

Title	Classification of polyhedral shapes from individual anisotropically resolved cryo-electron tomography reconstructions
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Publication date	2016-06-13
Original Citation	Bag, S., Prentice, M. B., Liang, M., Warren, M. J. and Roy Choudhury, K. (2016) 'Classification of polyhedral shapes from individual anisotropically resolved cryo-electron tomography reconstructions', BMC Bioinformatics, 17, 234 (14pp). doi: 10.1186/s12859-016-1107-5
Type of publication	Article (peer-reviewed)
Link to publisher's version	<a href="https://bmcbioinformatics.biomedcentral.com/articles/10.1186/s12859-016-1107-5">https://bmcbioinformatics.biomedcentral.com/articles/10.1186/s12859-016-1107-5</a> - <a href="https://doi.org/10.1186/s12859-016-1107-5">10.1186/s12859-016-1107-5</a>
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## Supplementary information for : Classification of polyhedral shapes from individual incomplete cryo-EM reconstructions

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Table S5: Categorization of features in the topological profile (TP) of a polyhedral graph (PG)

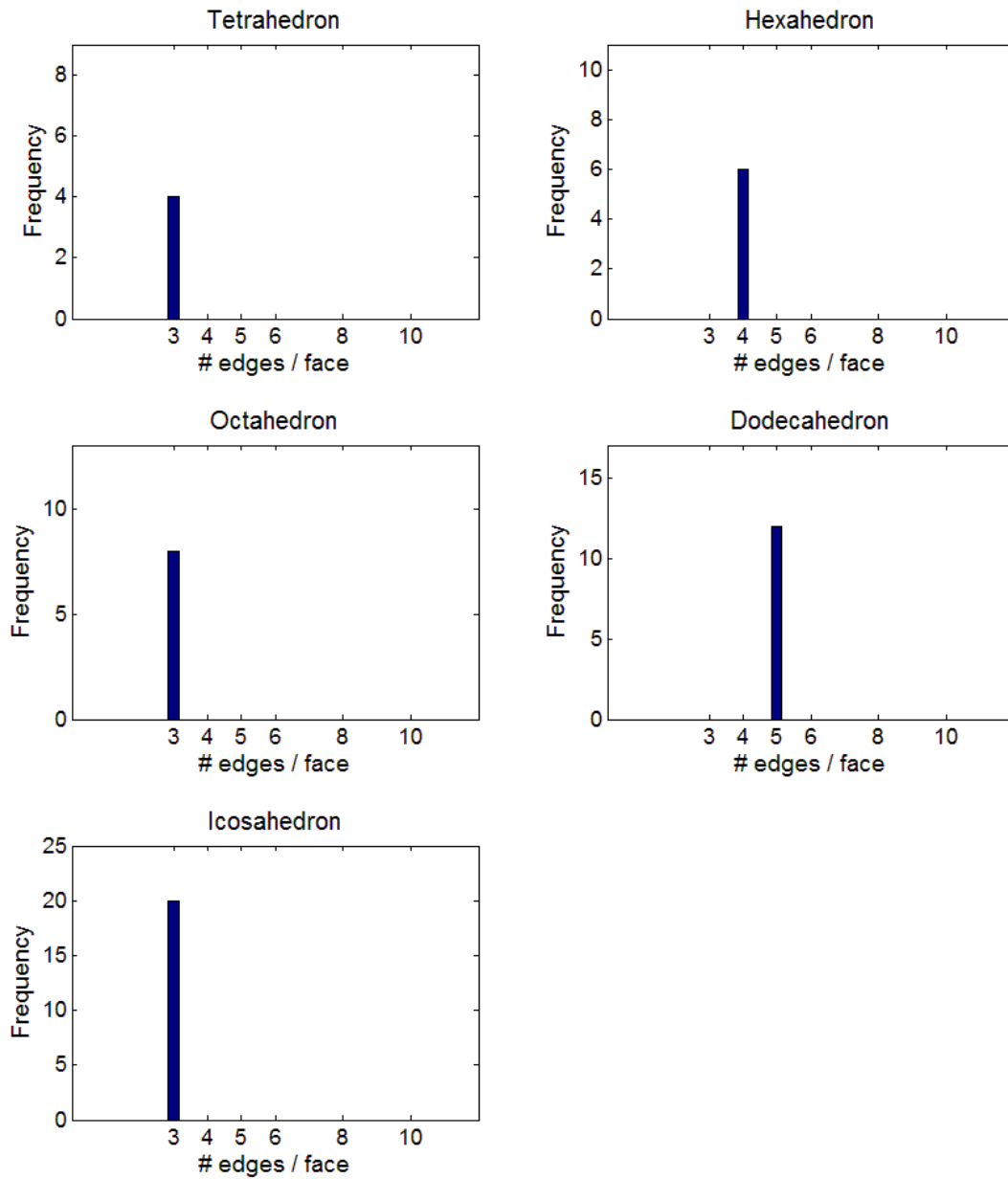


Figure S1: Distribution of number of edges per face for Platonic solids

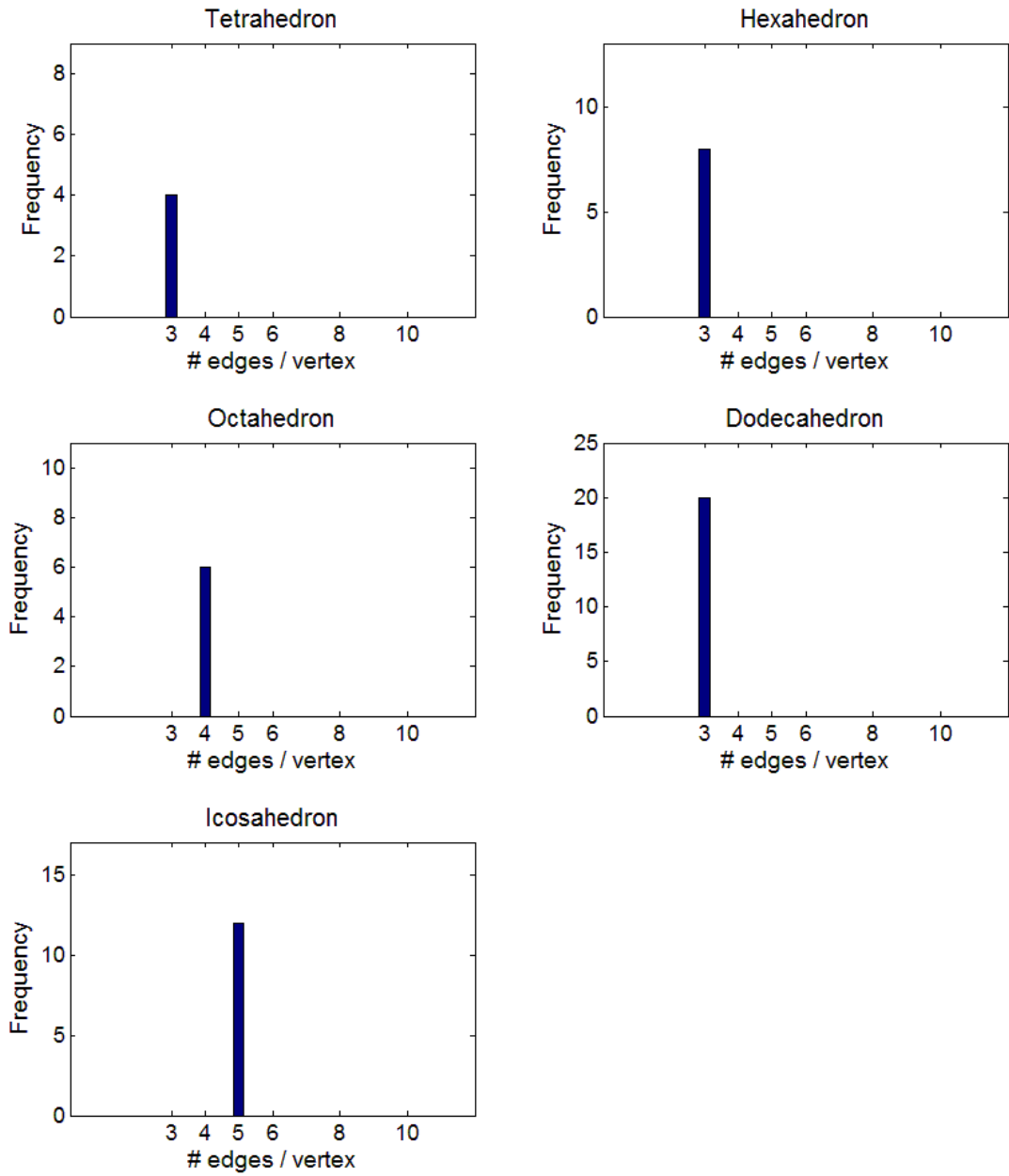


Figure S2: Distribution of vertex degree (number of edges meeting at a vertex) for Platonic solids

