

Volume Gradient Vector

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1 Abstract

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2 Introduction

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3 Methods

Essential modes (EMs) were extracted from 600ns production run and normalized to a length of 6 Å. Then, the average structure was displaced along each EM and the derivatives of the volumes (δV_i) calculated. Since higher order EMs tend to be localized in a few amino acids, applying the same magnitude of displacement along each EM could lead to excessive displacements, causing atom clashes. Thus, each displacement vector \mathbf{D}_i was scaled by the following formula:

$$\mathbf{D}_i = \frac{1}{l_i} \cdot \mathbf{Q}_i$$

where l_i is the frequency of the corresponding essential mode. The (δV_i) were compiled in a **Volume Gradient Vector (VGV)** which then was used to select the subset of modes that affect the cavity the most by means of the **Participation Number (P)**:

$$P = (\sum_i (\mathbf{VGV} \cdot \mathbf{Q}_i)^4)^{-1}$$

the P is rounded and used to determine the size of the subspace. The ' P ' modes that have the higher projections against the **VGV** are selected.

The **VGV** may be transformed to cartesian coordinates to determine which amino acids affect the cavity the most. Each EM can then be cutted to keep the displacements of the wall amino acids, discarding the rest of the vector. This cutting procedure was applied to the 2 sets of EMs: the whole subspace, and the ' P ' modes. **Collectivity** and **Participation Number** of each mode were recalculated to these cutted set of modes.

The **collectivity** of each mode was calculated using the formula from Tama et.al.:

formula

The **Participation Number** formula was also used to determine the number of amino acids that each EM mainly moves. These ' P ' amino acids of each mode was divided by the total number of amino acids to obtain the fraction of the protein that is affected the most by each mode.

4 Results

4.1 1HVR_APO

Fig.1 shows density of states histograms of the EM, weighted by the (δV_i) of each mode. Fig.1A corresponds to the full set of EM and Fig.1B for the reduced set of 149 'P' modes. These plots can be compared with a non-weighted density of states histogram (Fig.1C). **(se me ocurre q podríamos ponerlo acá)** Despite being the most numerous, middle frequency modes ($50cm^{-1}$ to $175cm^{-1}$) are not so relevant to the cavity volume and low frequency modes turn out to be even more important. Notably, a spike appears between the range of $175cm^{-1}$ to $200cm^{-1}$; these modes could indicate an alternative way of affecting the cavity volume. Besides a 'breathing' movement, encapsulated in the lower frequency amino acids, a protein could use the coordinated movement of several amino acids to affect the cavity volume or to function as a gate. If these residues undergo coordinated movement, then the gating dynamics should show up in middle frequency EM.

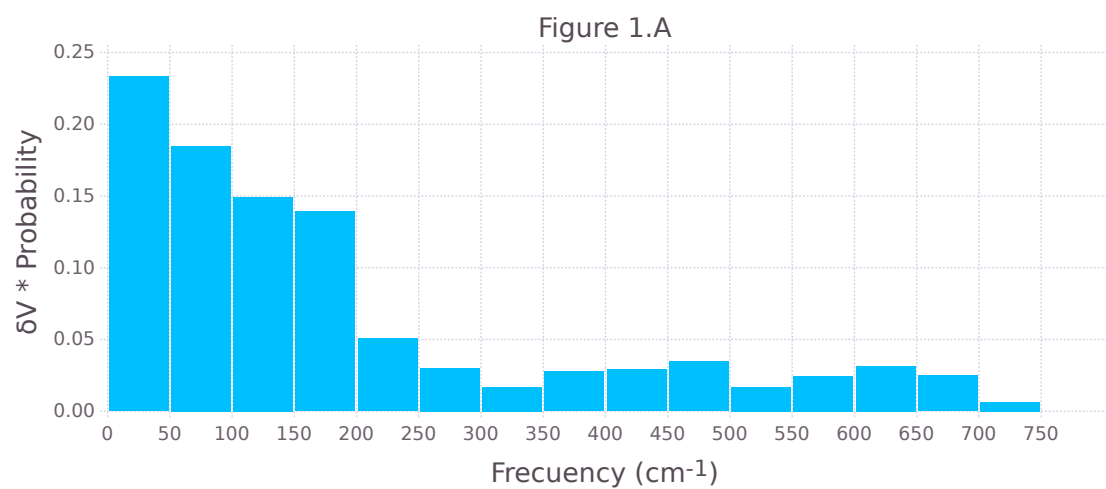


Figure 1. This is an inserted EPS graphic

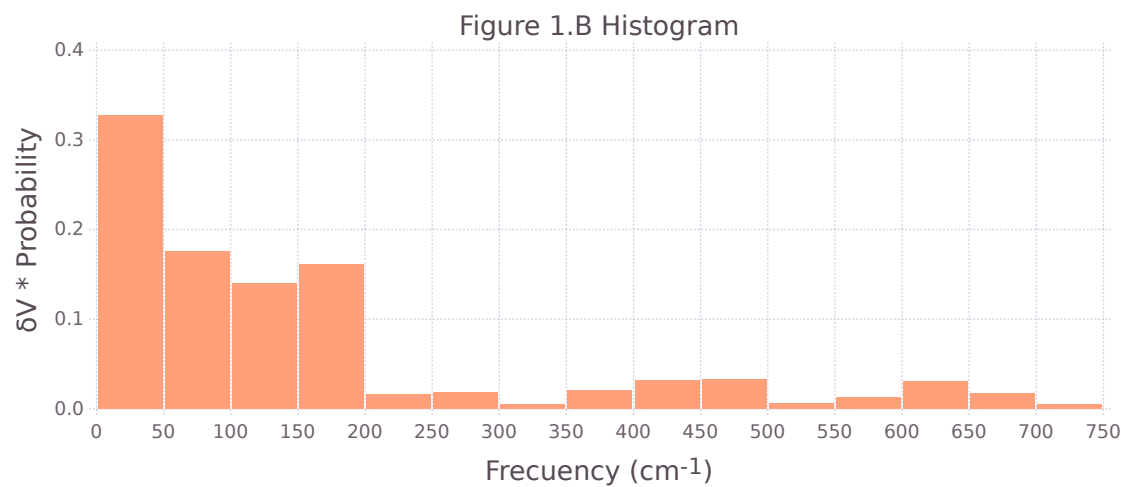


Figure 2. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

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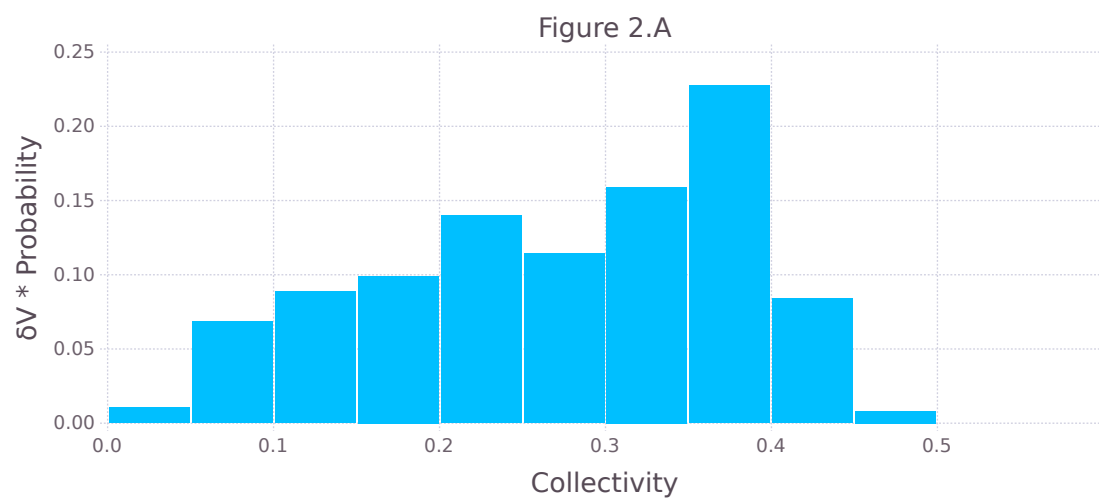


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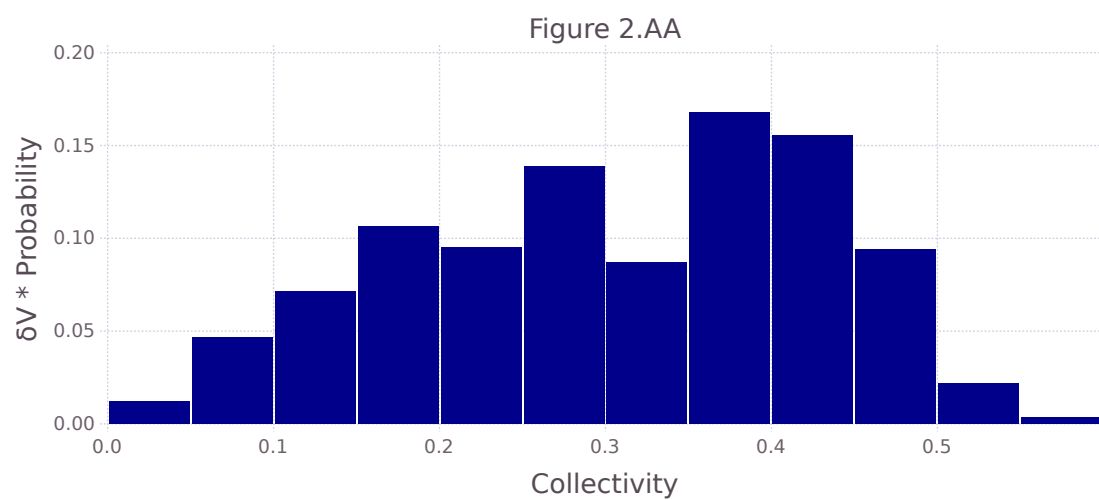


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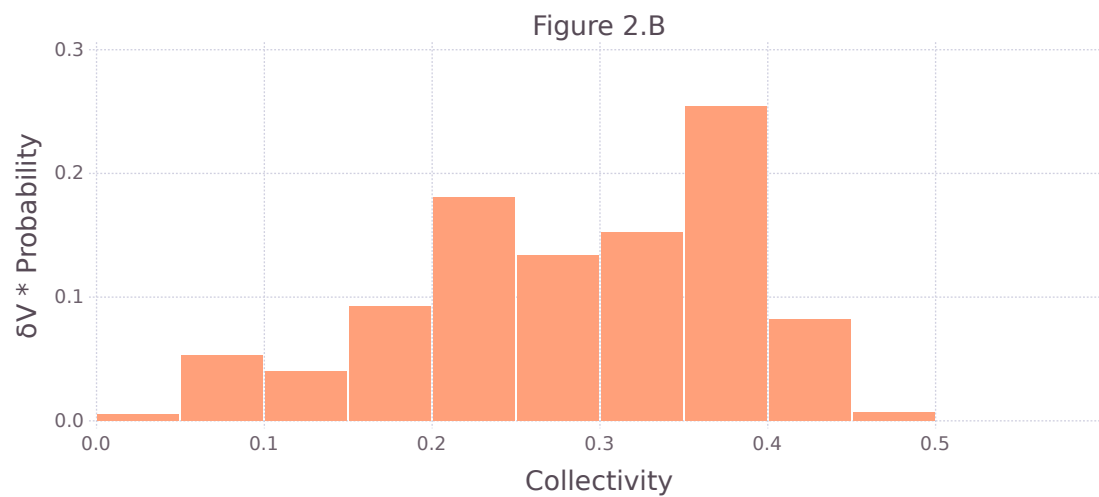


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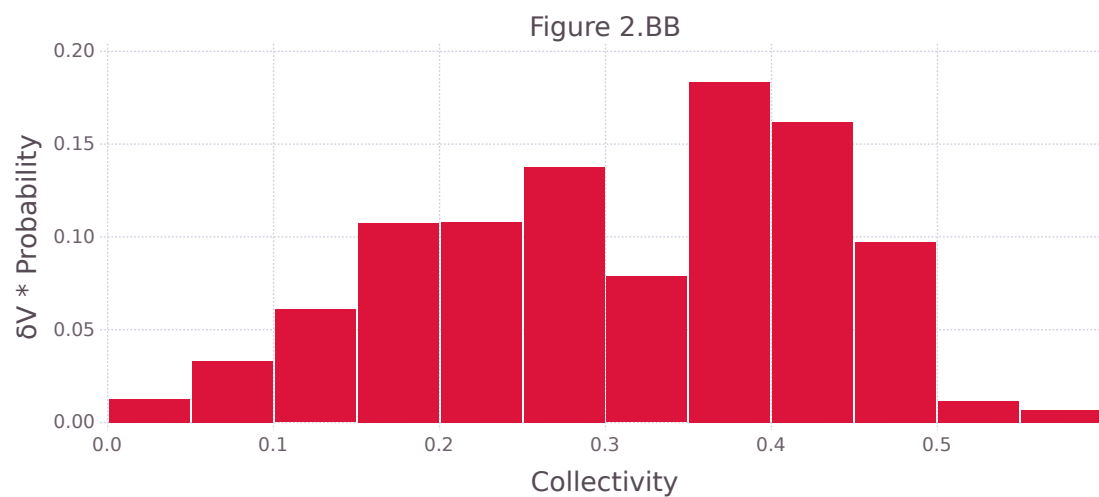


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As in Fig.1, the analogous can be done with the **Participation Number**, as Fig.2 shows.

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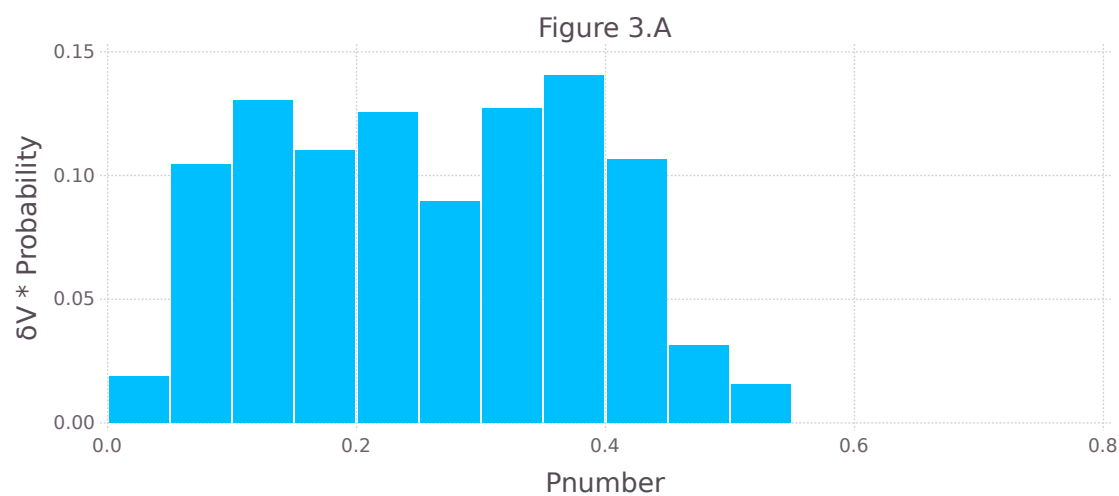


