	3.43	70.00	98.13	109.40
TCM-Mesh	374.50	430.31	252.68	2.59	2.52	3.20	81.98	111.39	105.05

	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	3.38	1.76
DC`	1	1.59	1.16	6	6.09	2.53	8	8.29	3.94
NP	3	4.06	3.59	6	8.29	5.87	5	5.50	4.23
IMPPAT	2	2.84	4.00	4	5.89	6.09	3	4.84	6.71
TCM-Mesh	2	3.13	3.81	5	6.97	6.41	4	5.03	5.82