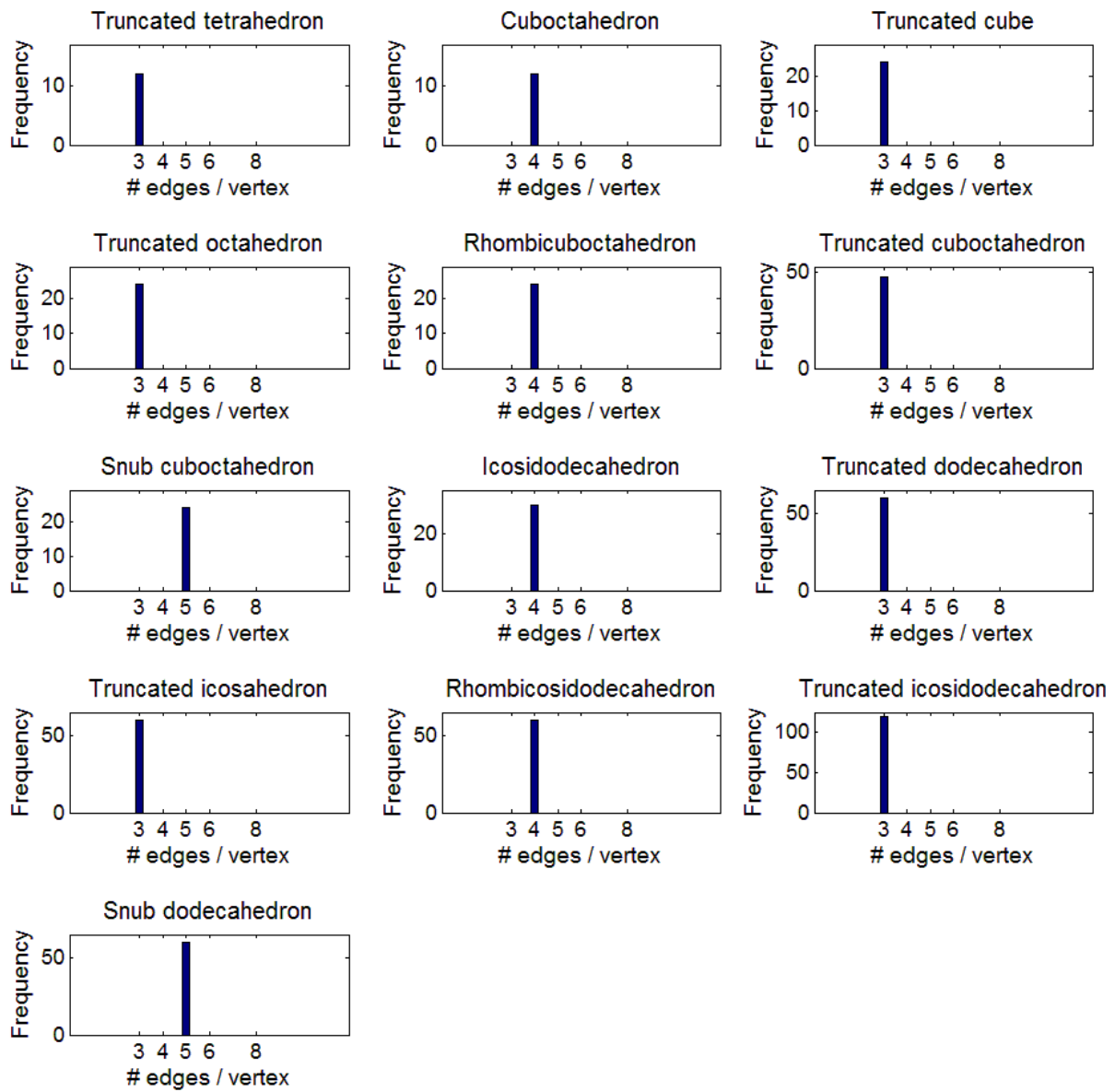


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