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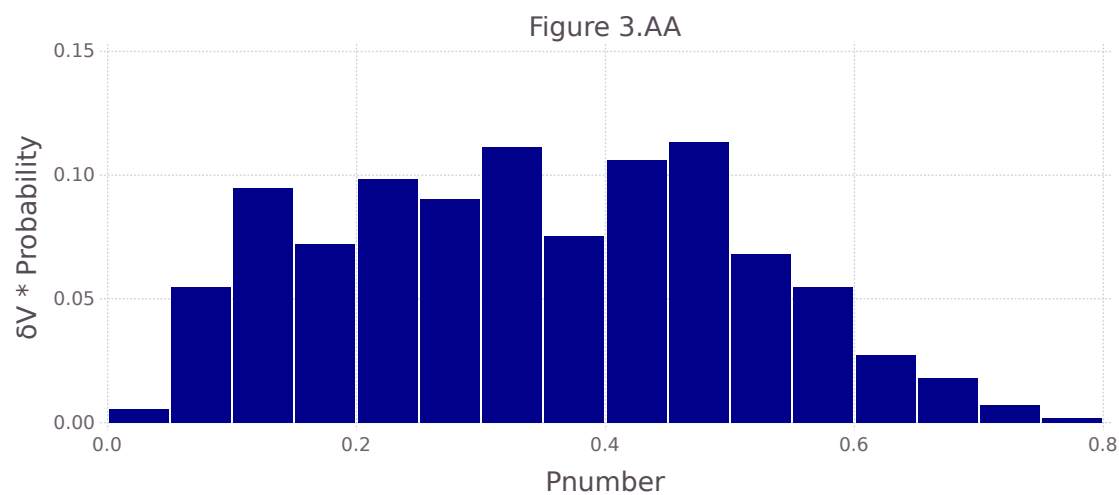


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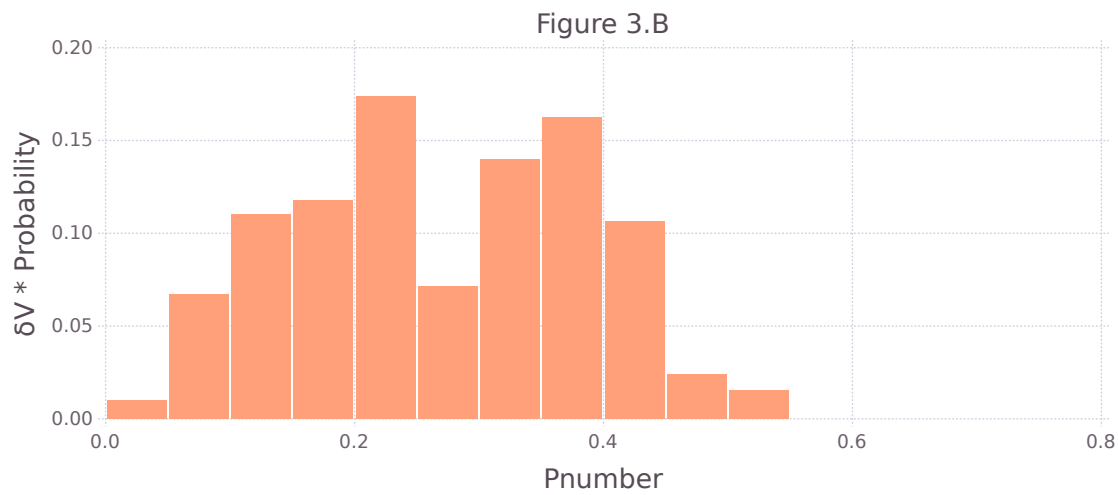


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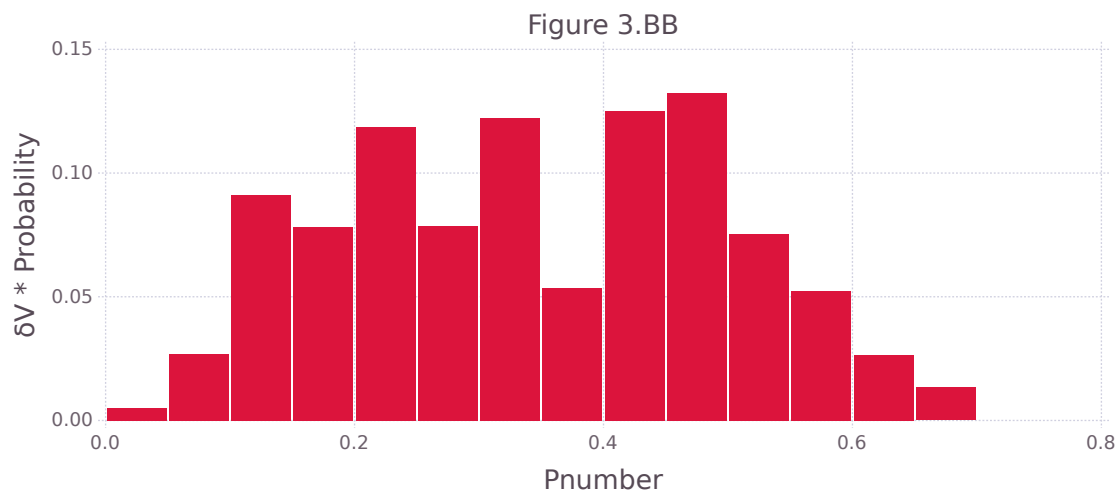


Figure 10. This is an inserted EPS graphic

VG can be translated into cartesian coordinates and the module of the X, Y, Z coordinates obtained.

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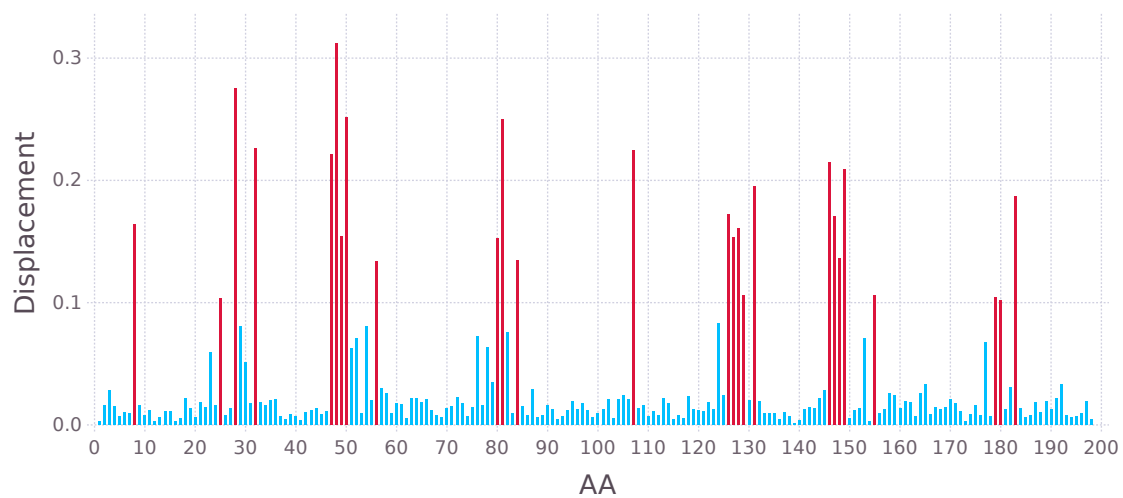


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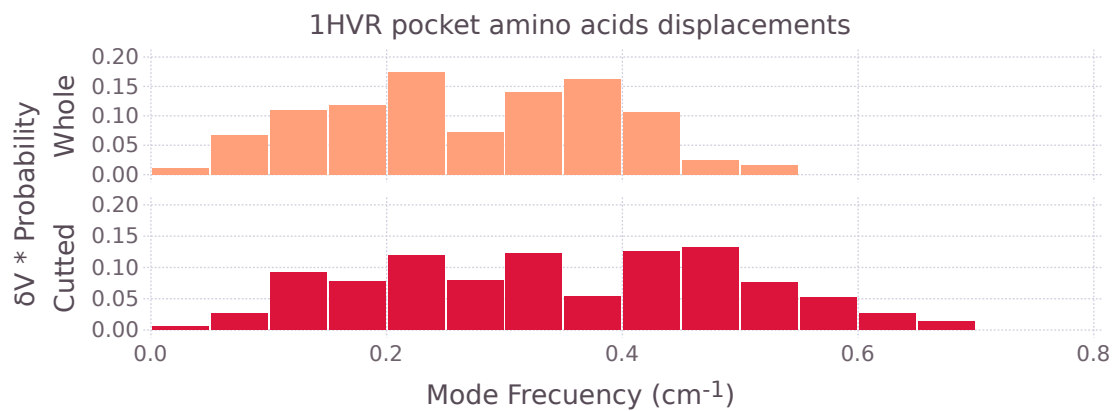


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4.2 1HVR_HOLO

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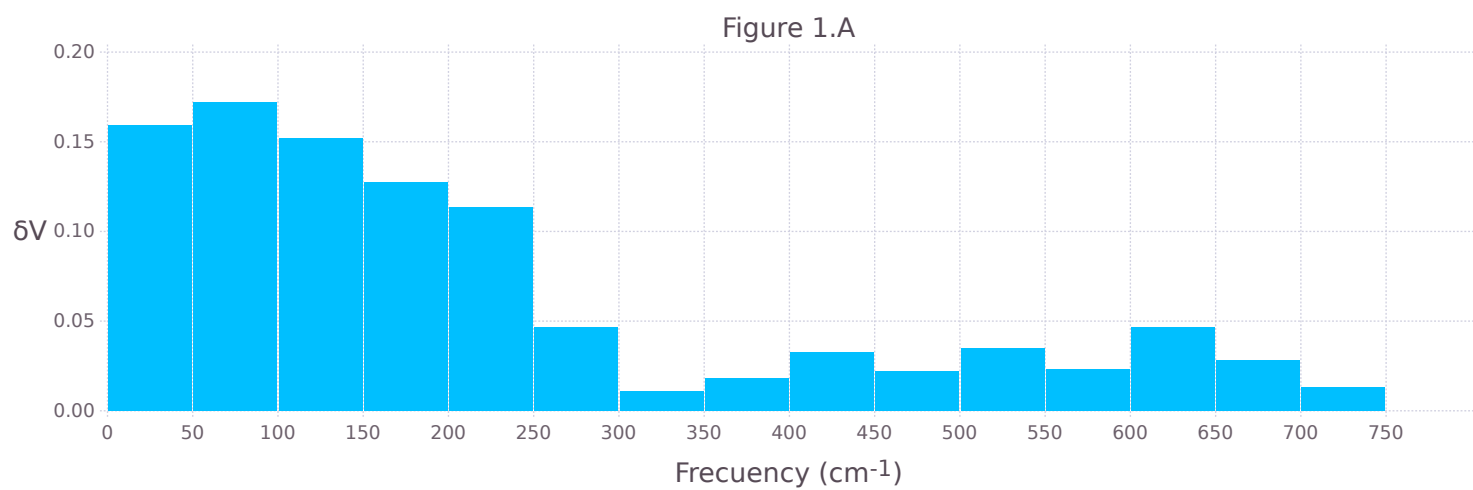


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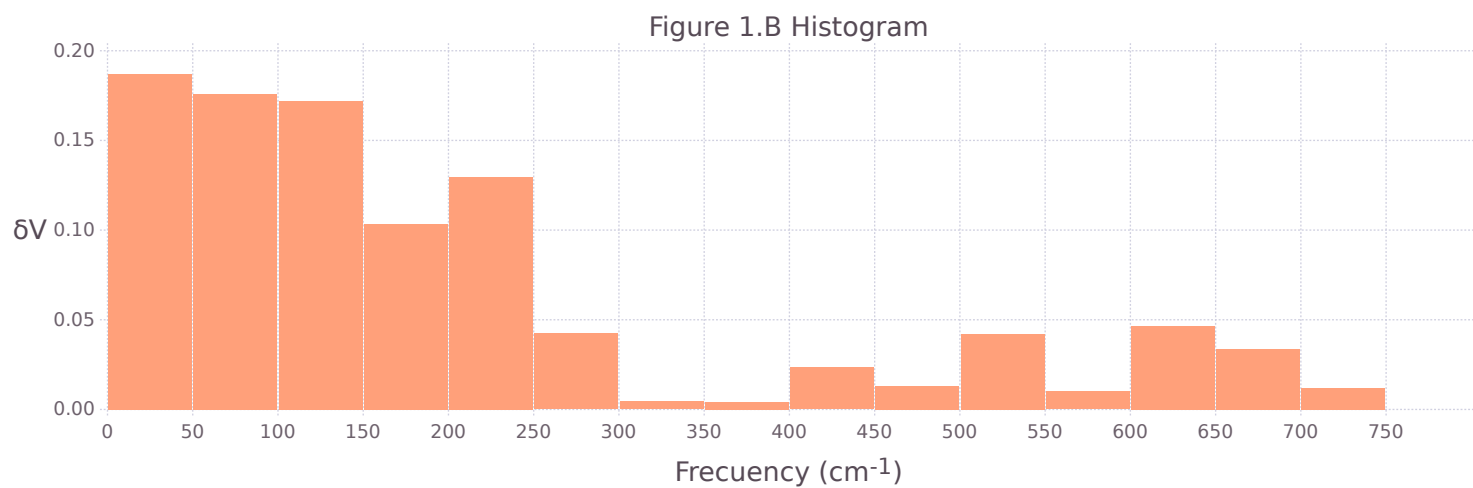


Figure 14. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

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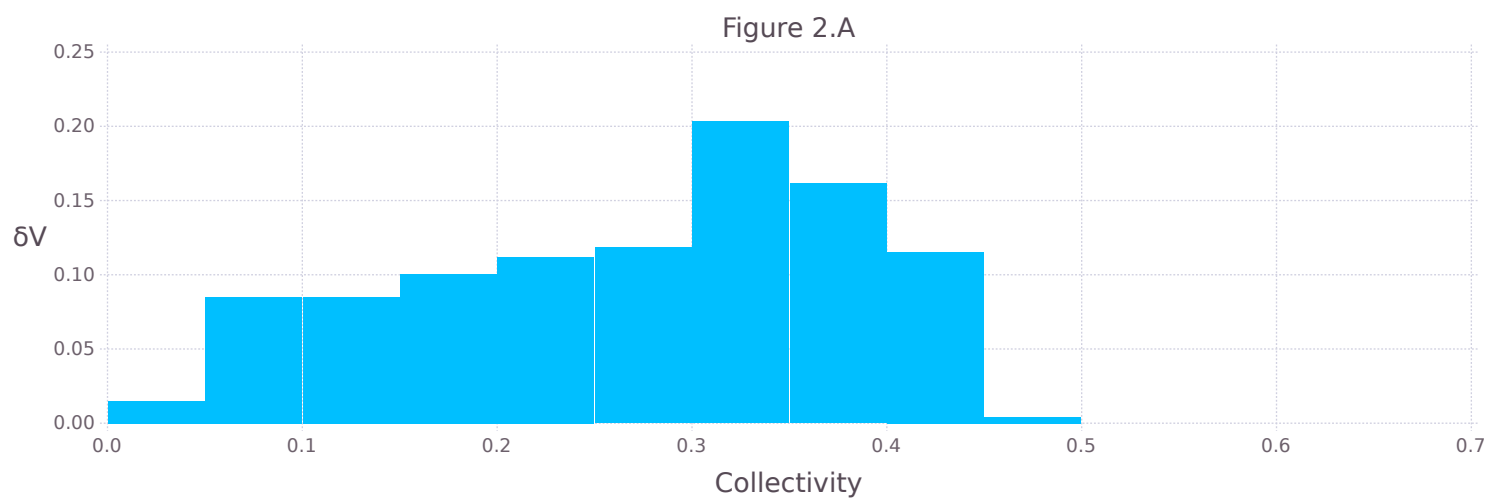


