Signatures of spatial organizations – From the universe of proteins to the universe in general*

Aditya Mittal

Kusuma School of Biological Sciences,

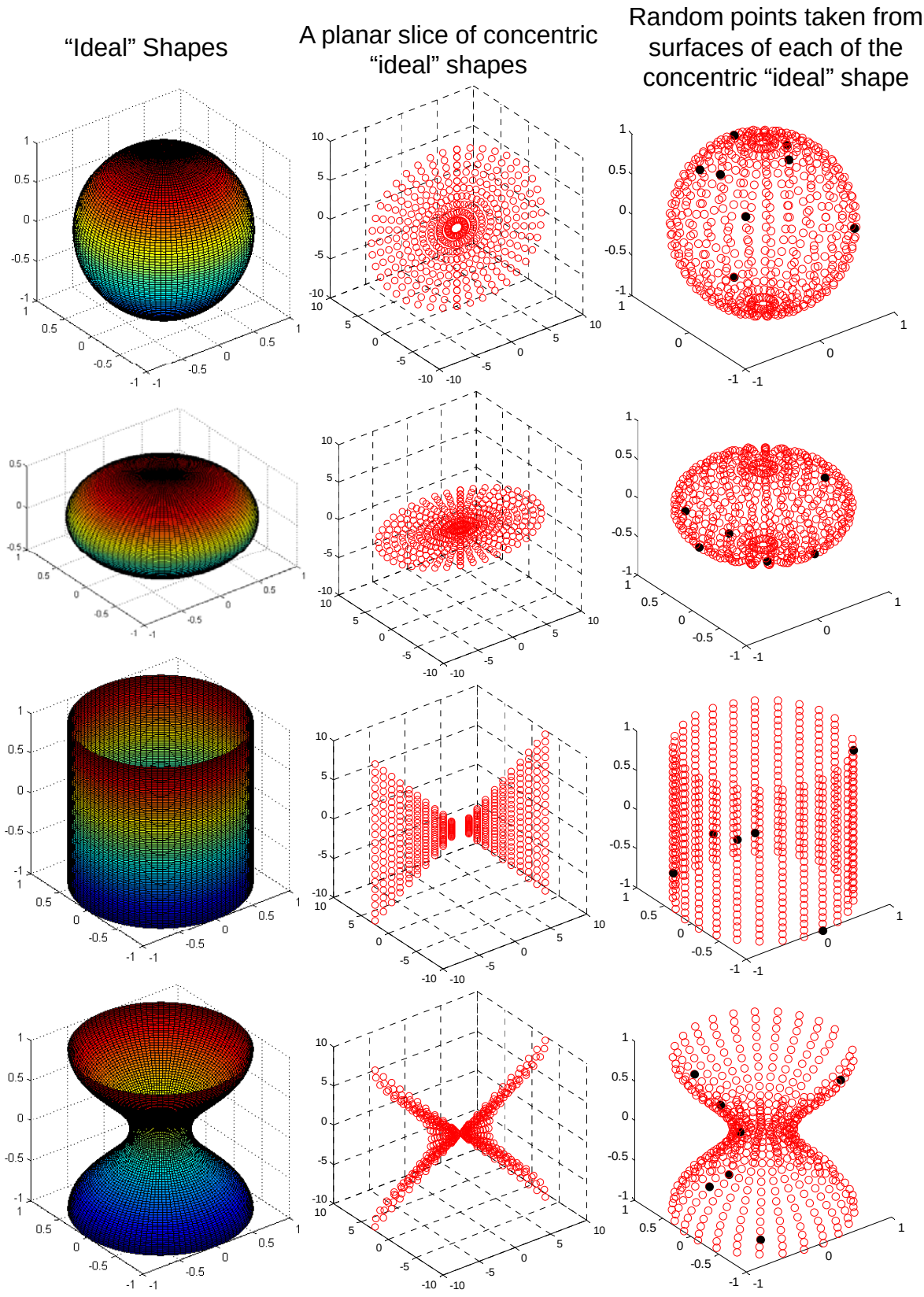
Indian Institute of Technology Delhi,

Hauz Khas, New Delhi 110016, India.

