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| Title | Classification of polyhedral shapes from individual anisotropically resolved cryo-electron tomography reconstructions |
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Table S4 (in separate Excel spreadsheet due to size): List of estimated polyhedral graphs for 30 micro-compartments of *E. coli*, as represented by their topological profiles.

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

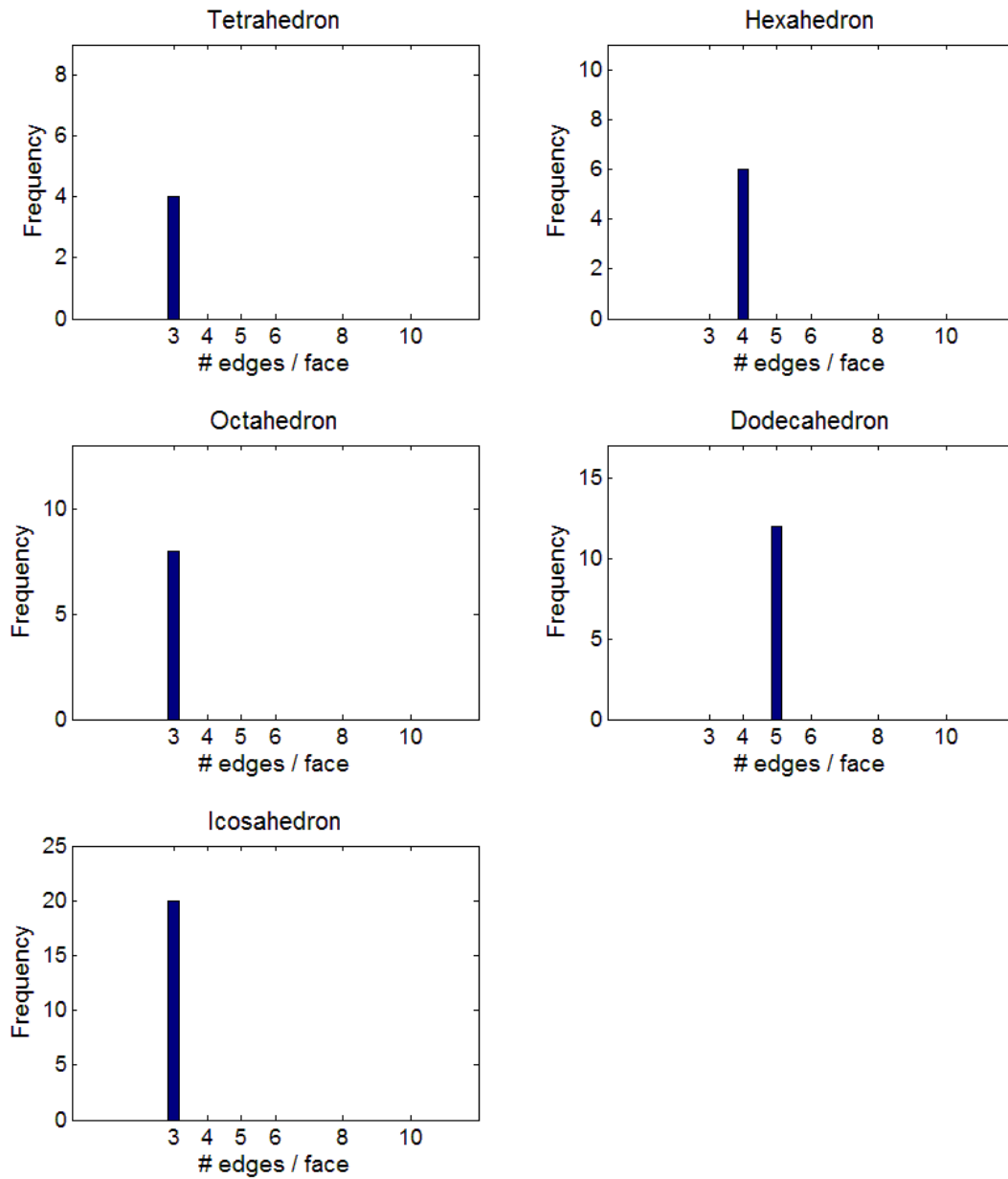


Figure S1: Distribution of number of edges per face for Platonic solids

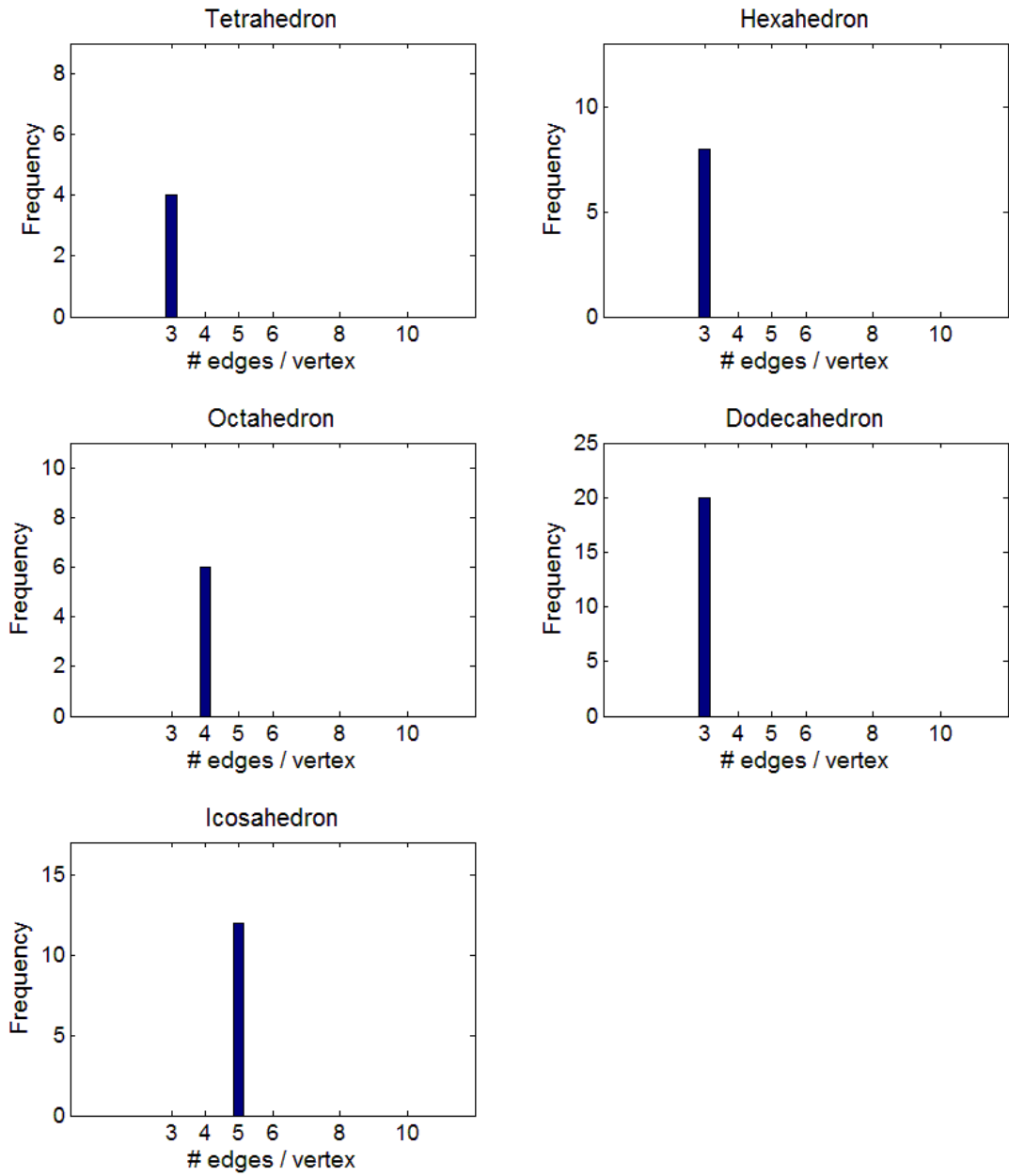


Figure S2: Distribution of vertex degree (number of edges meeting at a vertex) for Platonic solids