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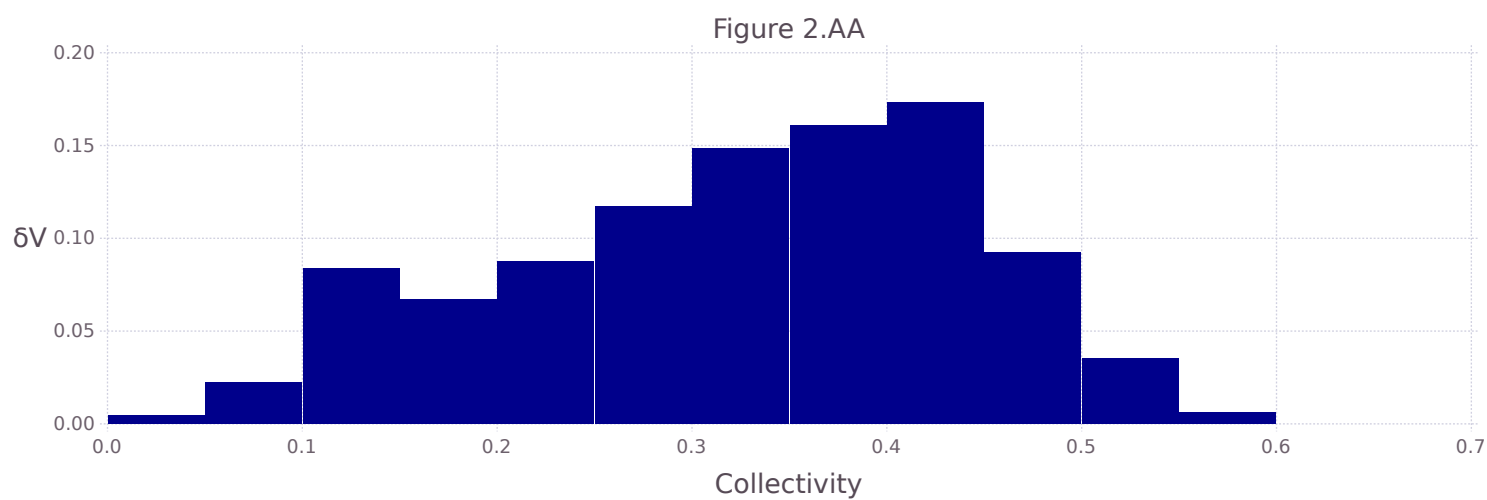


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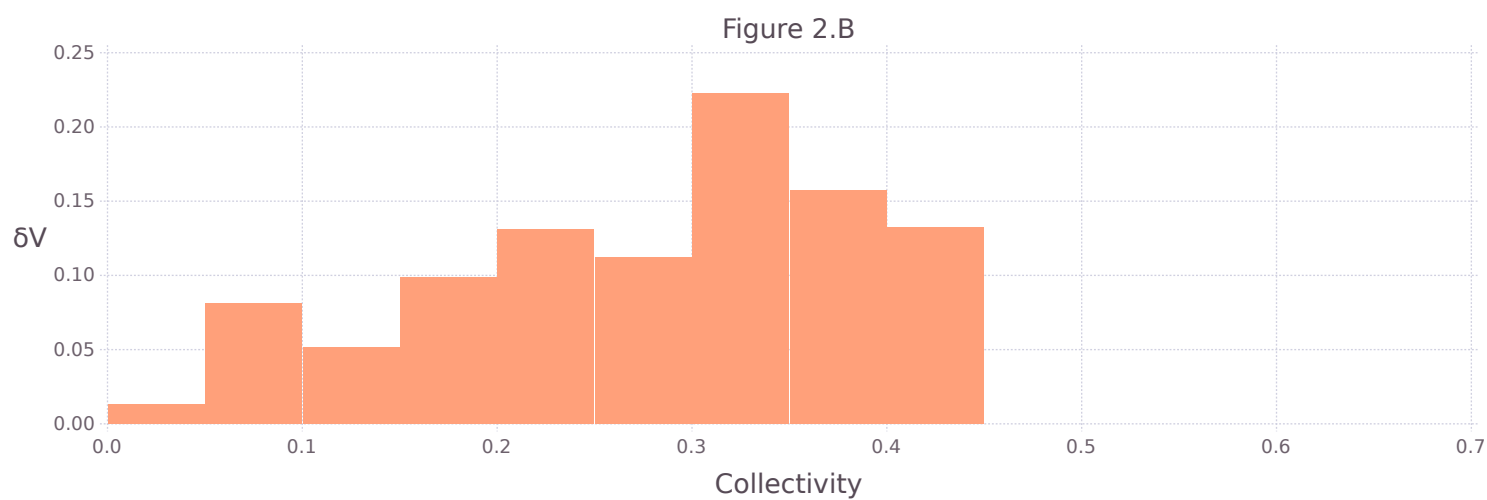


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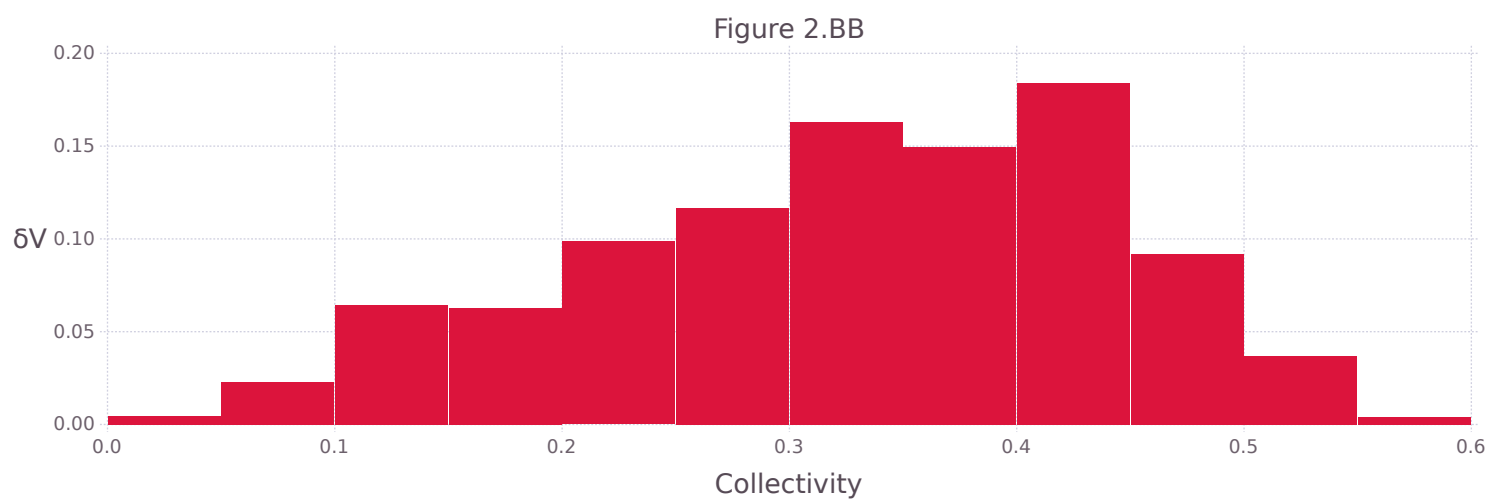


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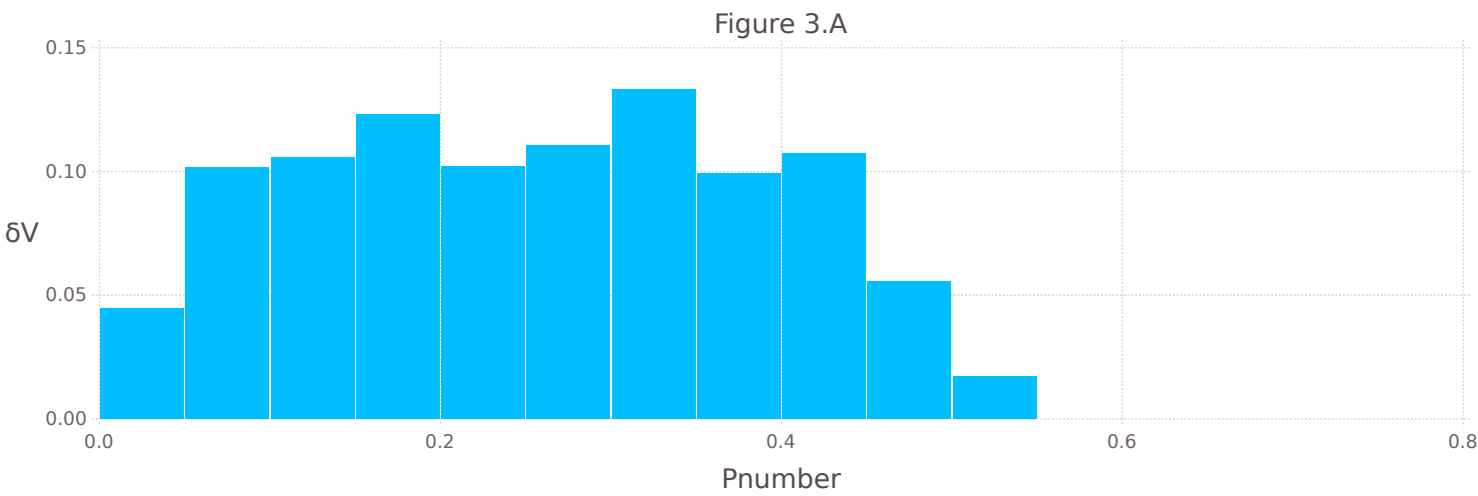


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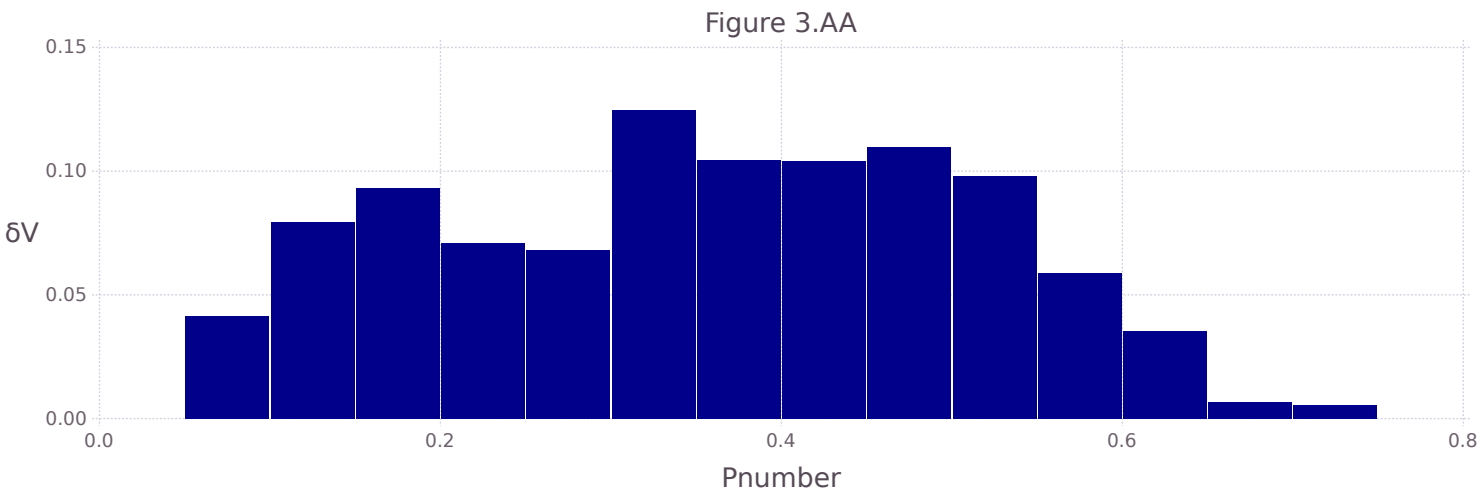


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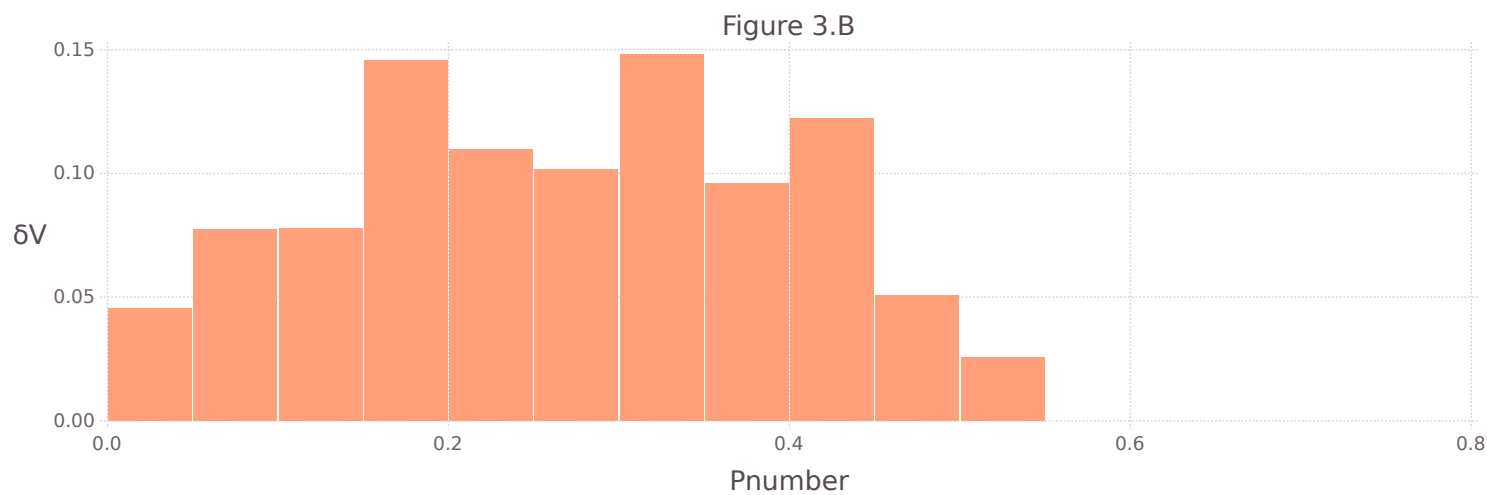


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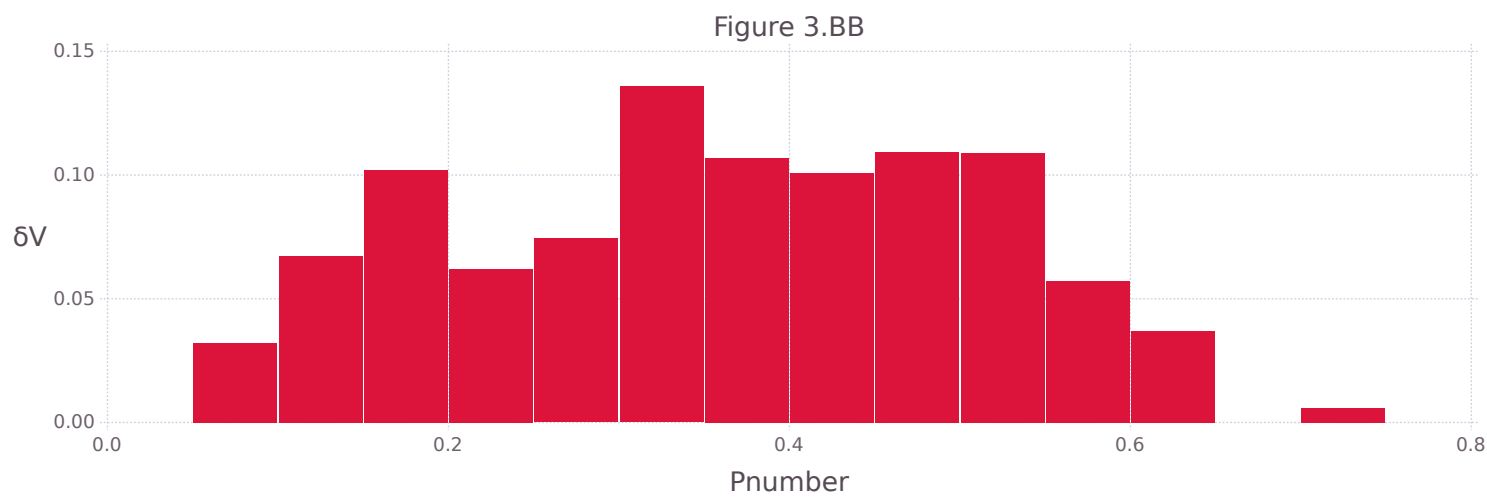


Figure 22. This is an inserted EPS graphic

VGV can be translated into cartesian coordinates and the module of the X,Y,Z
coordinates obtained.