Email: amittal@bioschool.iitd.ac.in

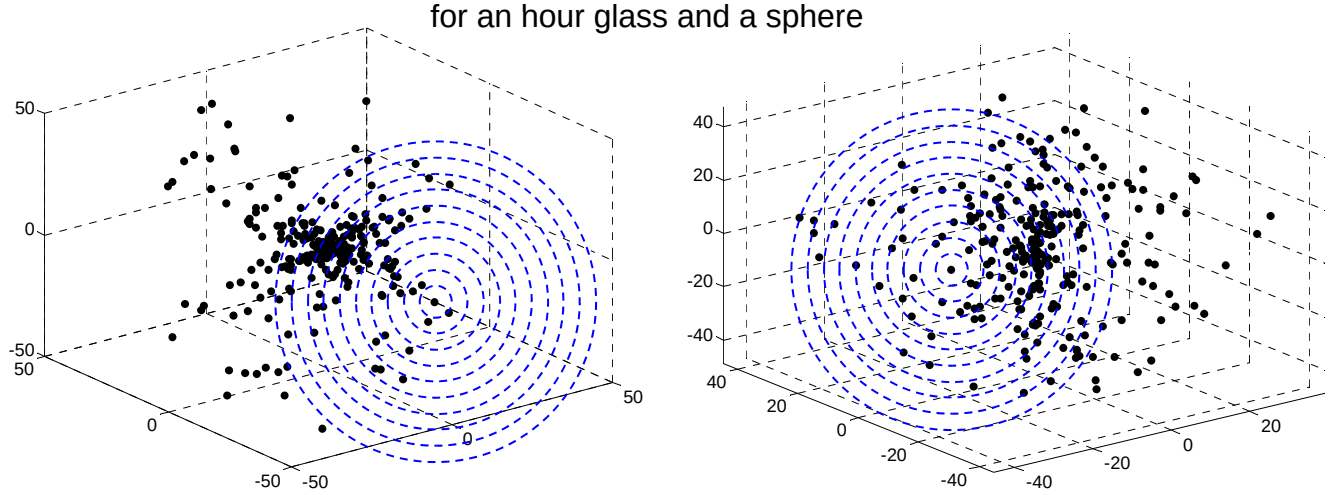
Web: http://web.iitd.ac.in/~amittal

How are (structures formed by) random points originating from ideal concentric shapes organized in space? Is there a signature of the underlying geometry in the final organization of these points?



