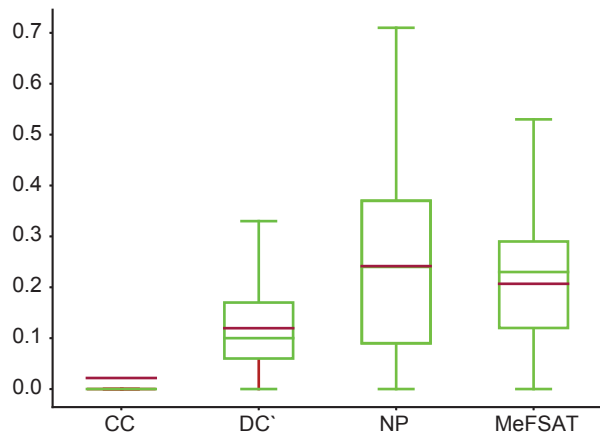


**A**

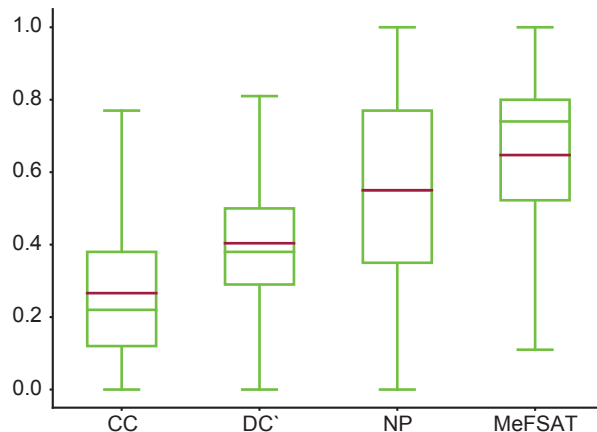
## Stereochemical complexity



Median: 0.0      0.10      0.24      0.23  
Mean: 0.02      0.12      0.24      0.21  
SD: 0.05      0.08      0.17      0.12

**B**

## Shape complexity



Median: 0.22      0.38      0.55      0.74  
Mean: 0.27      0.40      0.55      0.65  
SD: 0.20      0.17      0.26      0.23

**C**

## Molecular weight (g/mol)

	Median	Mean	SD
CC	311.34	314.19	74.62
DC	495.54	509.50	158.65
NP	386.53	457.22	231.65
MeFSAT	440.62	419.81	154.63

## Log P

	Median	Mean	SD
CC	3.30	3.21	1.50
DC	3.97	3.98	2.14
NP	1.94	1.64	2.35
MeFSAT	3.88	4.10	2.64

Topological Polar surface Area  
(TPSA) Å<sup>2</sup>

	Median	Mean	SD
CC	55.98	58.33	26.06
DC	94.56	97.08	40.68
NP	105.20	136.56	93.56
MeFSAT	86.99	91.18	45.88

## Hydrogen bond donors

	Median	Mean	SD
CC	1	0.94	0.89
DC	1	1.59	1.16
NP	3	4.06	3.59
MeFSAT	2	2.34	1.66

## Hydrogen bond acceptors

	Median	Mean	SD
CC	4	4.01	1.79
DC	6	6.09	2.53
NP	6	8.29	5.87
MeFSAT	5	4.94	2.41

## Rotatable bonds

	Median	Mean	SD
CC	4	4.13	2.09
DC	9	9.50	4.78
NP	5	6.04	4.67
MeFSAT	5	6.03	5.89