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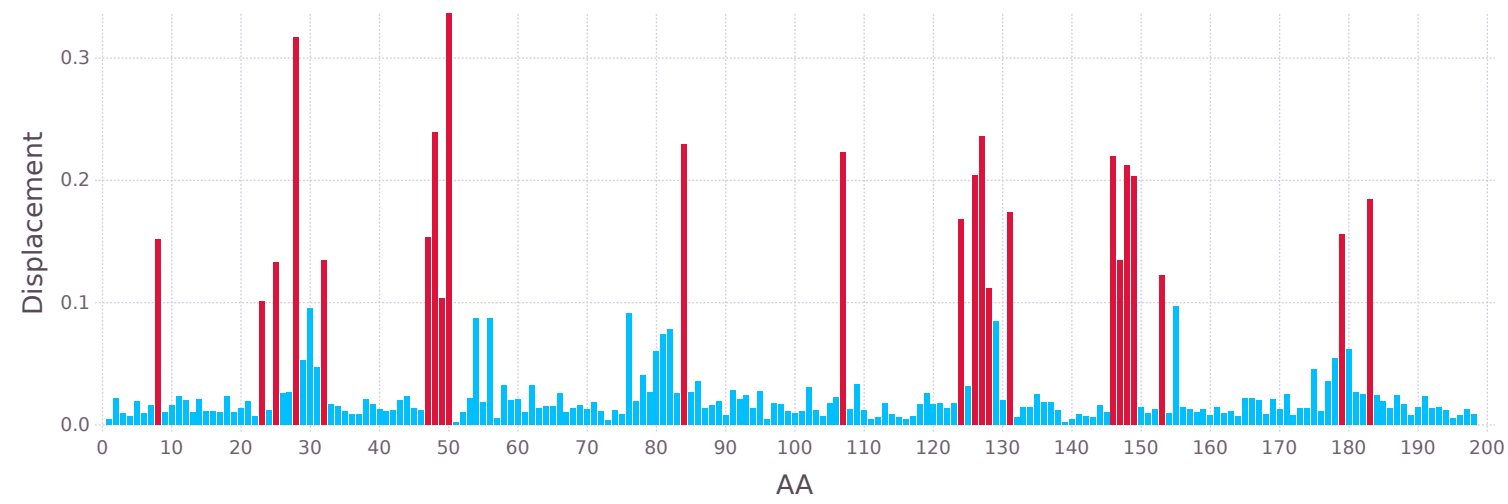


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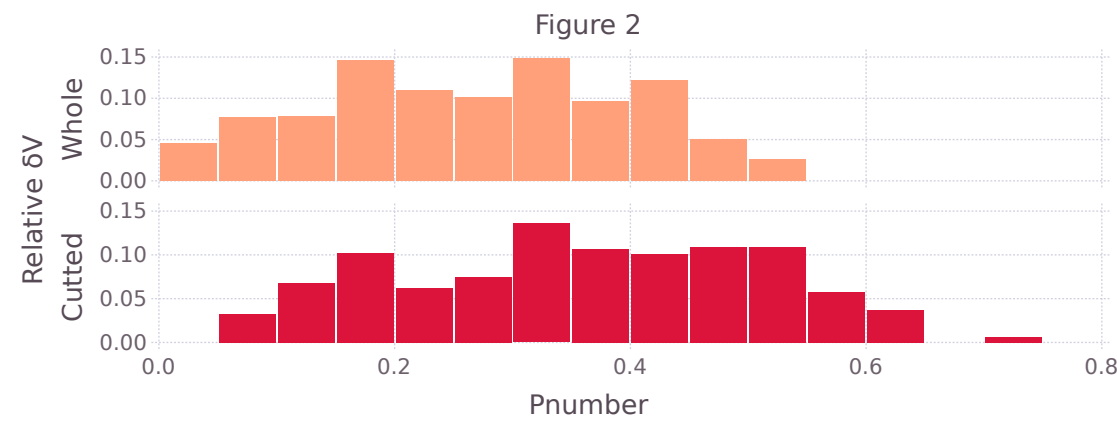
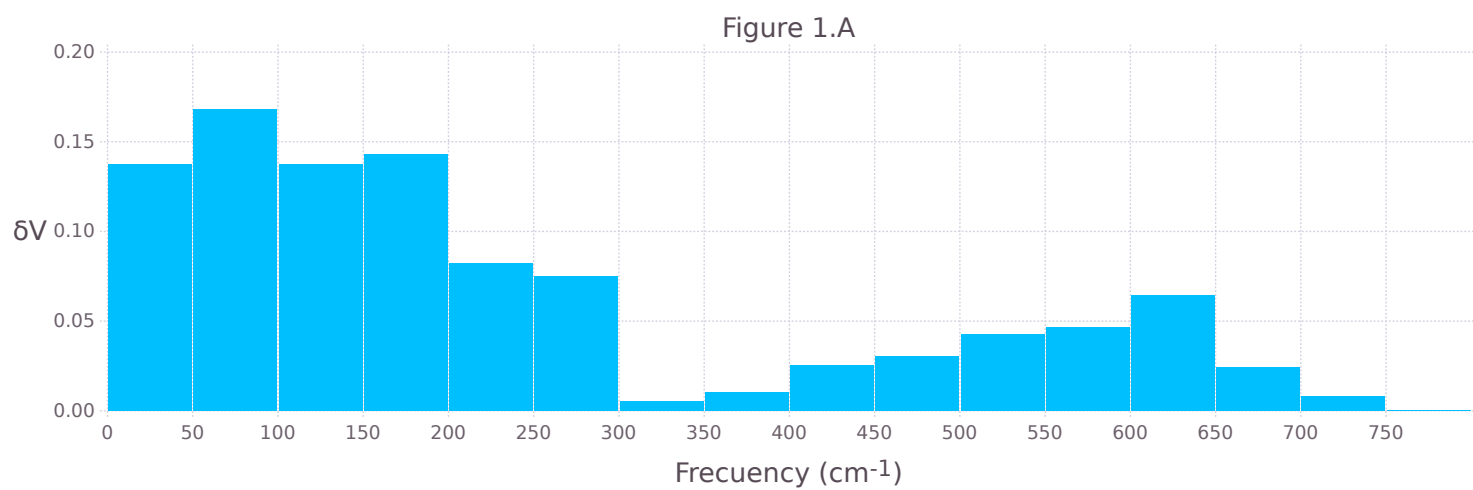
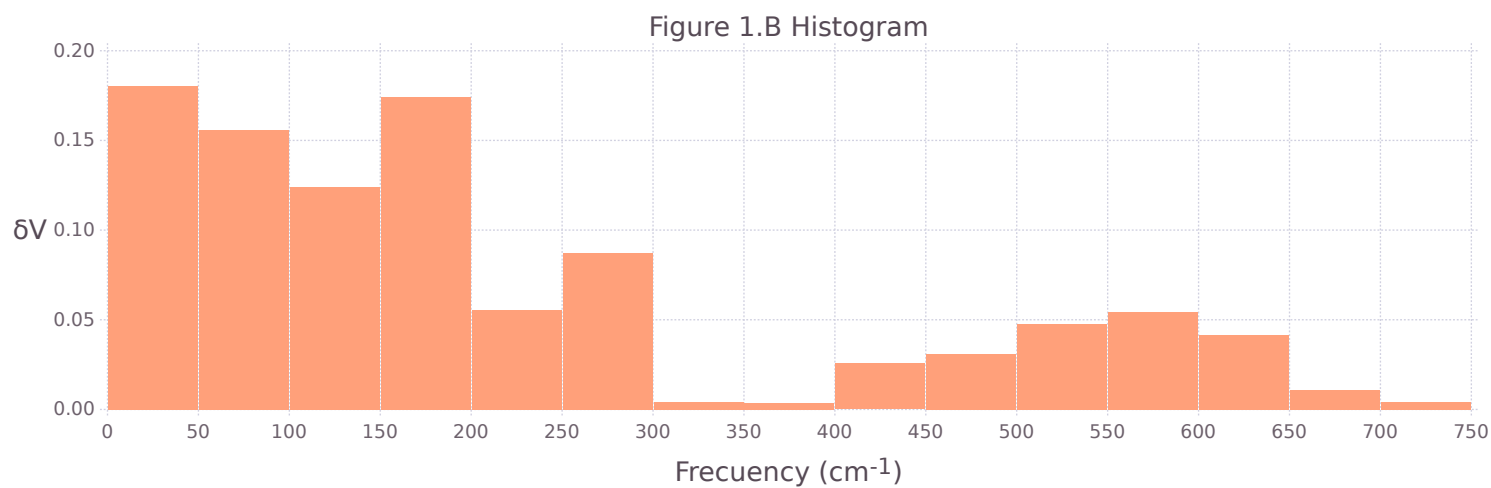


Figure 24. This is an inserted EPS graphic

4.3 1XKK

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**Figure 25.** This is an inserted EPS graphic**Figure 26.** This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

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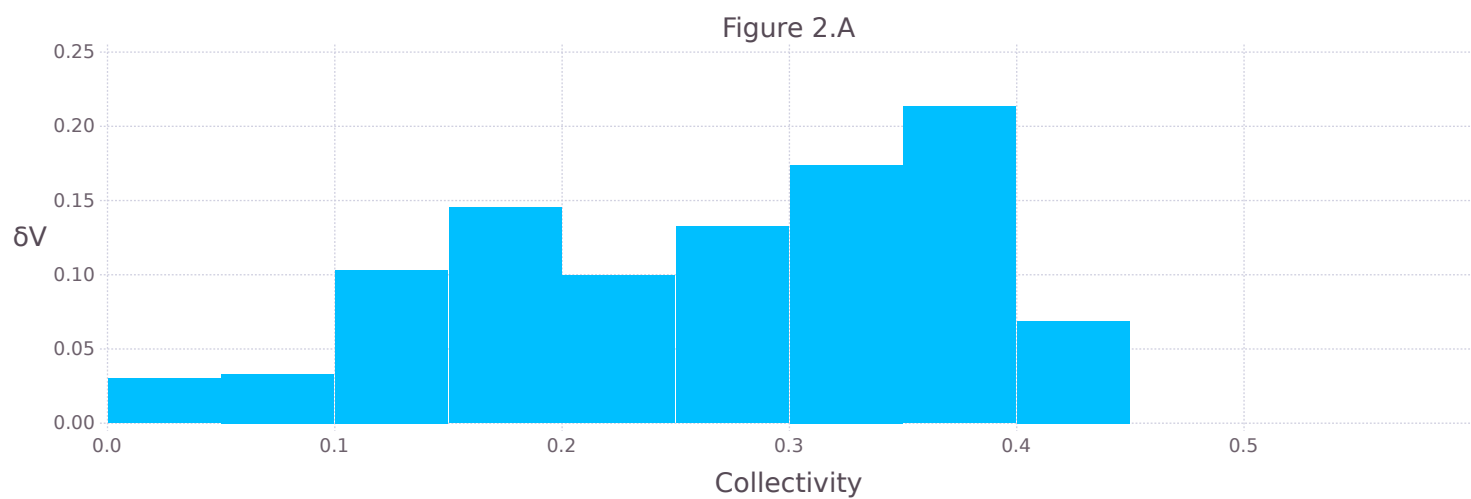


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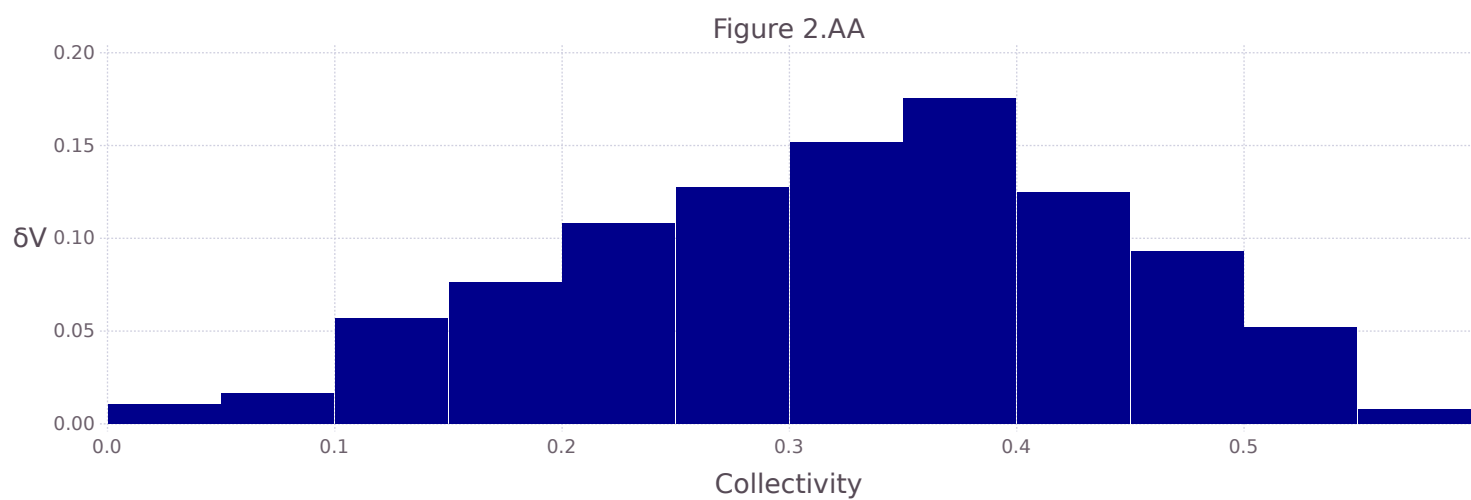


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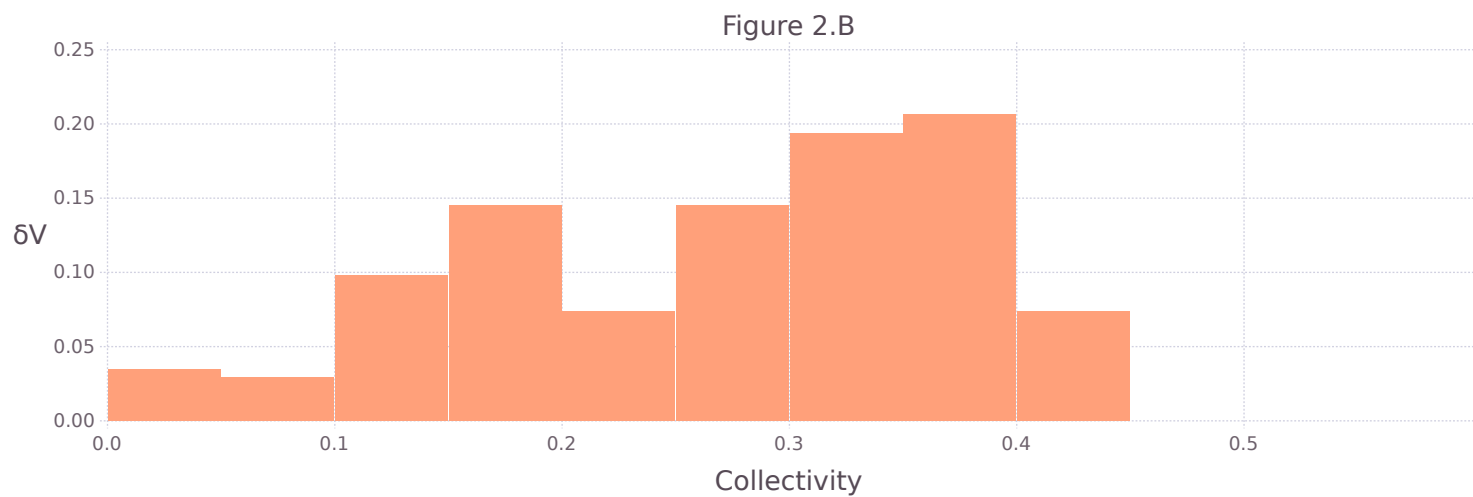