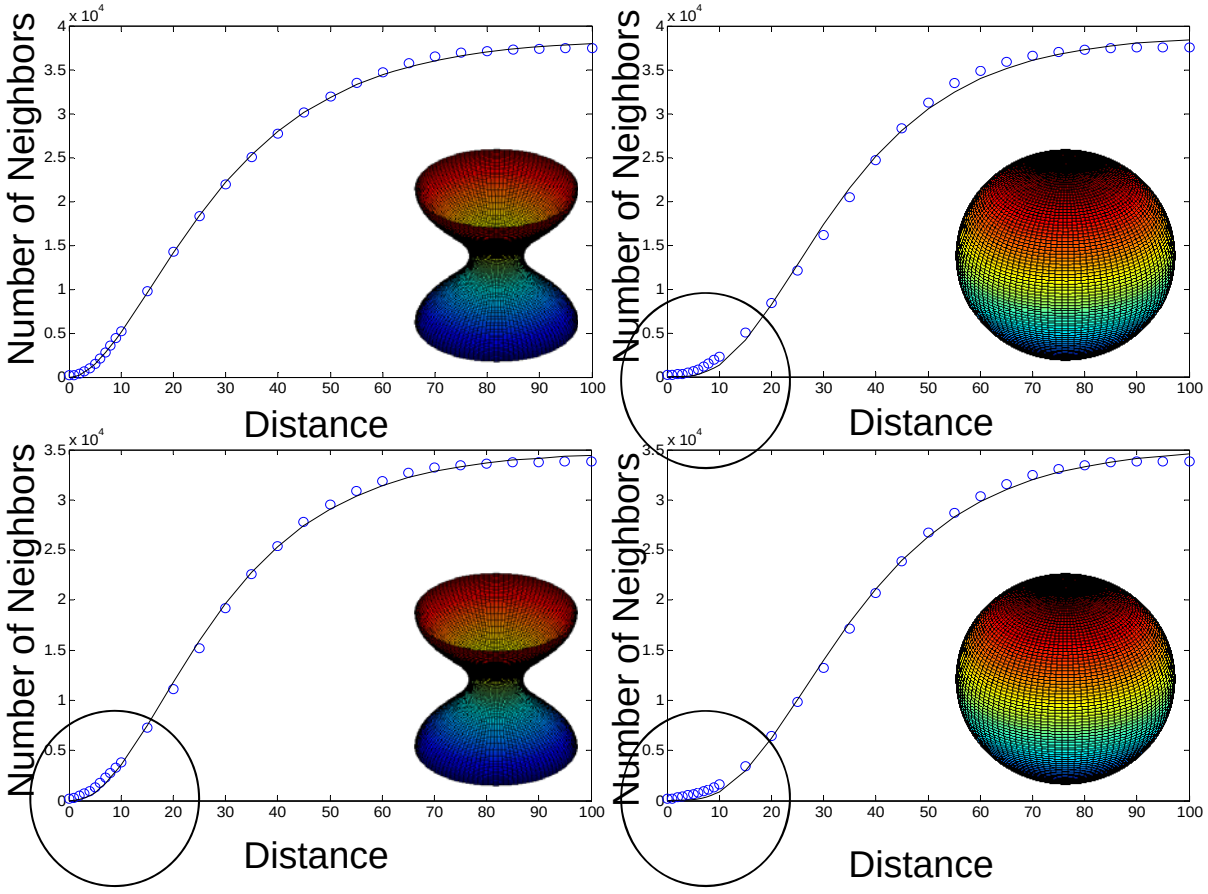
Deciphering spatial organization of points originating from ideal concentric shapes

Organization of random points taken from surfaces of 50 concentric “ideal” shape, example shown for an hour glass and a sphere



The points are analyzed as in Mittal et al., J. Biomol. Struct. Dyn. (2010) ; Mittal & Jayaram , J. Biomol Struct. Dyn. (2011), with slight modifications (no exclusion of peptide-bonded neighbors)