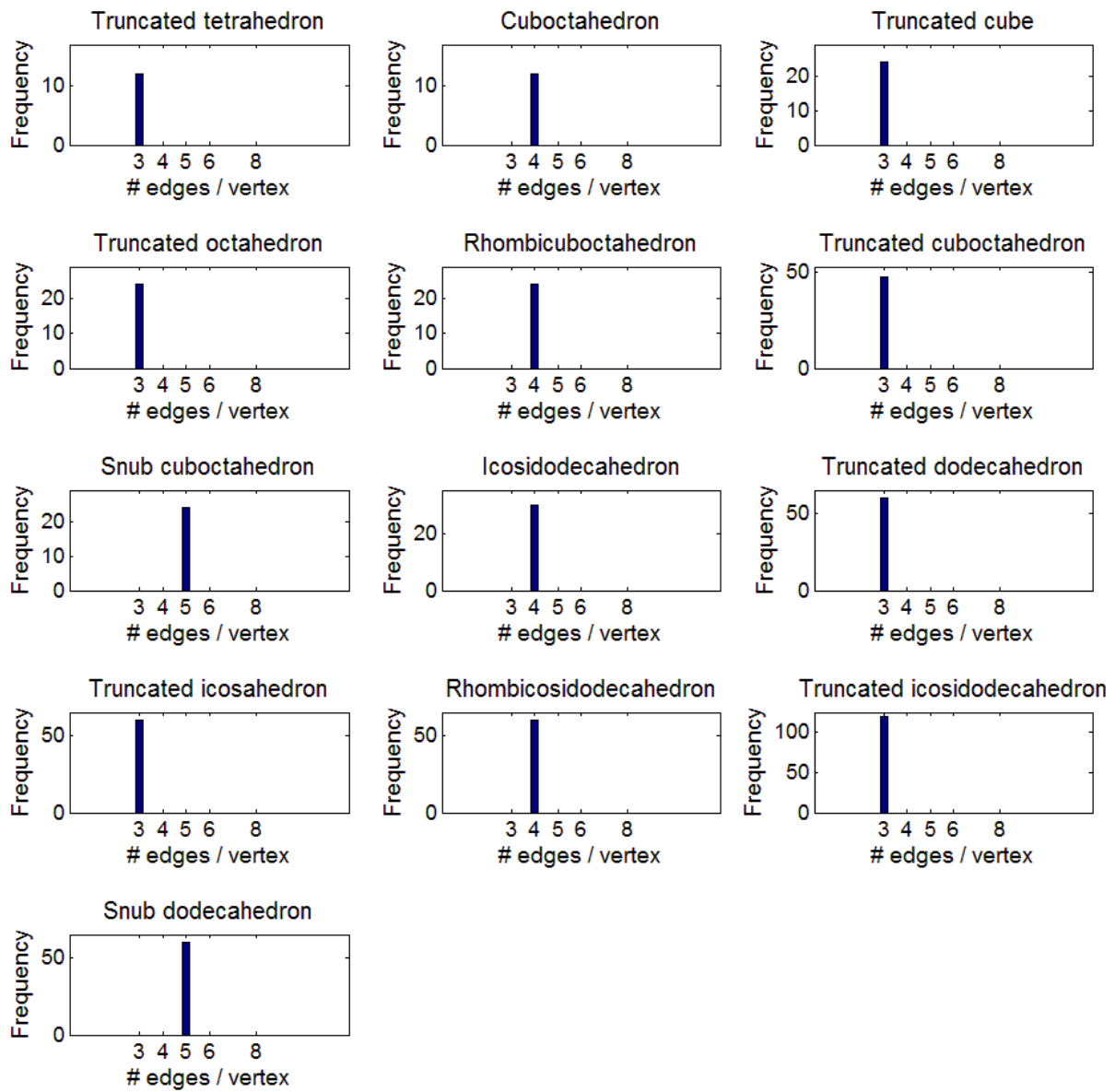


Figure S3: Distribution of vertex degree for Archimedean solids

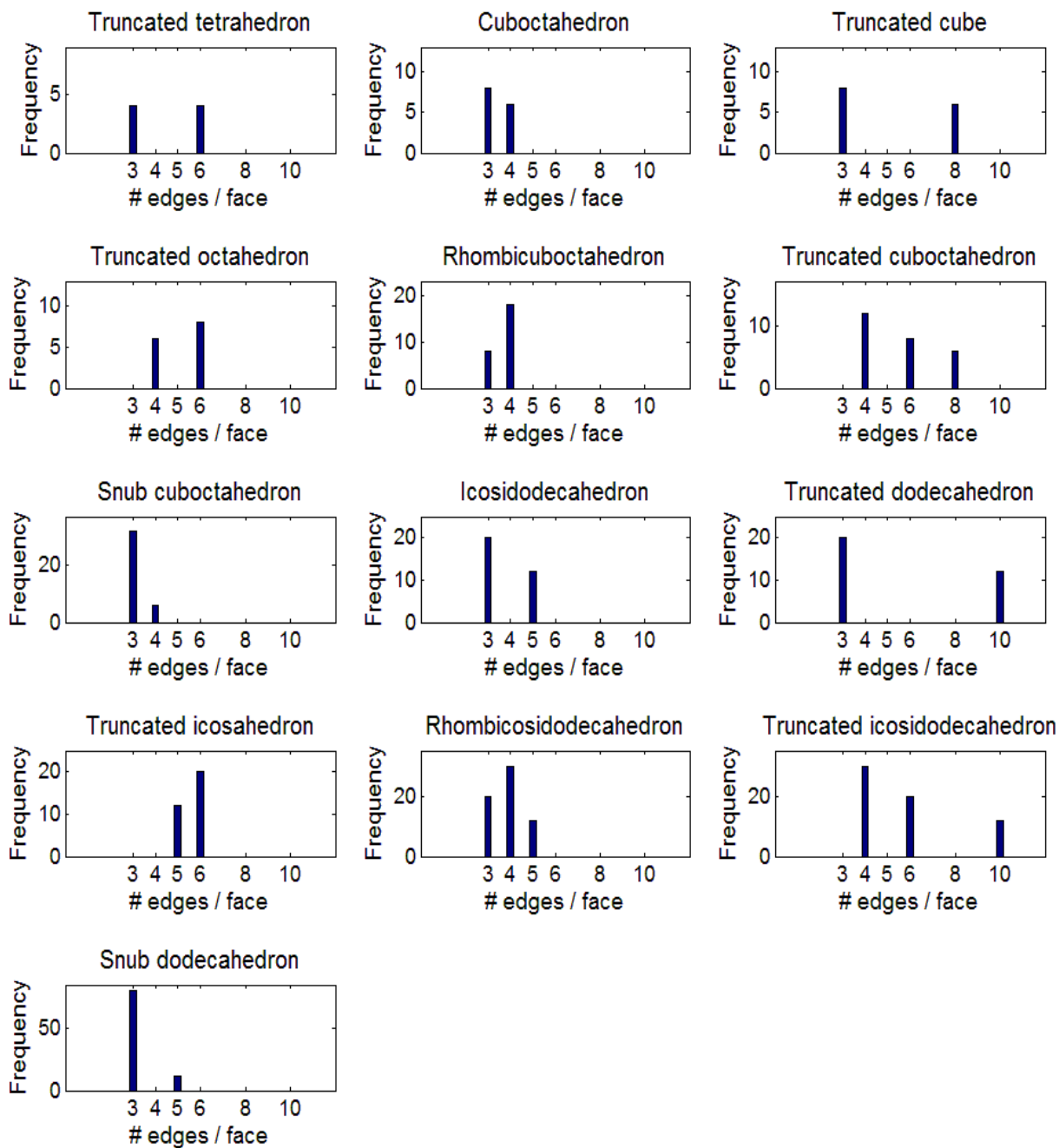


Figure S4: Distribution of number of edges per face for Archimedean solids

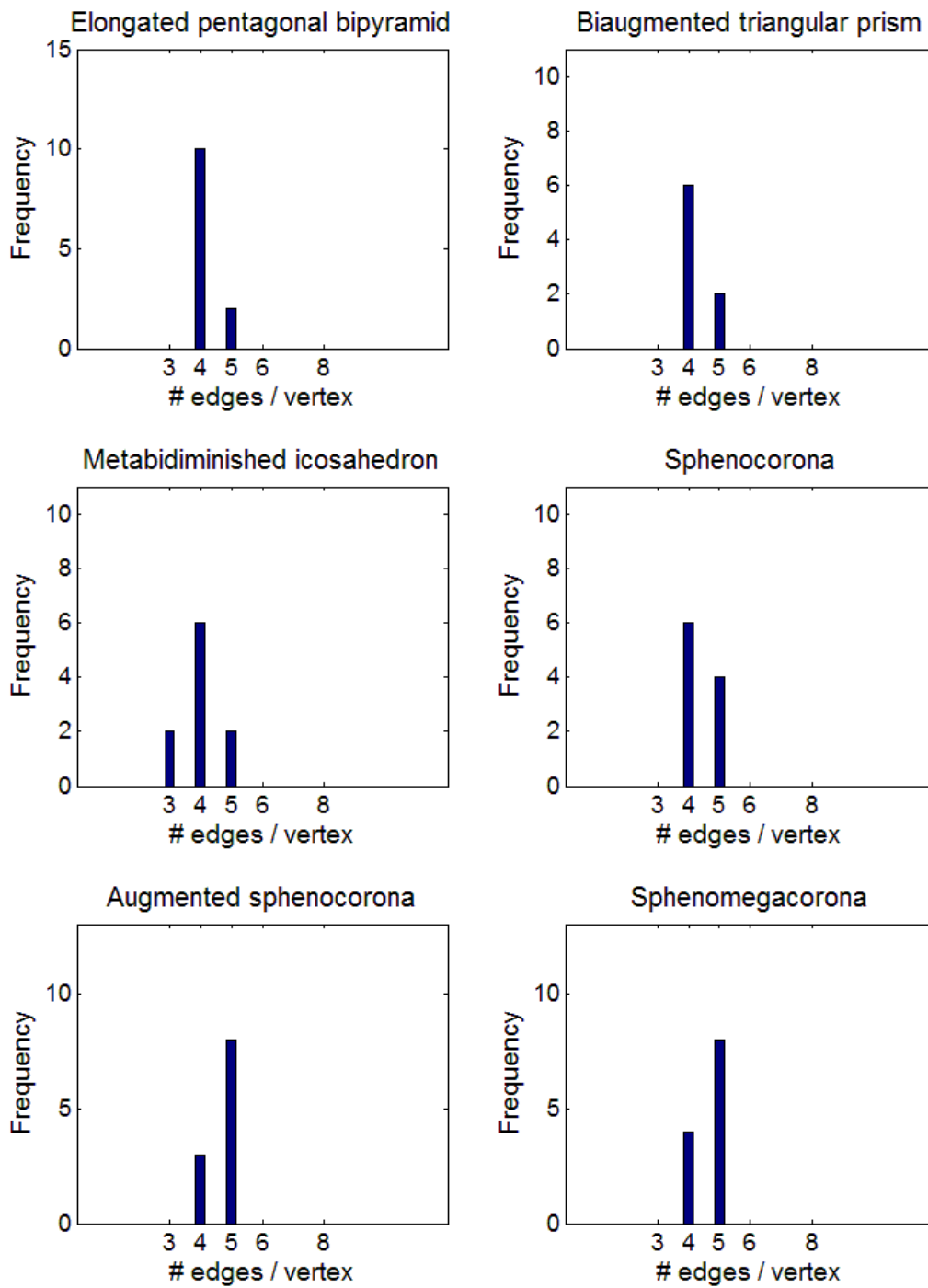