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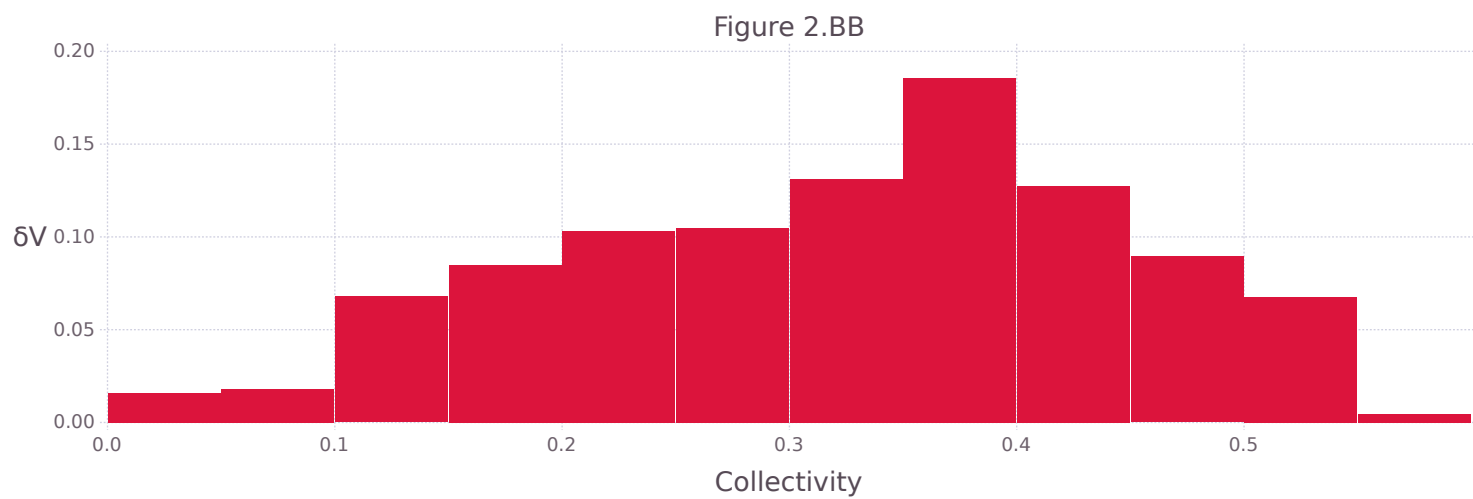


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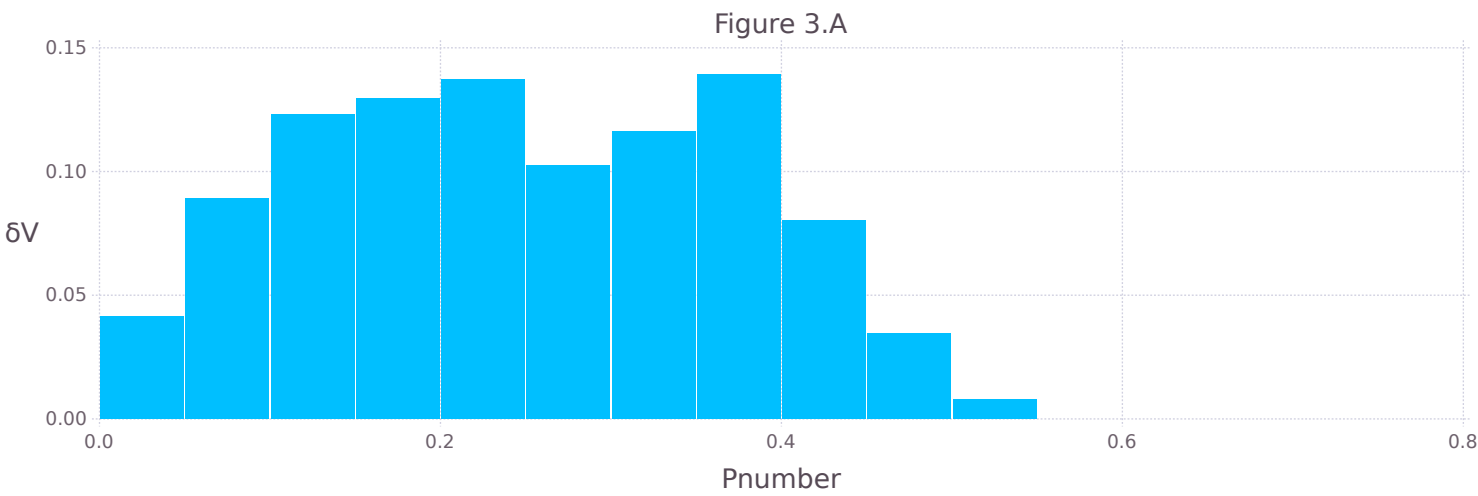


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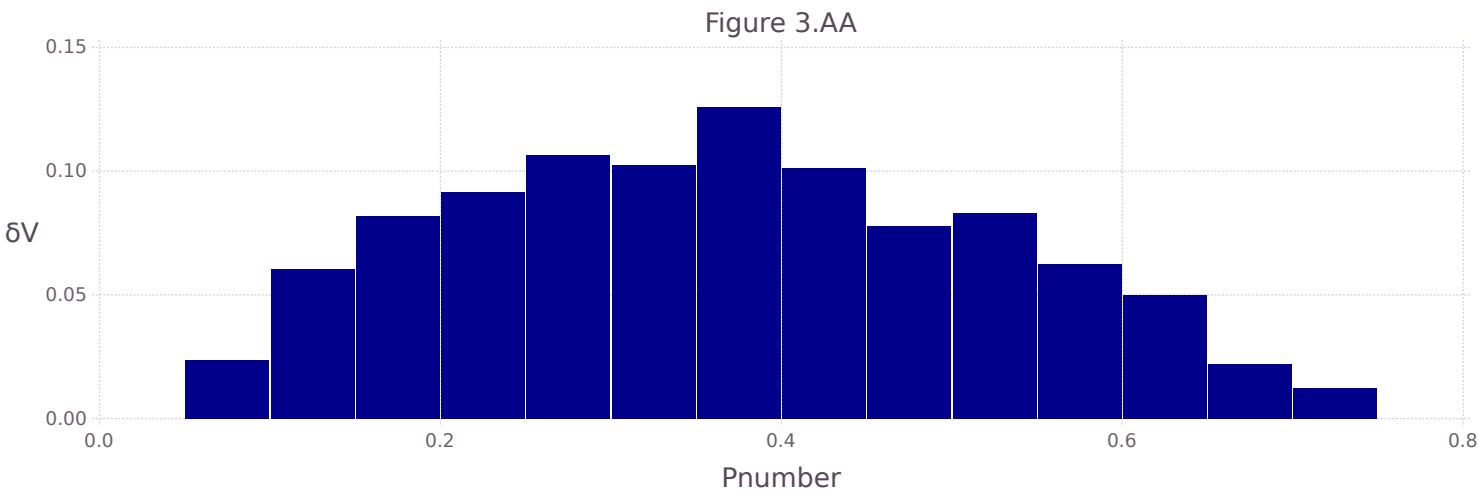


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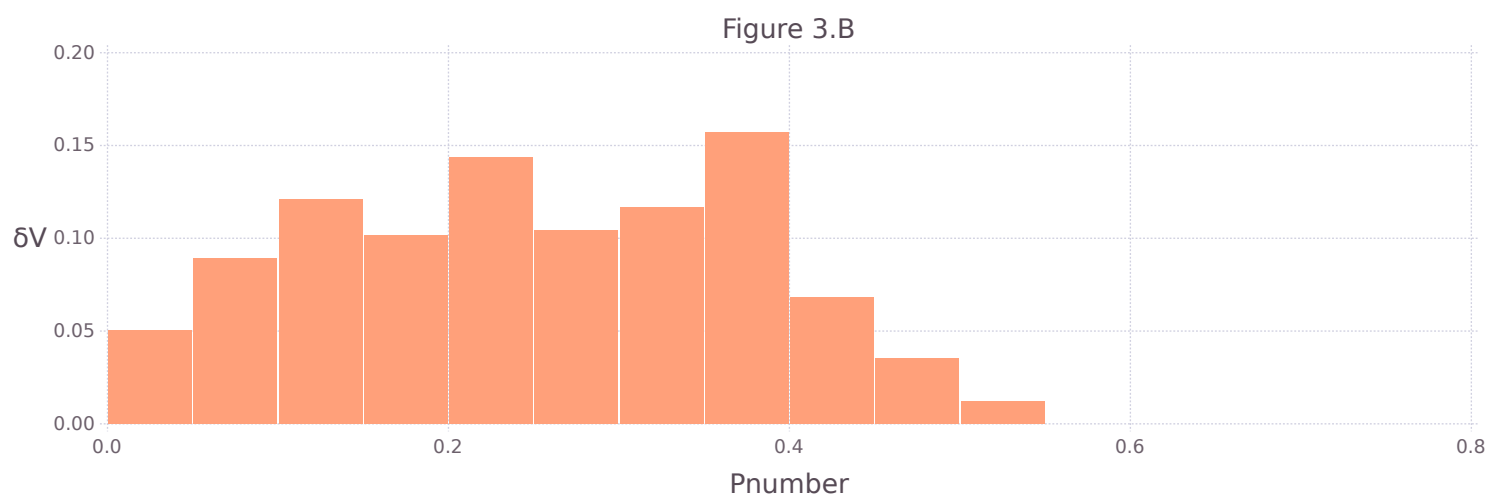


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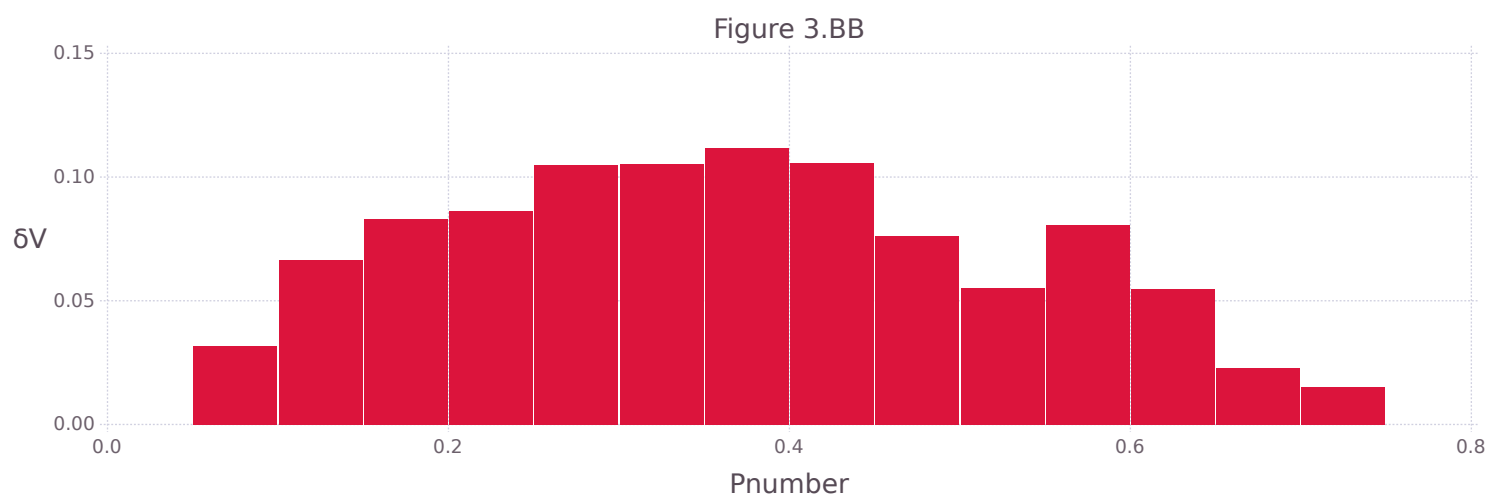


Figure 34. This is an inserted EPS graphic

VGV can be translated into cartesian coordinates and the module of the X, Y, Z coordinates obtained.

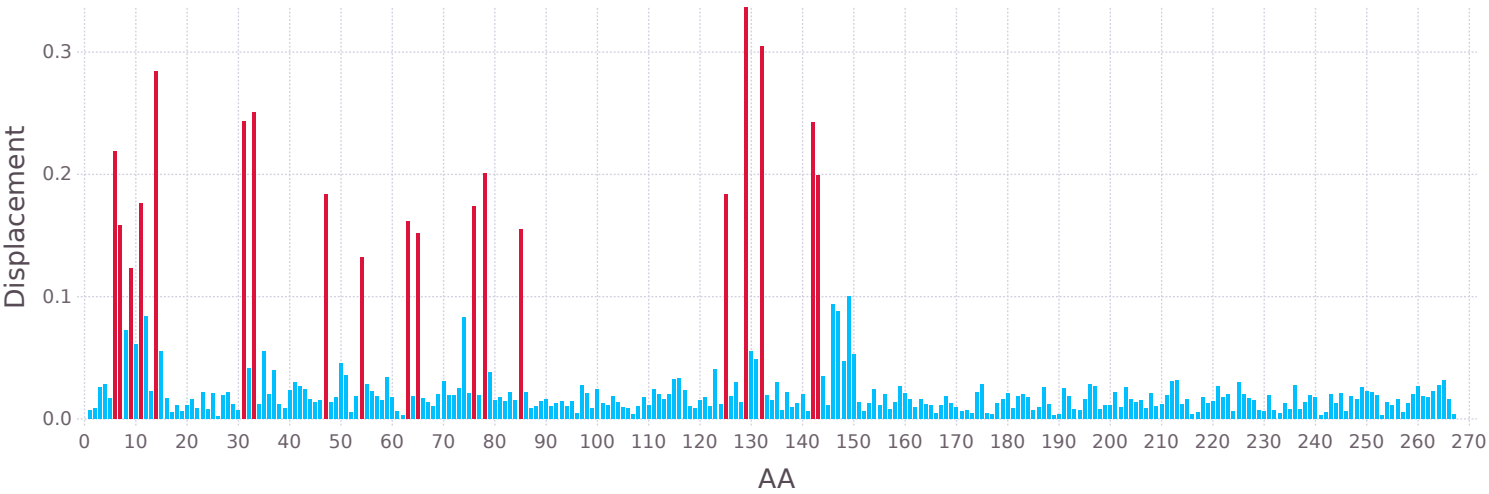


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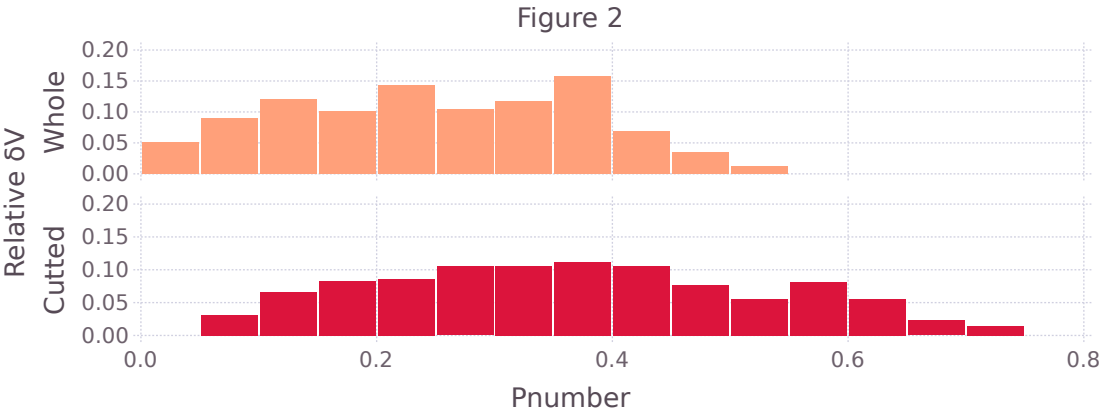