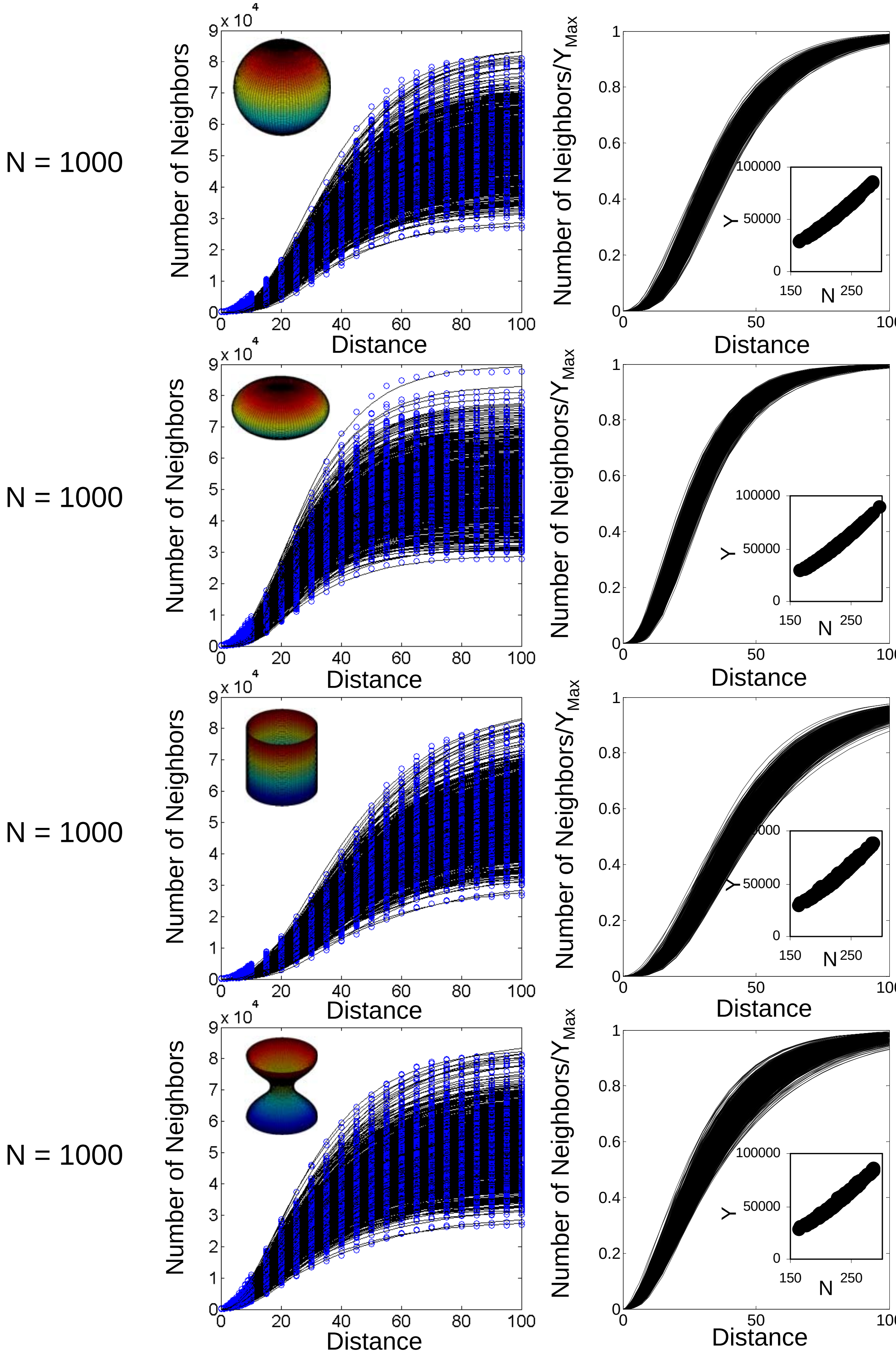
Smooth lines → Data fit using $Y = Y_{Max}(1-e^{-kX})^n$



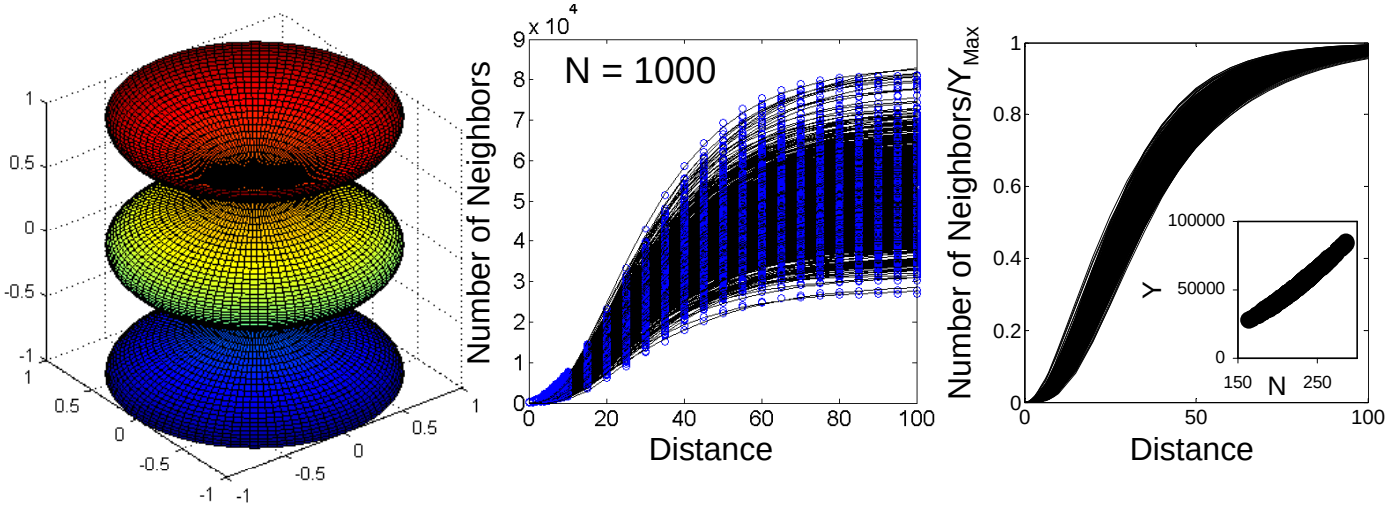
At “close range” even random points show some deviations from the fits. Over the last 40 years deviations equivalent or even smaller than these observed in protein structures have lead to an incorrect development of statistical potentials.