Figure S5: Distribution of vertex degree for 6 Johnson solids

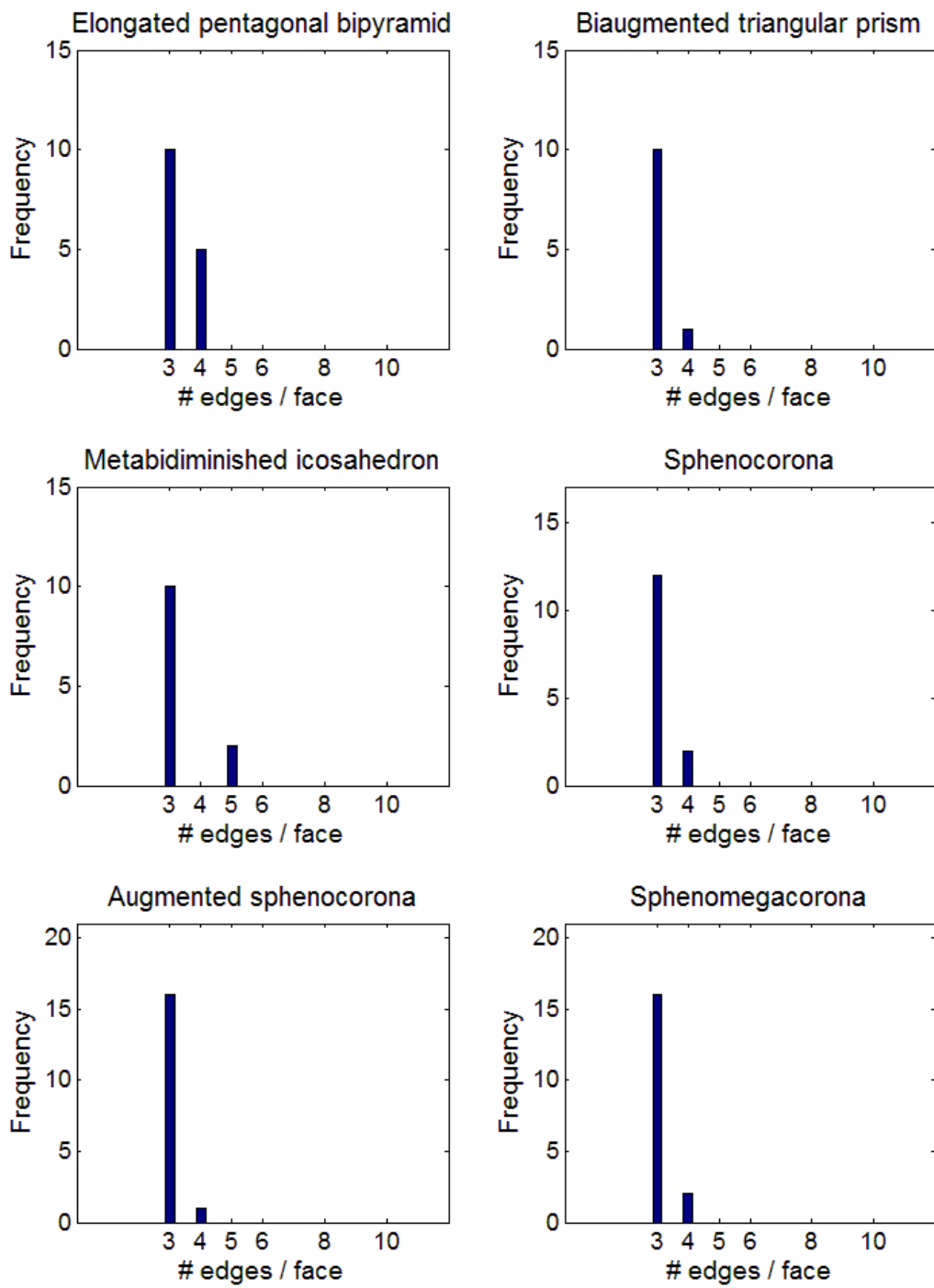


Figure S6: Distribution of number of edges per face for Johnson solids

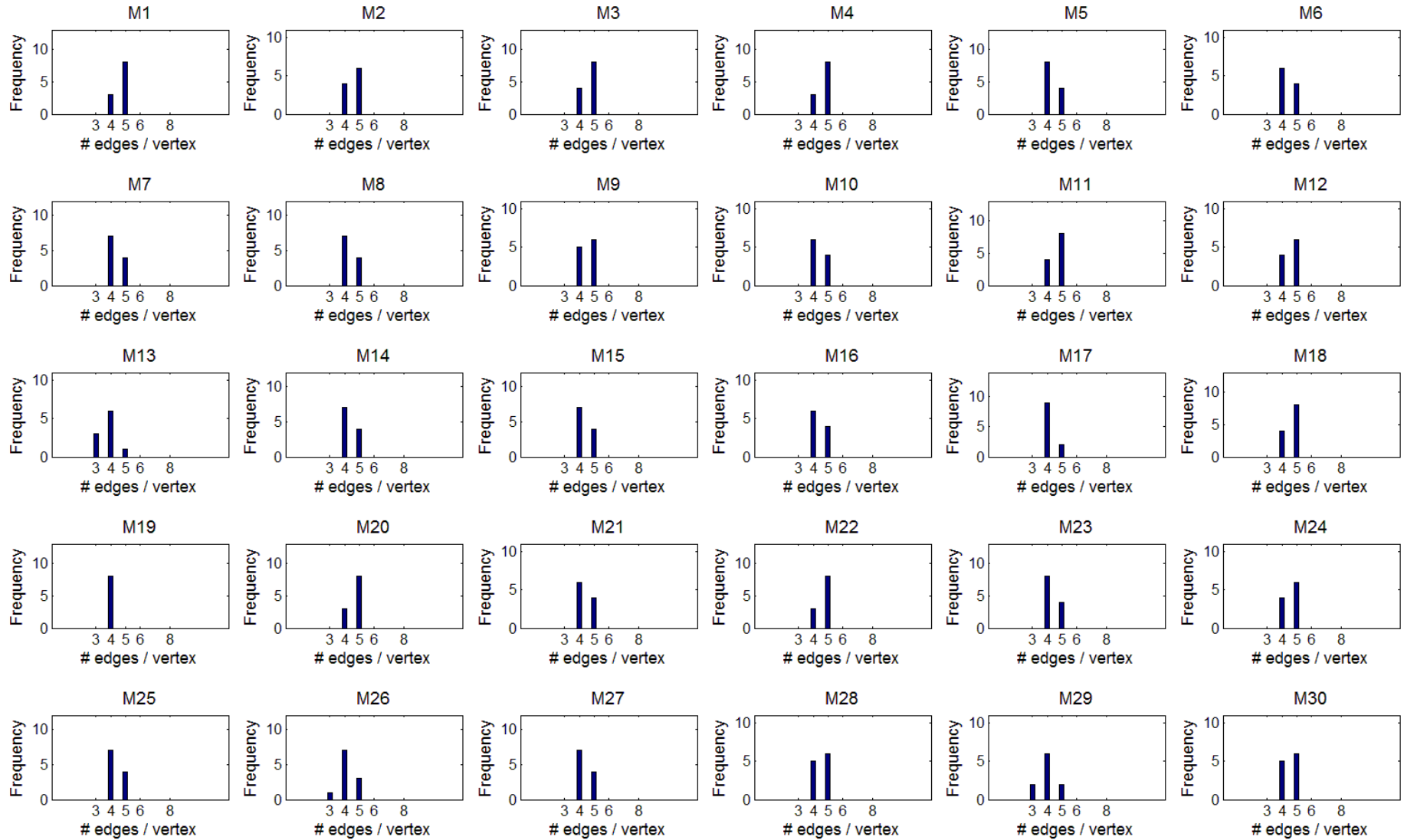


Figure S7: The distribution of vertex degree in MCs

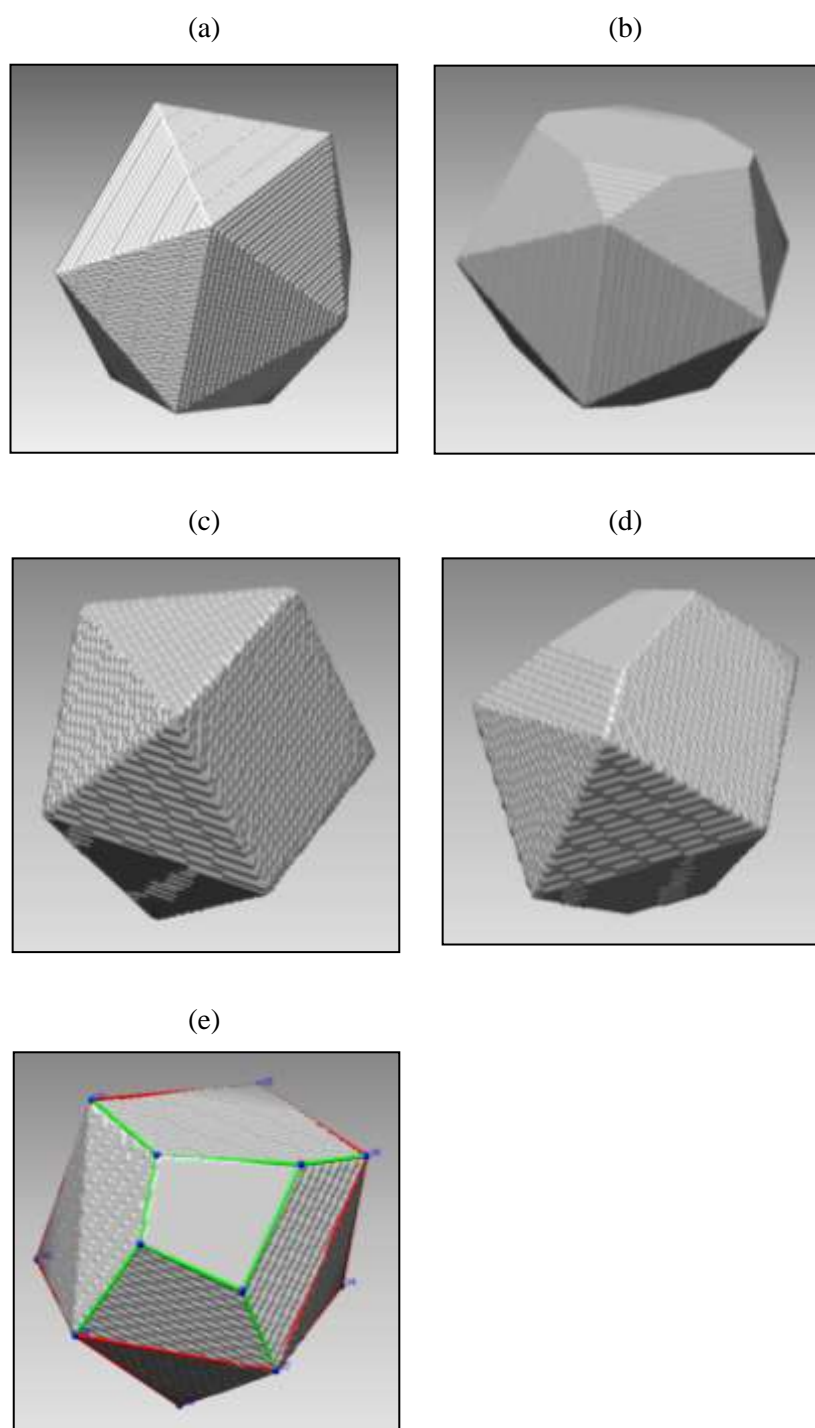