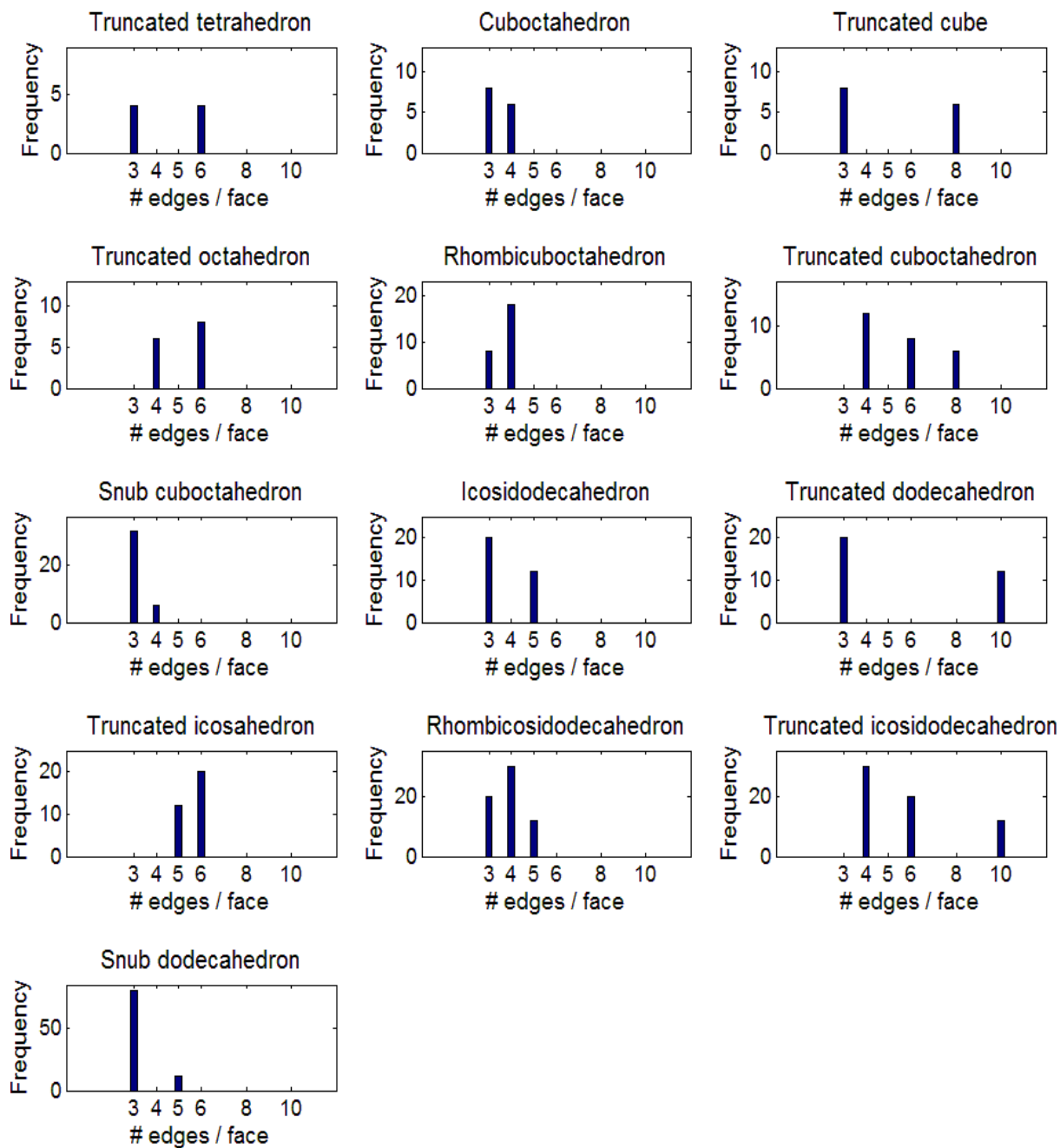