Spatial organization of points originating from a ideal shapes

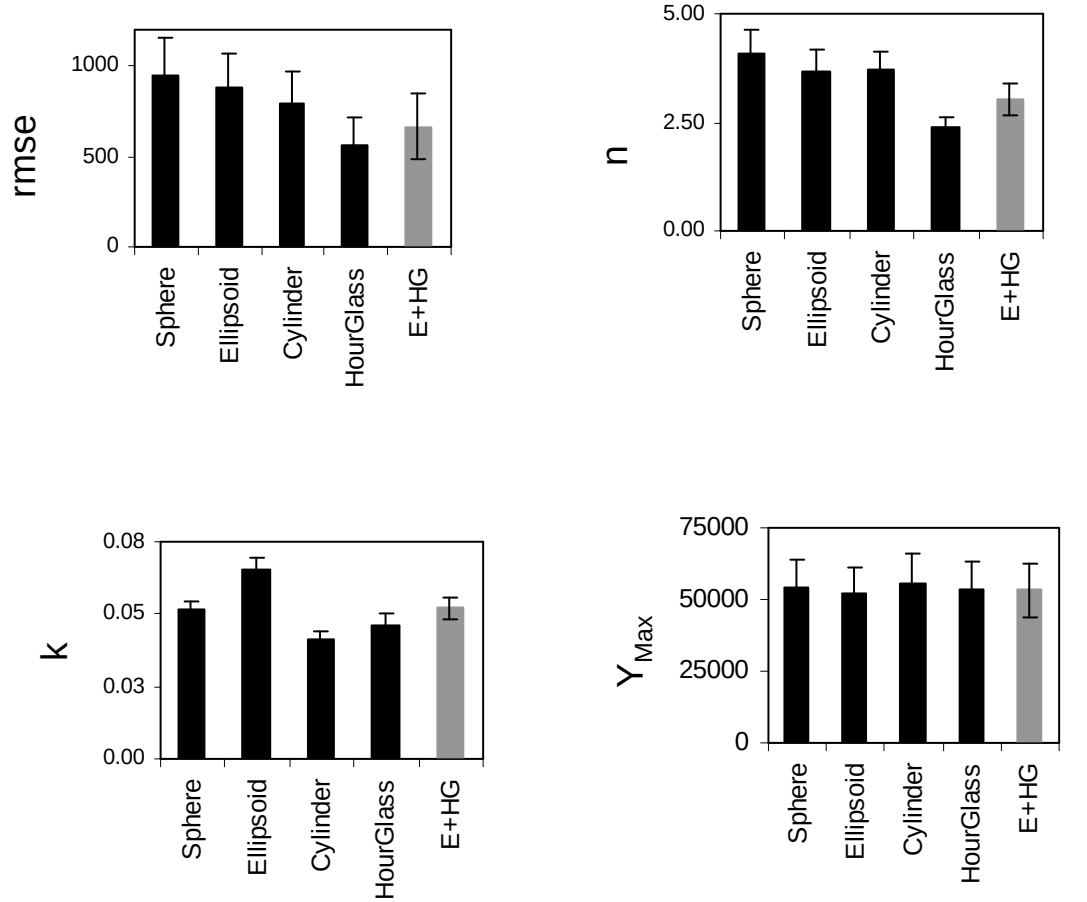
Each curve represents one set of points. Right panels show that all distributions collapse into a narrow band on normalization with the asymptote and asymptote is directly correlated to the total number of points