Figure S8: **Simulated standard Polyhedron and their view after truncation - (a) A simulated icosahedron, (b) the icosahedron with missing top, (c) A simulated sphenocorona, (d) the sphenocorona with missing top and (e) the ball-stick diagram on (d)**

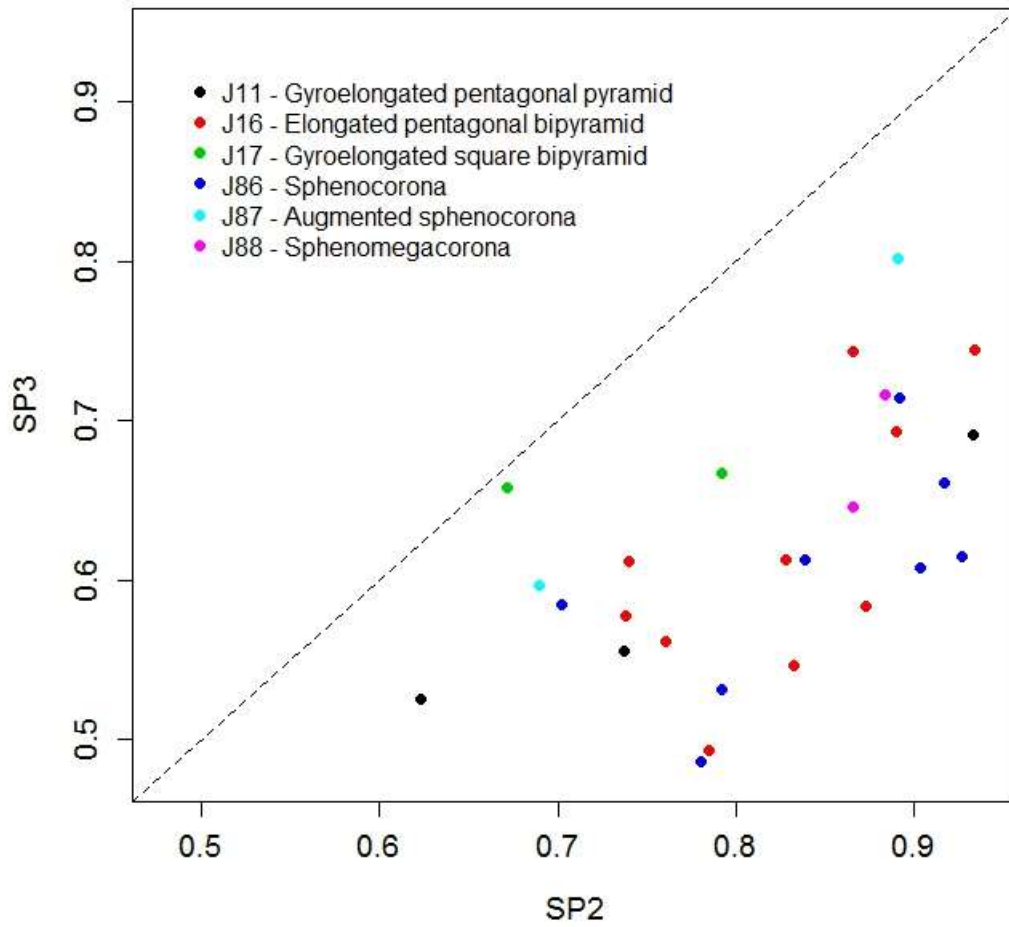


Figure S9: Distribution of aspect ratios by identified structure of BMCs. $SP2 = \lambda_2/\lambda_1$, $SP3 = \lambda_3/\lambda_1$, where $\lambda_1 \geq \lambda_2 \geq \lambda_3$ are the principal axes of an ellipsoid fitted to each reconstructed BMC.

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 |
| Platonic Solids | 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 |
| Archimedean Solids | 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 |
| Catalan Solids | 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 |
|---------------------|------------------------------|---------------------------|
|---------------------|------------------------------|---------------------------|

| | | (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 |
| Mean PPV | | 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 | | | | |