Figure S4: Distribution of number of edges per face for Archimedean solids

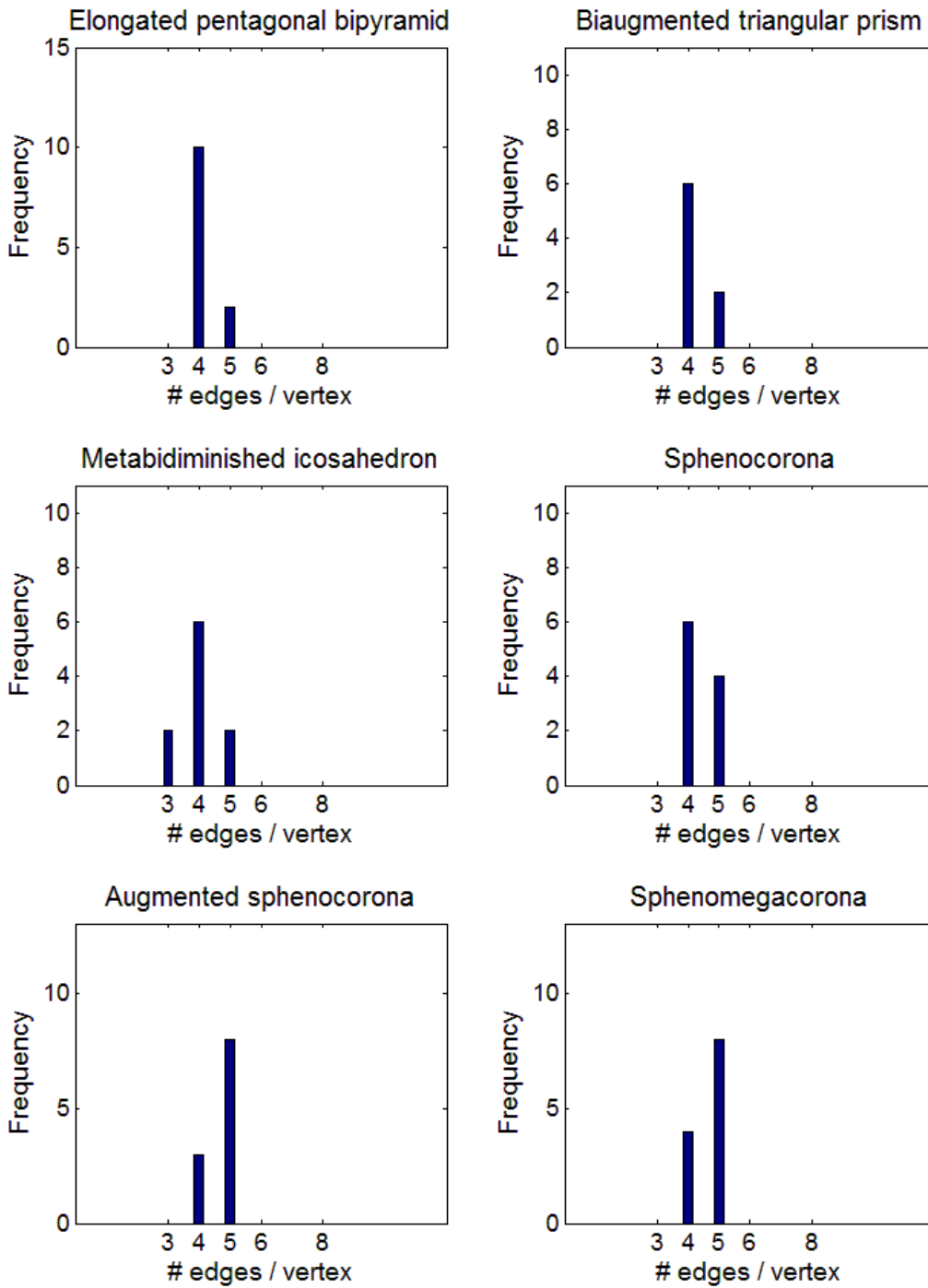


Figure S5: Distribution of vertex degree for 6 Johnson solids



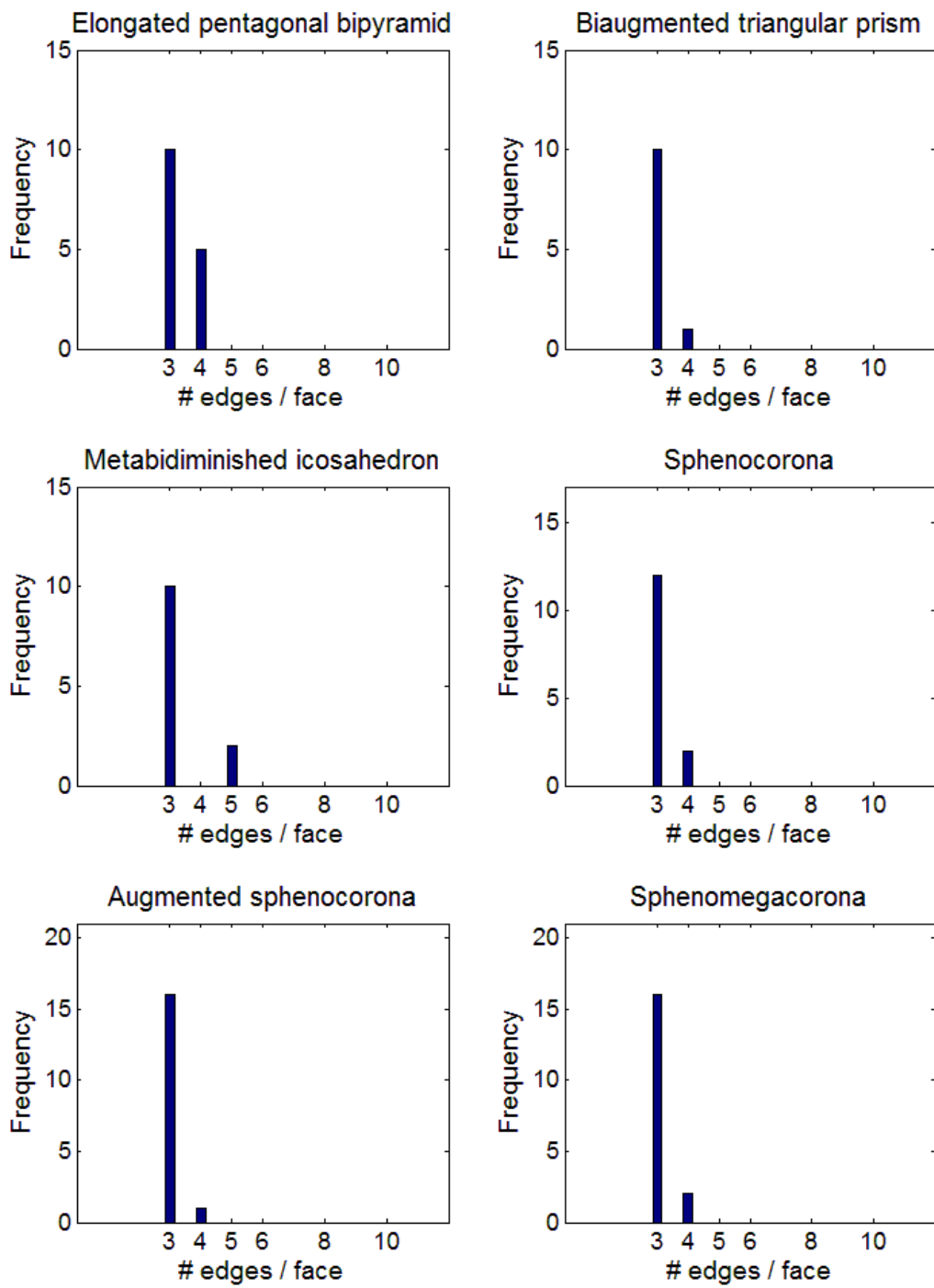