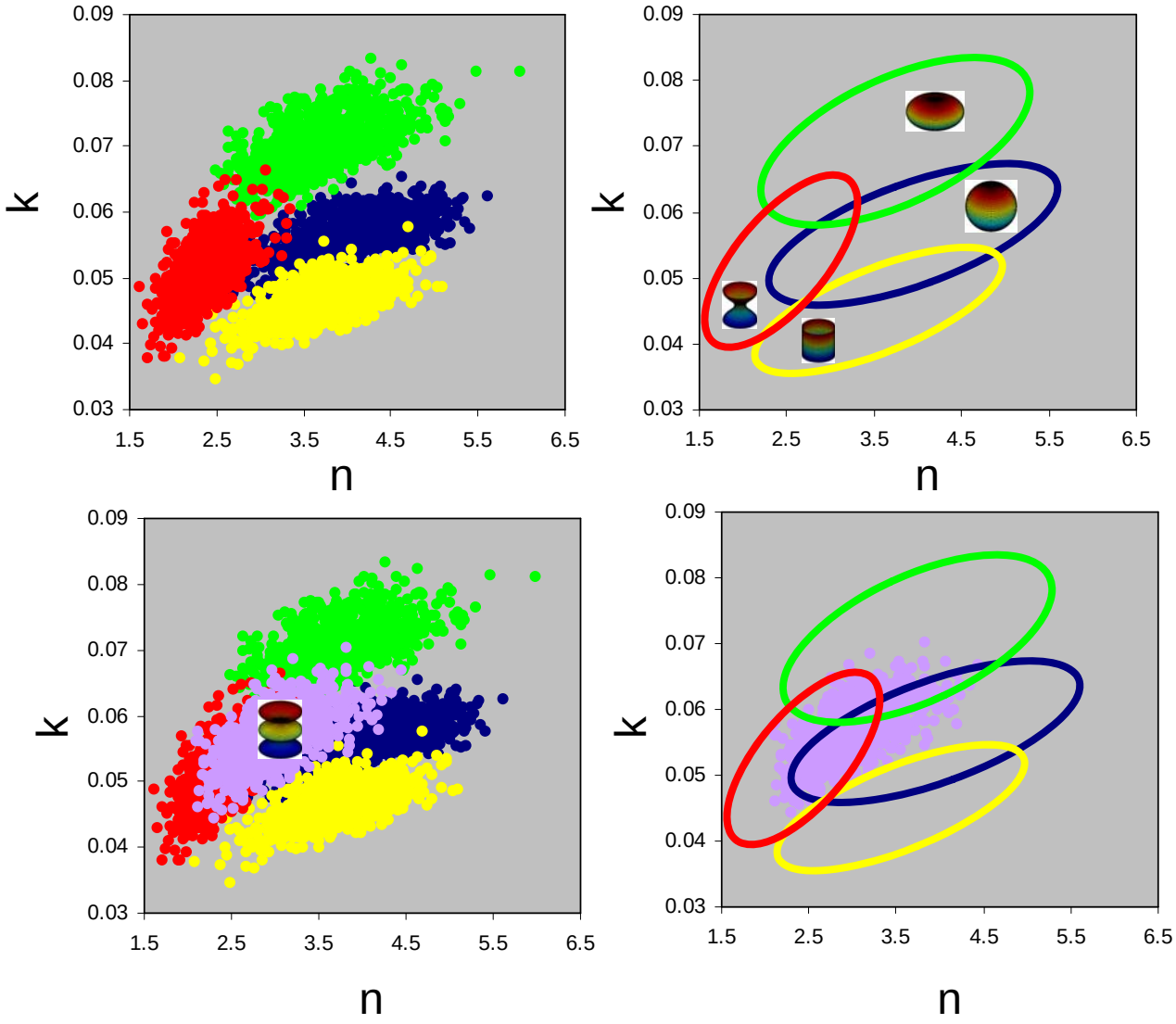
Spatial organization of points originating from a “hybrid” shape (HourGlass + Ellipsoid – E+HG)