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4.4 1M14

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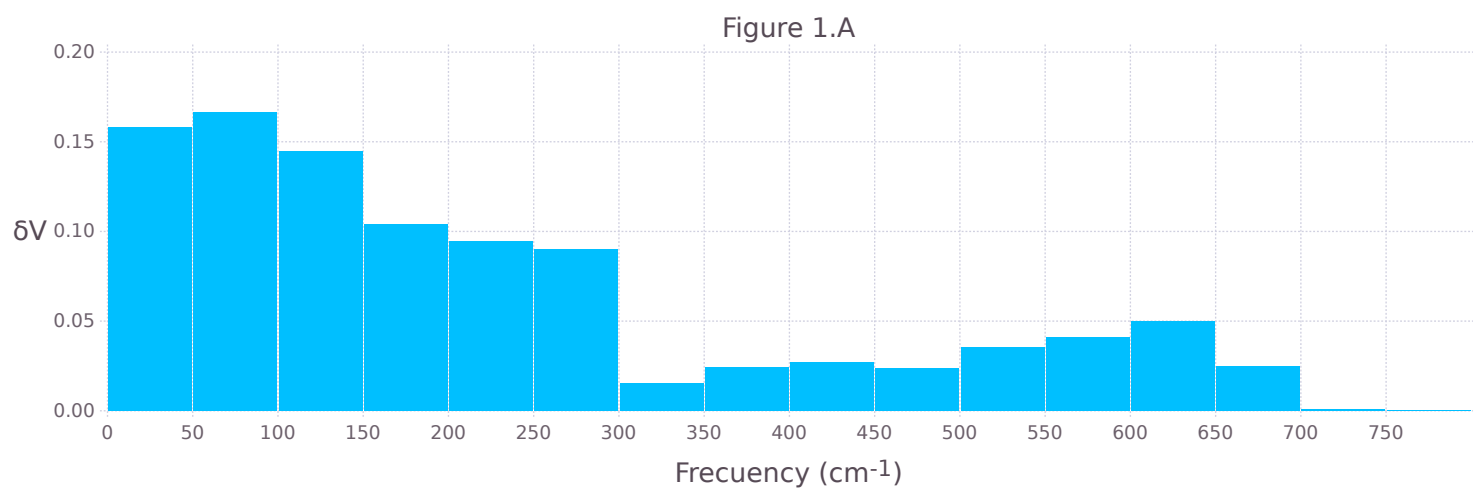


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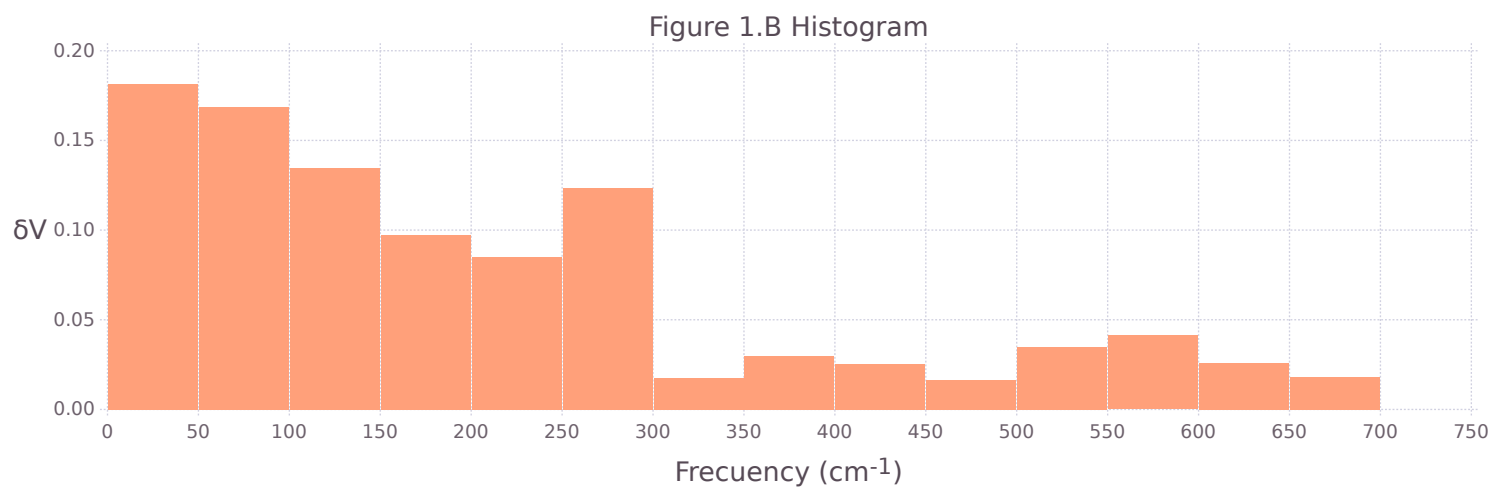


Figure 38. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

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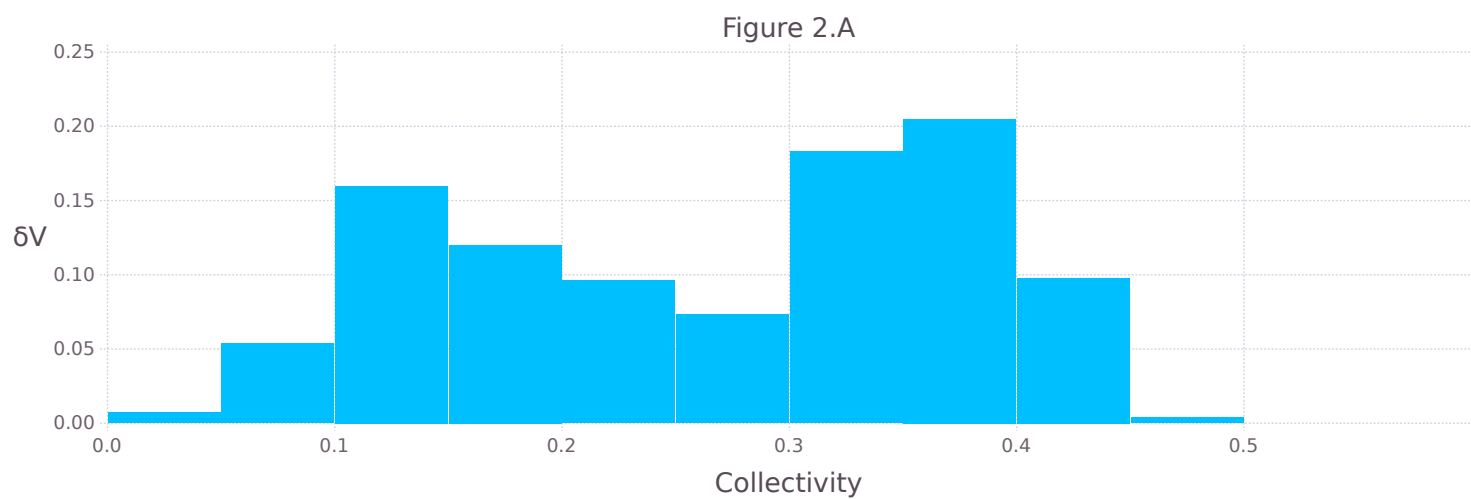


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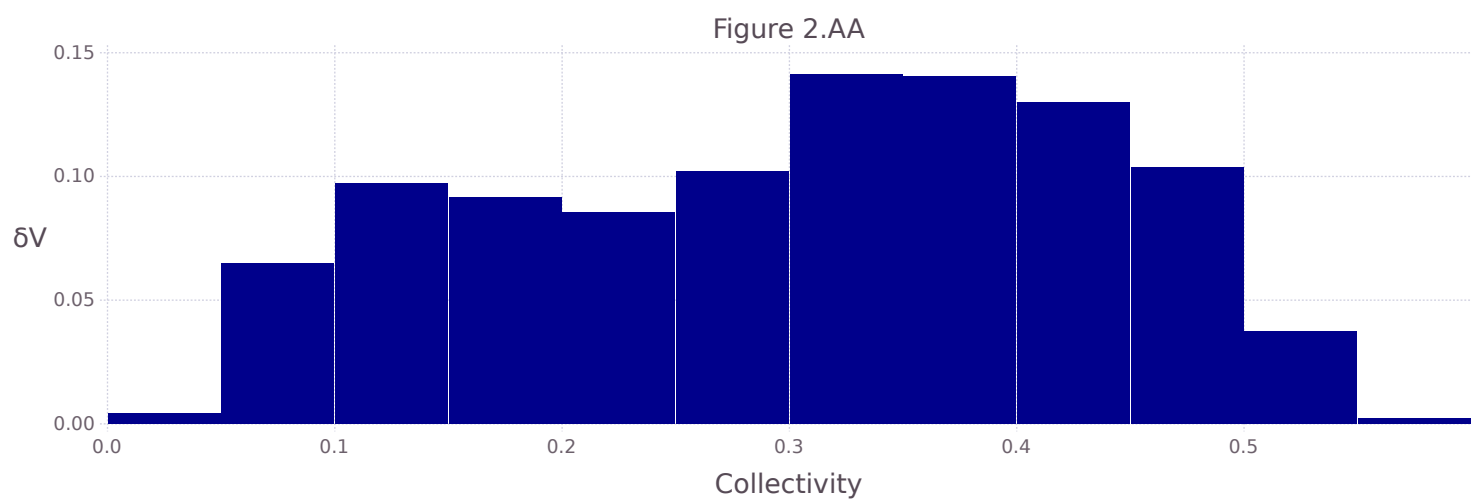


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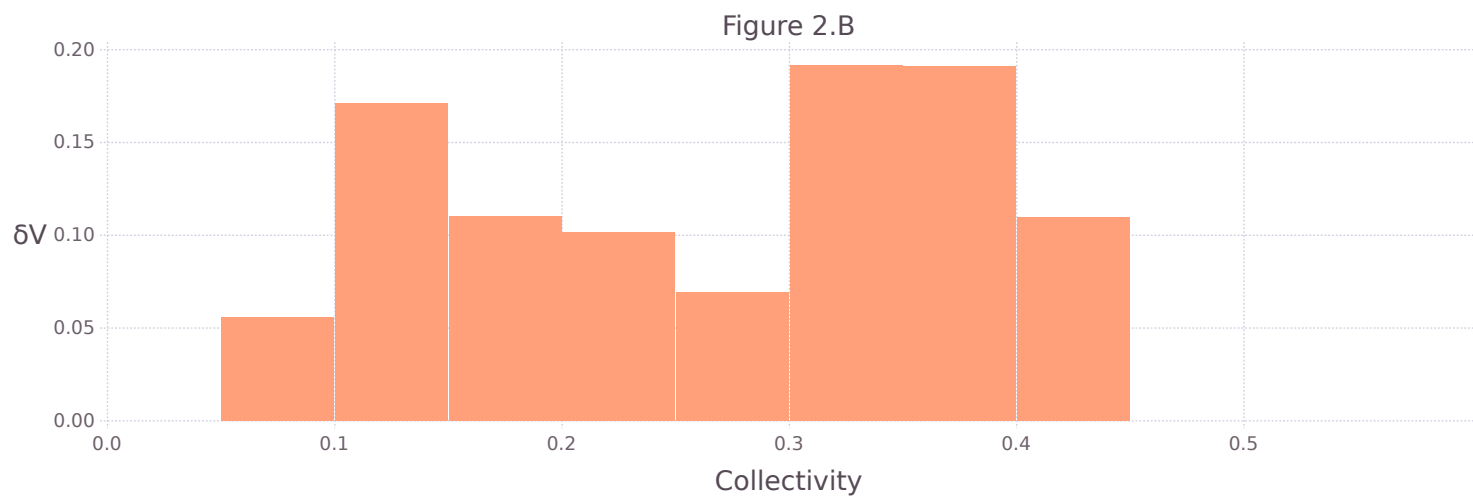


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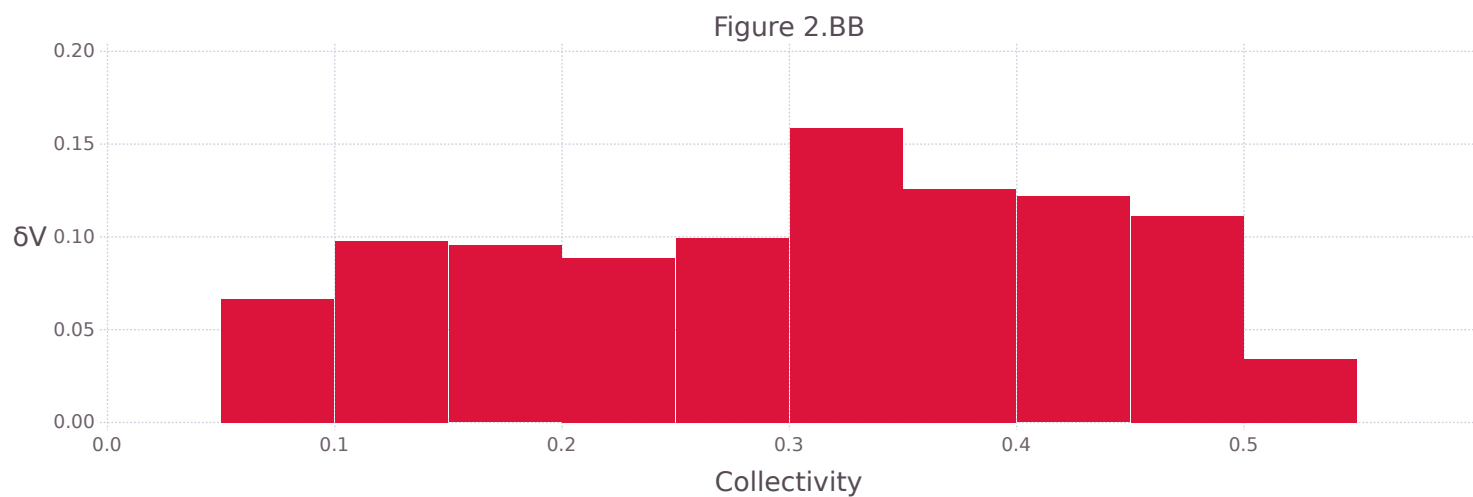


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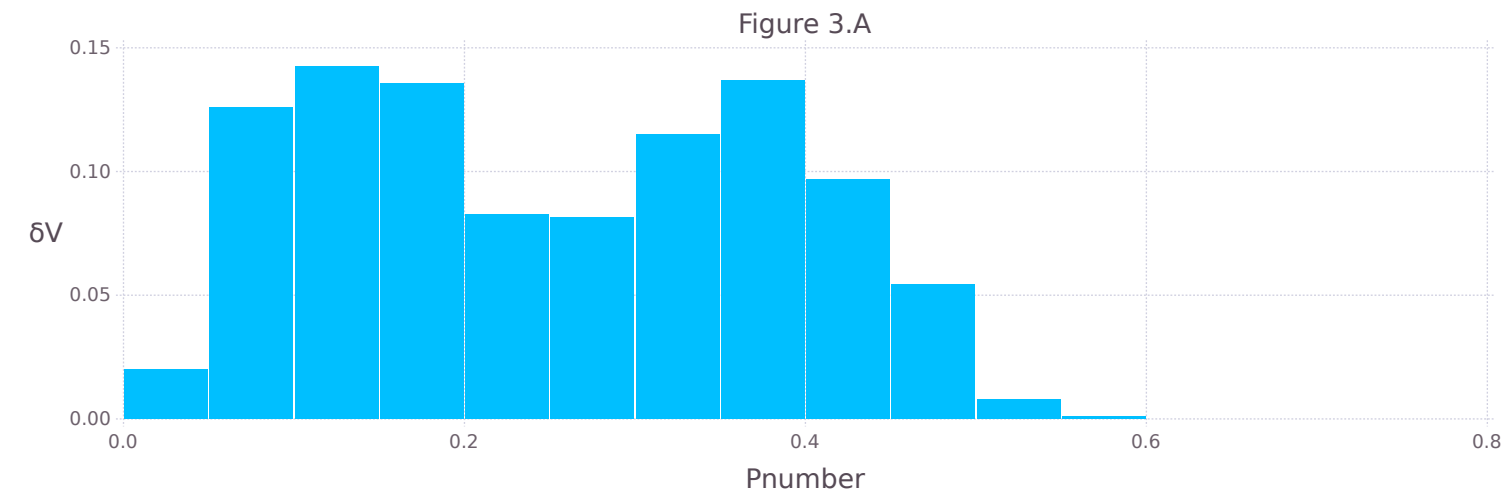