Figure S6: Distribution of number of edges per face for Johnson solids

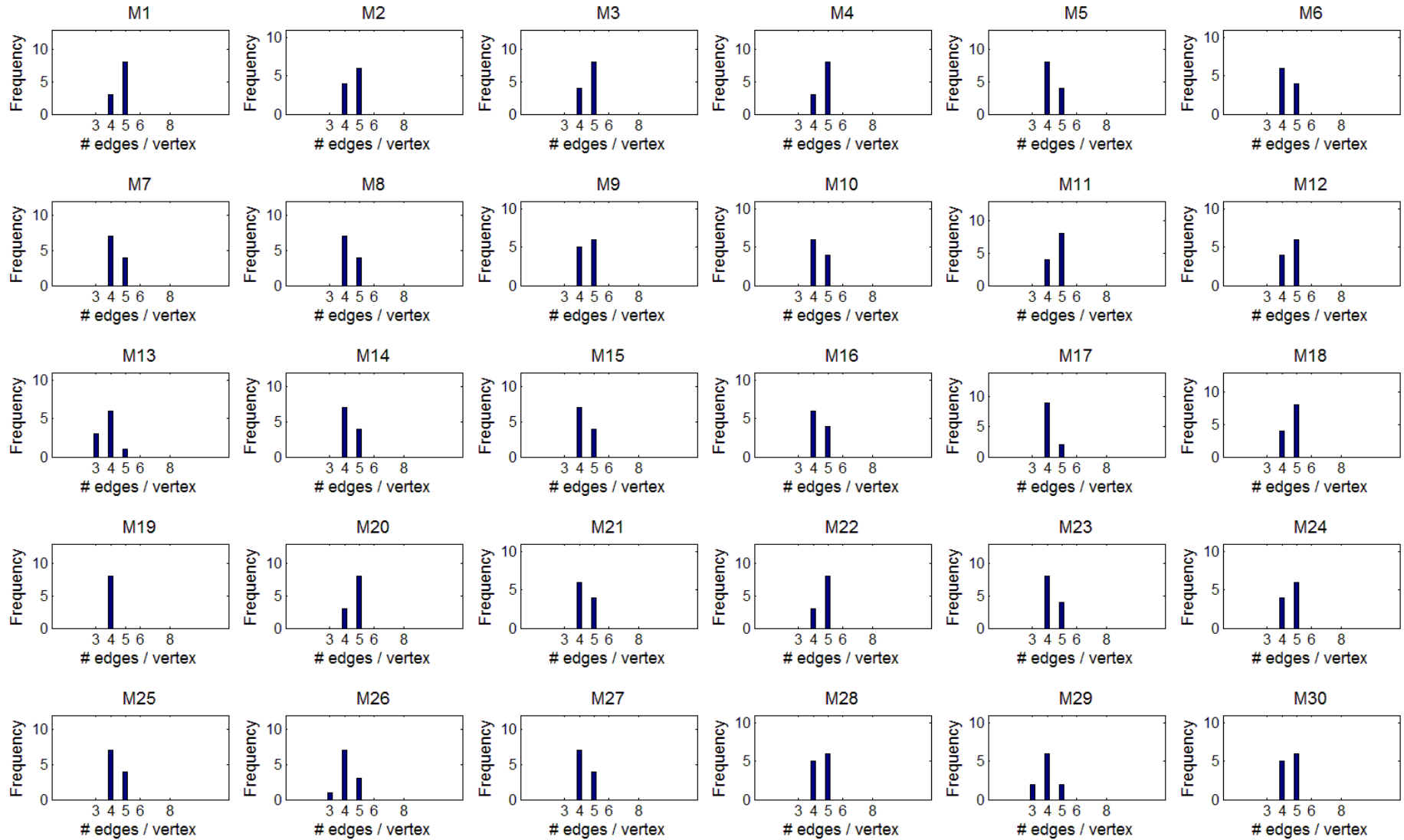


Figure S7: The distribution of vertex degree in MCs

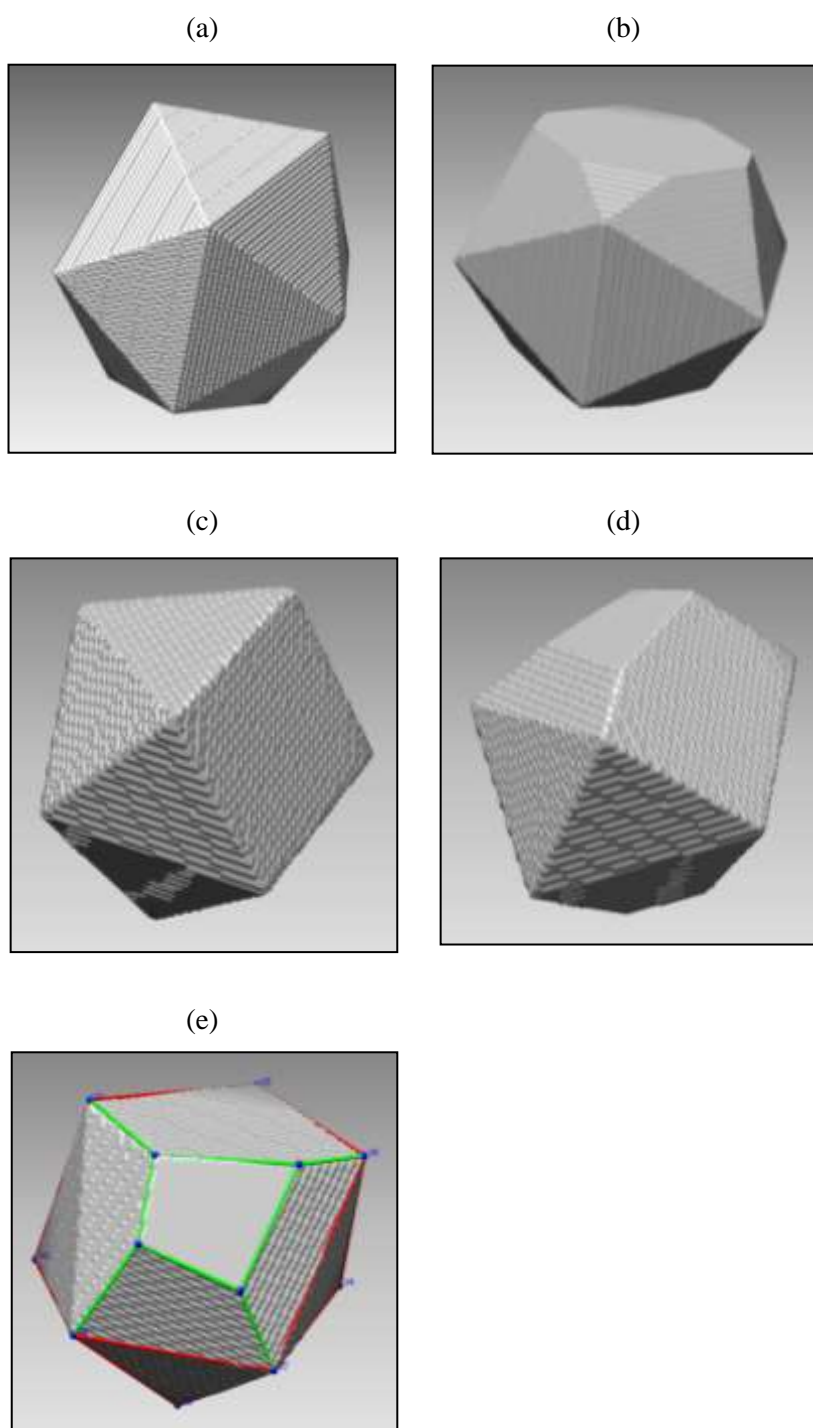


Figure S8: **Simulated standard Polyhedron and their view after truncation - (a) A simulated icosahedron, (b) the icosahedron with missing top, (c) A simulated sphenocorona, (d) the sphenocorona with missing top and (e) the ball-stick diagram on (d)**