Smooth lines → Data fit using $Y = Y_{Max}(1-e^{-kX})^n$

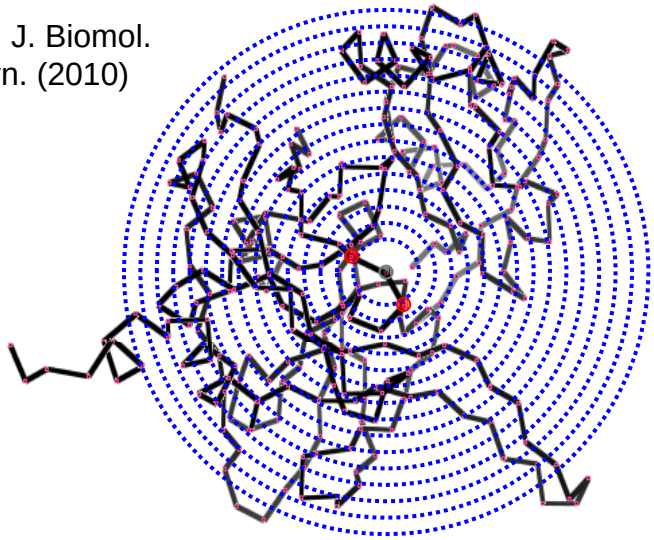


Spatial signatures of known shapes in “n-k” space



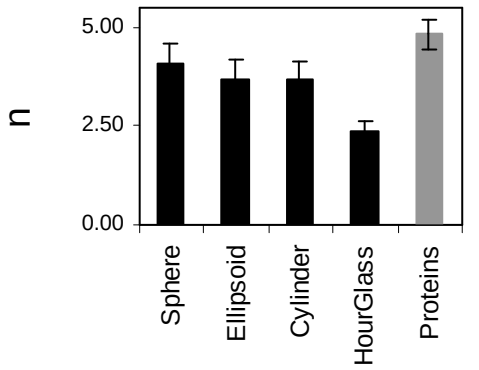
Spatial signatures of proteins - Universal spatial organization

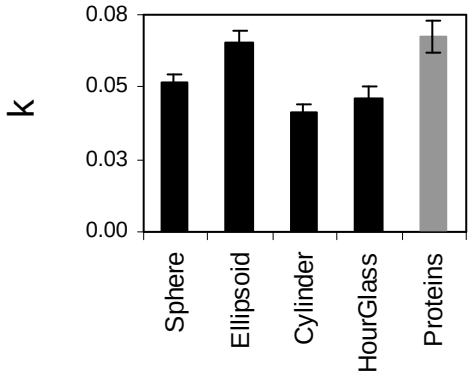
Mittal et al., J. Biomol. Struct. Dyn. (2010)

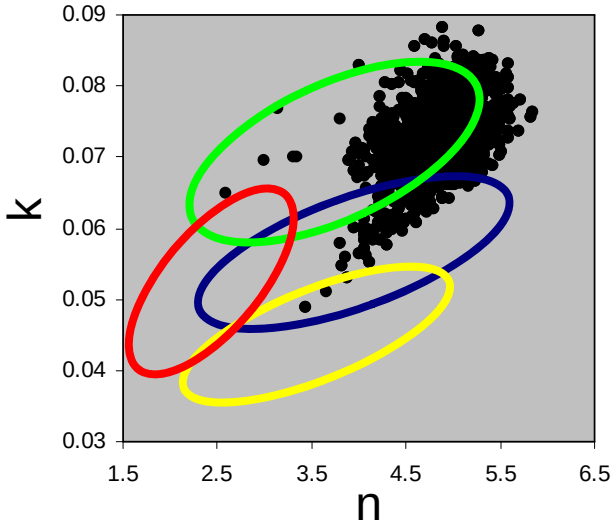


SCOP Classifications

Alpha	2066
Alpha/Beta	4877
Alpha+Beta	3476
Beta	3131
Membrane	97







Outliers

k	n	AA2	AA1
5.99E-02	2.59	10	10
6.46E-02	2.98	10	10
7.18E-02	3.14	10	10
6.50E-02	3.31	10	10
6.50E-02	3.34	10	10
4.40E-02	3.43	16	19
4.40E-02	3.43	19	16
4.62E-02	3.65	19	19

1	A
2	V
3	I
4	L
5	Y
6	F
7	W
8	P
9	M
10	C
11	T
12	S
13	Q
14	N
15	D
16	E
17	H
18	R
19	K
20	G

Hence "Stoichiometrically driven universal Spatial Organization for folded proteins" **Proved (Q. E. D.) – Thank You!**

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