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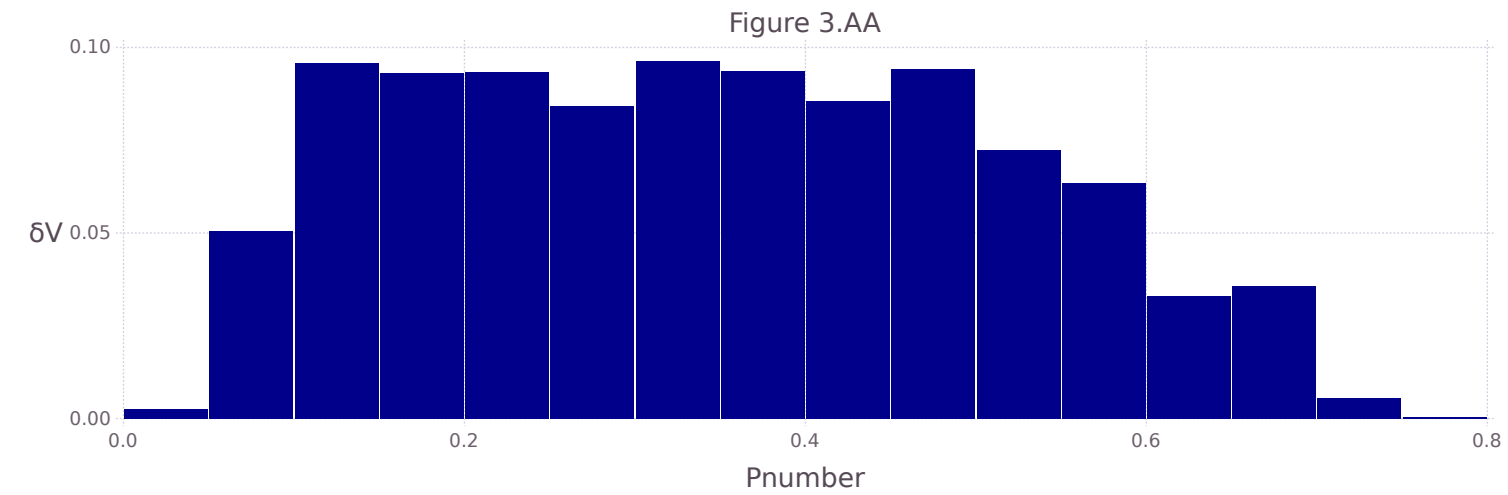


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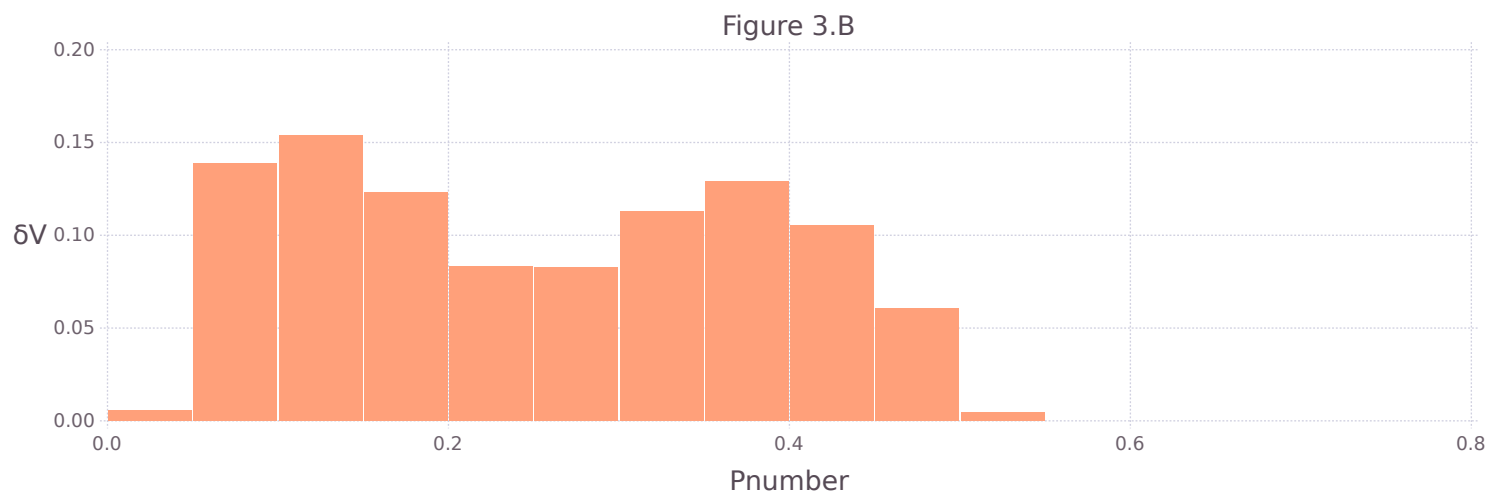


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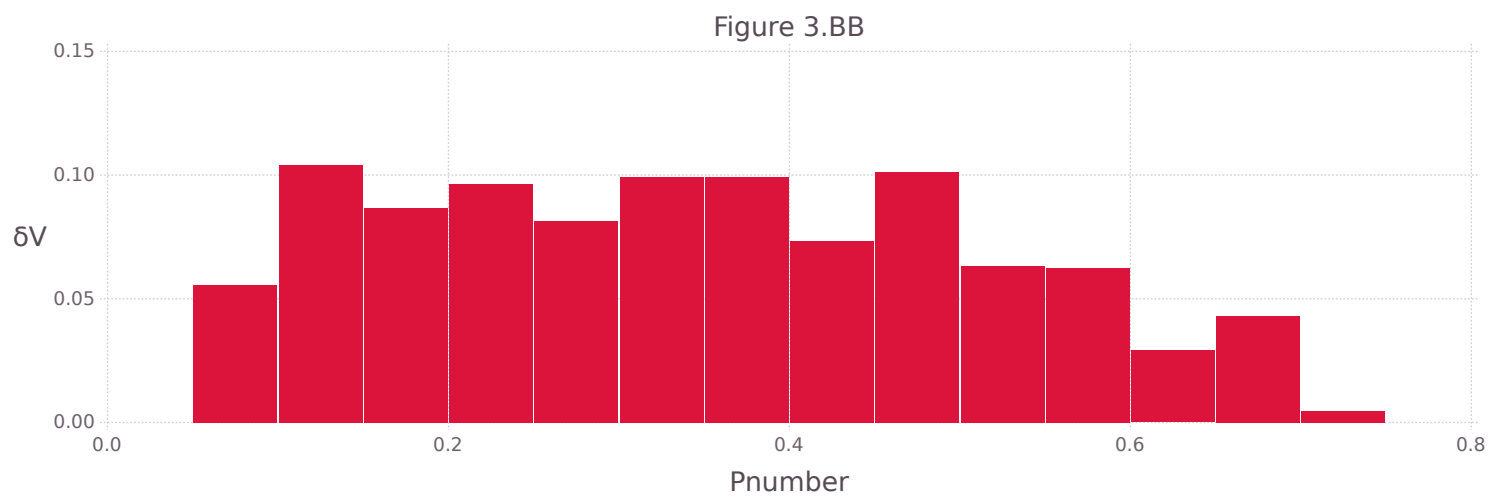


Figure 46. This is an inserted EPS graphic

VGV can be translated into cartesian coordinates and the module of the X,Y,Z coordinates obtained.

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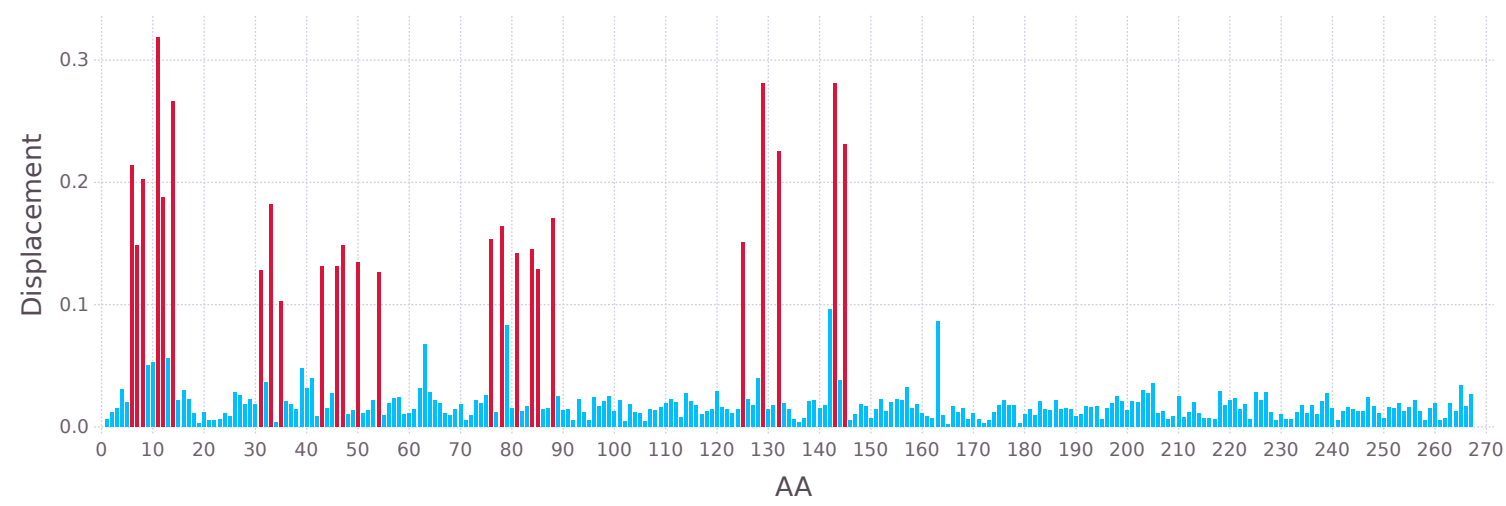


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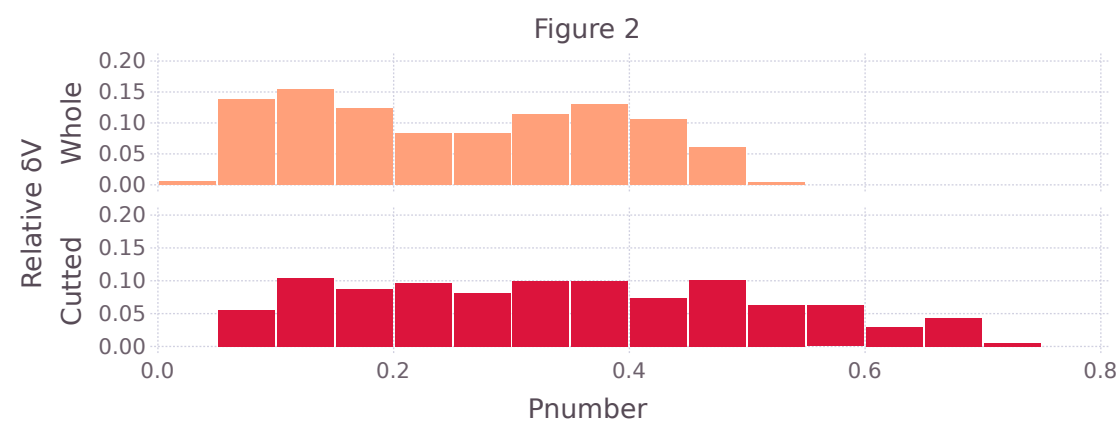


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4.5 1PRN

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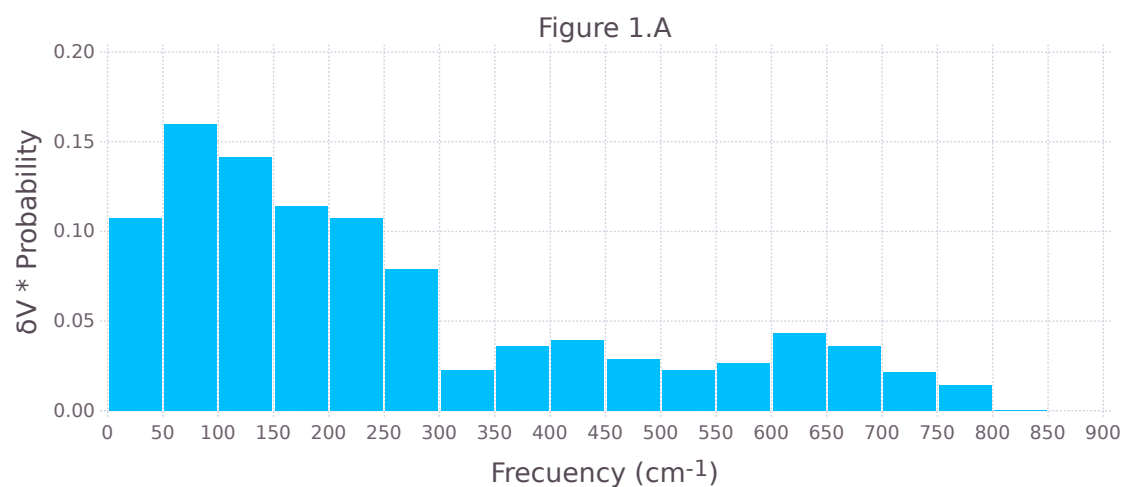


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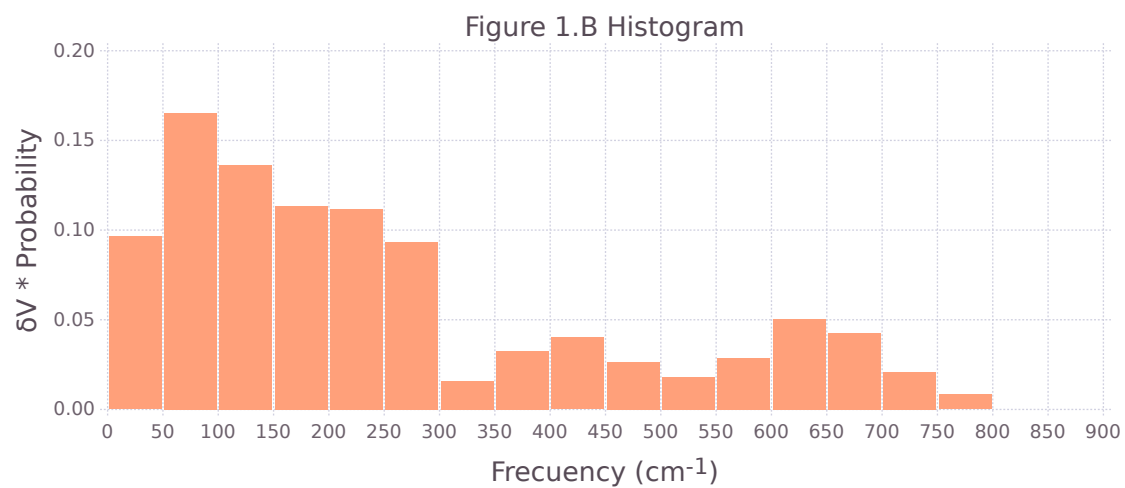