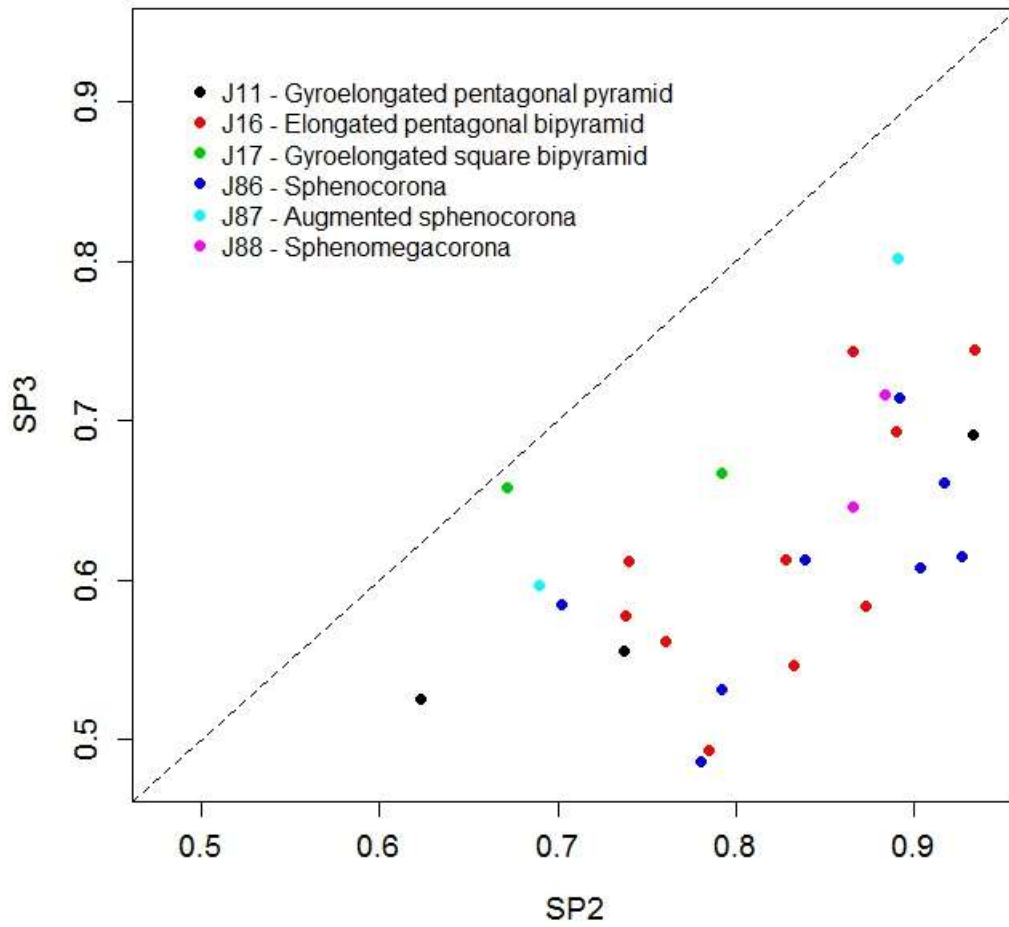


Figure S9: Distribution of aspect ratios by identified structure of BMCs.  $SP2 = \lambda_2/\lambda_1$ ,  $SP3 = \lambda_3/\lambda_1$ , where  $\lambda_1 \geq \lambda_2 \geq \lambda_3$  are the principal axes of an ellipsoid fitted to each reconstructed BMC.

Table S1: Test set misclassification error for SVM classifier summarised by class of solid. This analysis is based on the set of 54 solids with 20 vertices or less. The highlighted section refers to the chance of misclassification of a symmetric Platonic solid as a Johnson solid.

Predicted shape class	Misclassification error	Actual shape class			
		Johnson Solids	Platonic Solids	Archimedean Solids	Catalan Solids
Johnson Solids	Minimum	0.0120	0.0000	0.0200	0.0000
	Maximum	0.5240	0.0540	0.4620	0.0020
	Median	0.2680	0.0320	0.2410	0.0000
	Mean	0.2763	0.0287	0.2410	0.0005

	SD	0.1462	0.0272	0.3125	0.0010
	5th Percentile	0.0520	0.0000	0.0200	0.0000
	95th Percentile	0.4990	0.0540	0.4620	0.0020
<b>Platonic Solids</b>	Minimum	0.0000	0.0000	0.0000	0.0000
	Maximum	0.0320	0.3200	0.2900	0.0000
	Median	0.0000	0.0320	0.1450	0.0000
	Mean	0.0014	0.1173	0.1450	0.0000
	SD	0.0063	0.1762	0.2051	0.0000
	5th Percentile	0.0000	0.0000	0.0000	0.0000
	95th Percentile	0.0085	0.3200	0.2900	0.0000
<b>Archimedean Solids</b>	Minimum	0.0000	0.0000	0.0040	0.0000
	Maximum	0.3960	0.0020	0.5400	0.0000
	Median	0.0000	0.0000	0.2720	0.0000
	Mean	0.0120	0.0007	0.2720	0.0000
	SD	0.0603	0.0012	0.3790	0.0000
	5th Percentile	0.0000	0.0000	0.0040	0.0000
	95th Percentile	0.0520	0.0020	0.5400	0.0000
<b>Catalan Solids</b>	Minimum	0.0000	0.0000	0.0000	0.0000
	Maximum	0.0380	0.0000	0.0000	0.0340
	Median	0.0000	0.0000	0.0000	0.0160
	Mean	0.0015	0.0000	0.0000	0.0165
	SD	0.0059	0.0000	0.0000	0.0154
	5th Percentile	0.0000	0.0000	0.0000	0.0000
	95th Percentile	0.0080	0.0000	0.0000	0.0340

Table S2: Predicted polyhedral shapes for 30 E. coli microcompartments using the SVM classifier. The names of the solids corresponding the serial numbers are given in Table S3. The positive predictive value (PPV) is the chance that the correct solid was identified, based on estimated misclassification errors obtained using a mis-specified polyhedral graph test set.

Microcompartment No	Predicted Shape (Serial No.)	Positive Predictive Value
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		(PPV)
1	17	0.70
2	11	0.69
3	16	0.75
4	11	0.69
5	16	0.75
6	86	0.69
7	86	0.69
8	86	0.69
9	16	0.75
10	86	0.69
11	88	0.59
12	86	0.69
13	54	0.62
14	16	0.75
15	86	0.69
16	86	0.69
17	16	0.75
18	88	0.59
19	50	0.76
20	87	0.60
21	86	0.69
22	87	0.60
23	16	0.75
24	17	0.70
25	16	0.75
26	16	0.75
27	16	0.75
28	16	0.75
29	62	0.81
30	11	0.69
<b>Mean PPV</b>		0.70

Table S5: Categorization of features in the topological profile (TP) of a polyhedral graph (PG)

Topological profile component	Dimension	Feature type			
		Complete	Incomplete	Global	Local
V,E,F	3	x		x	
Face type distribution	6	x			x

Vertex degree distribution	6	x			x
At least face type distribution	8		x		x
At least vertex type distribution	8		x		x
Edge adjacency matrix	10x10 = 100	x			x
Face adjacency matrix	10x10 = 100	x			x
Total	231				