Figure 50. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

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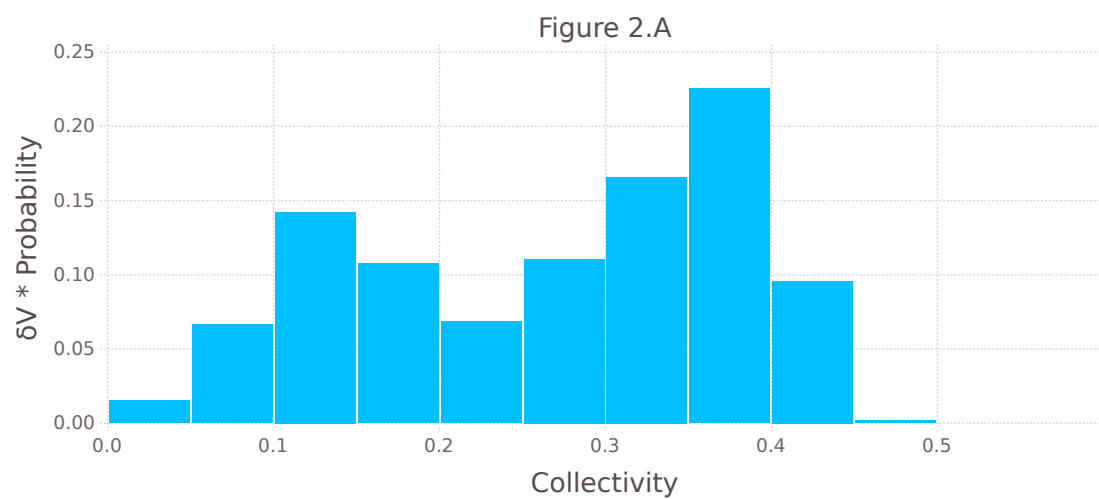


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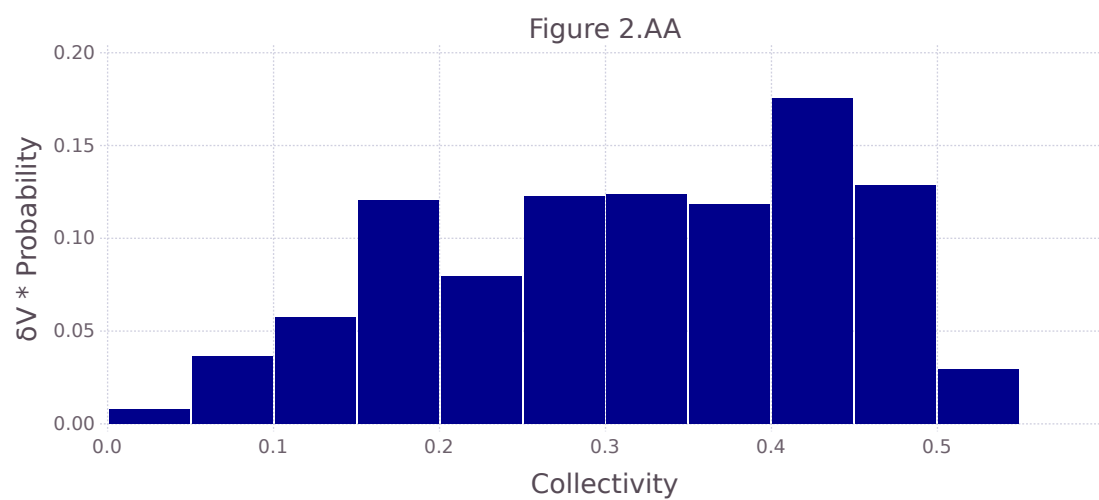


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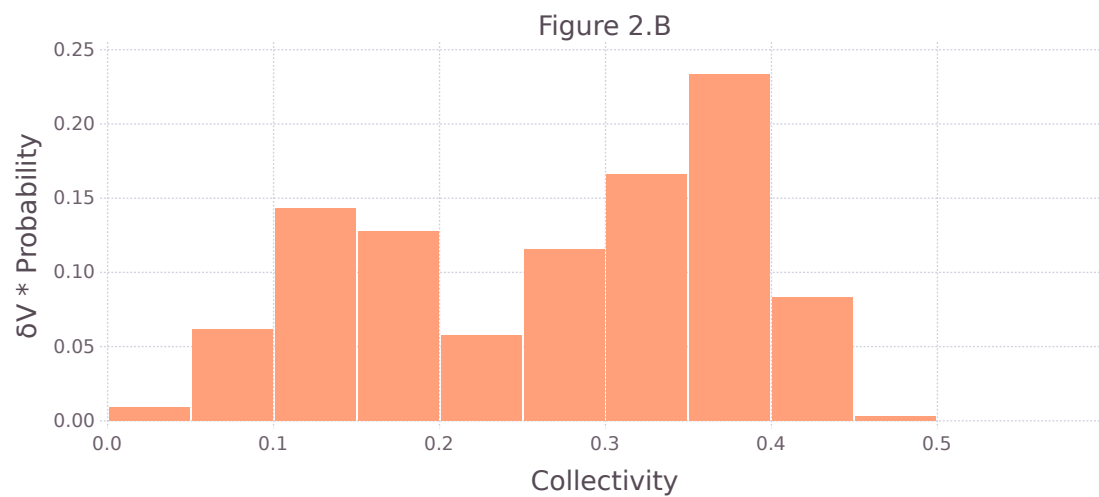


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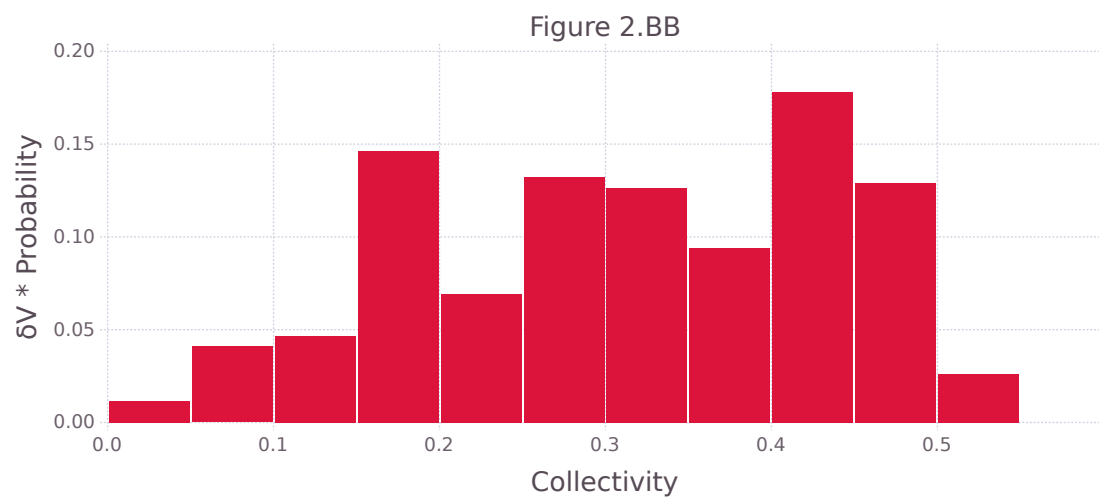


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As in Fig.1, the analogous can be done with the **Participation Number**, as Fig.2 shows.

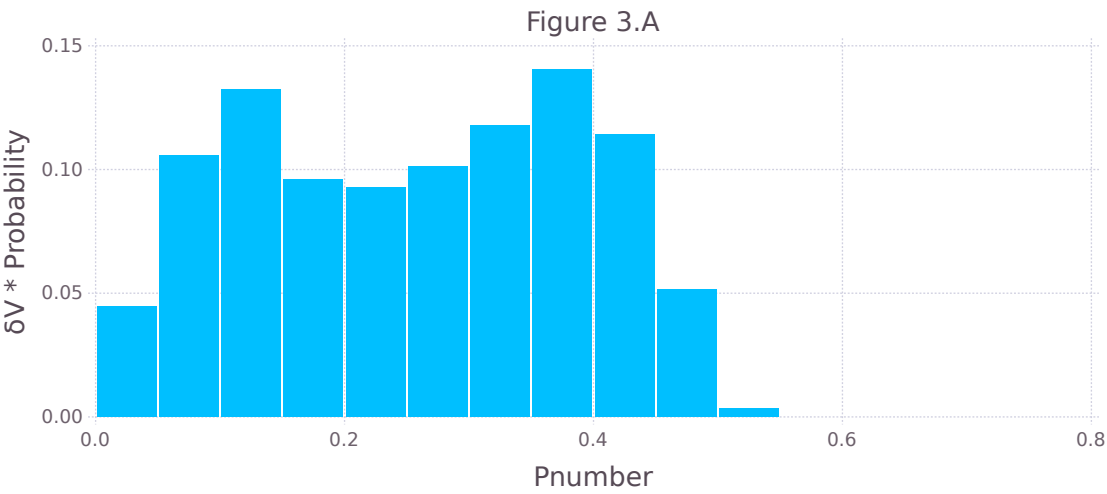


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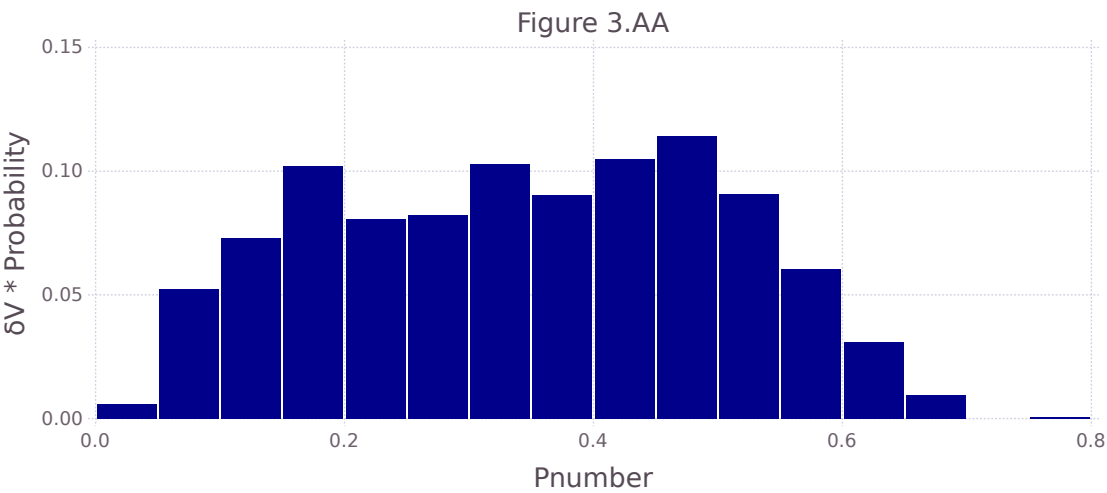


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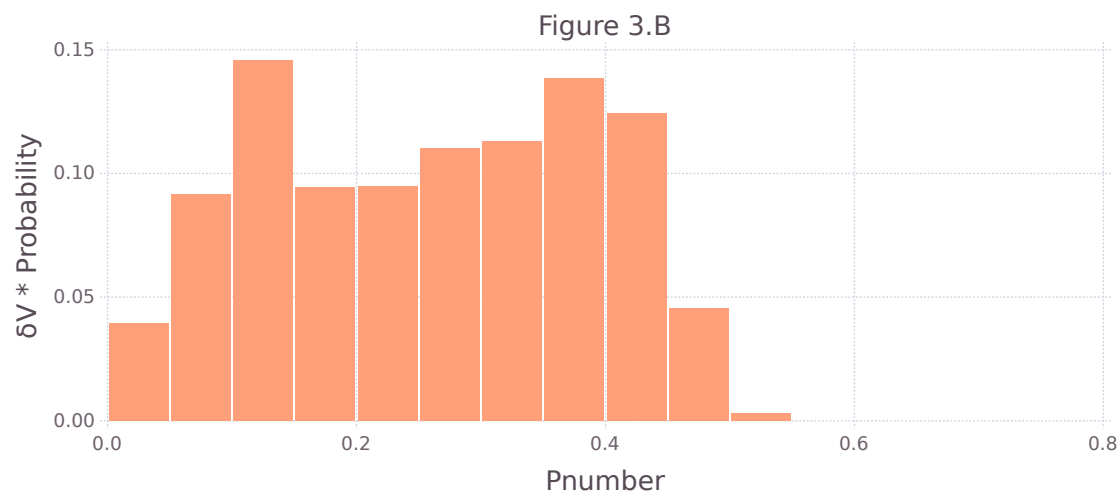


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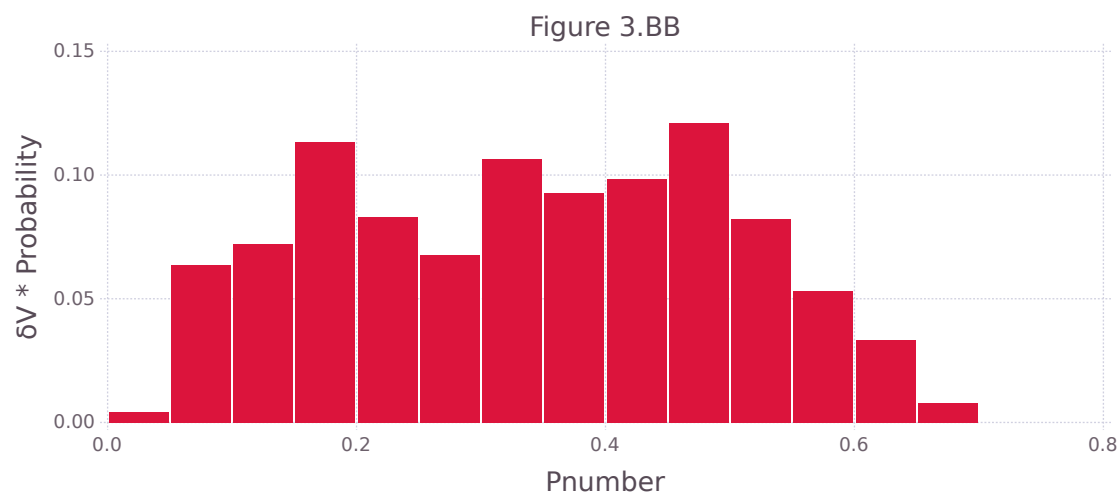


Figure 58. This is an inserted EPS graphic

VGW can be translated into cartesian coordinates and the module of the X, Y, Z coordinates obtained.

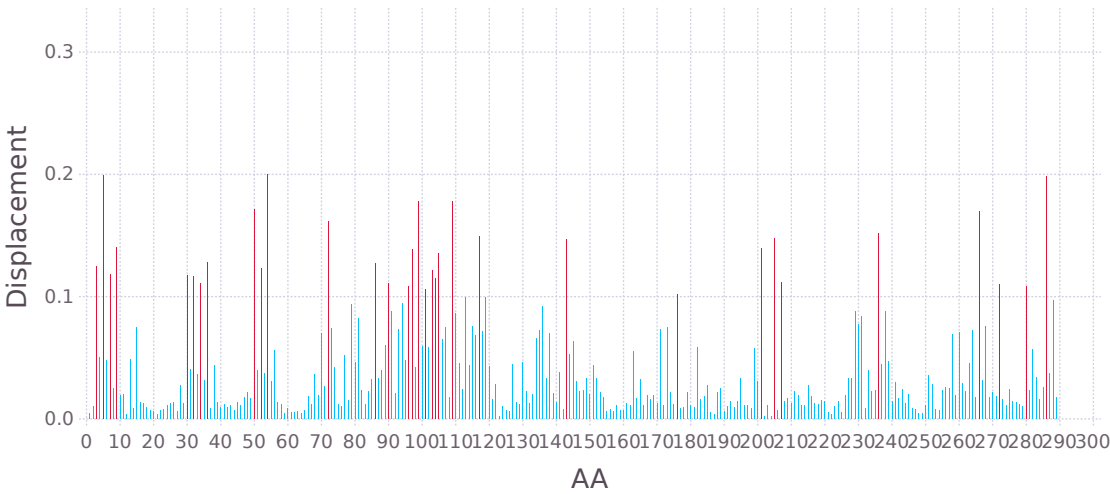


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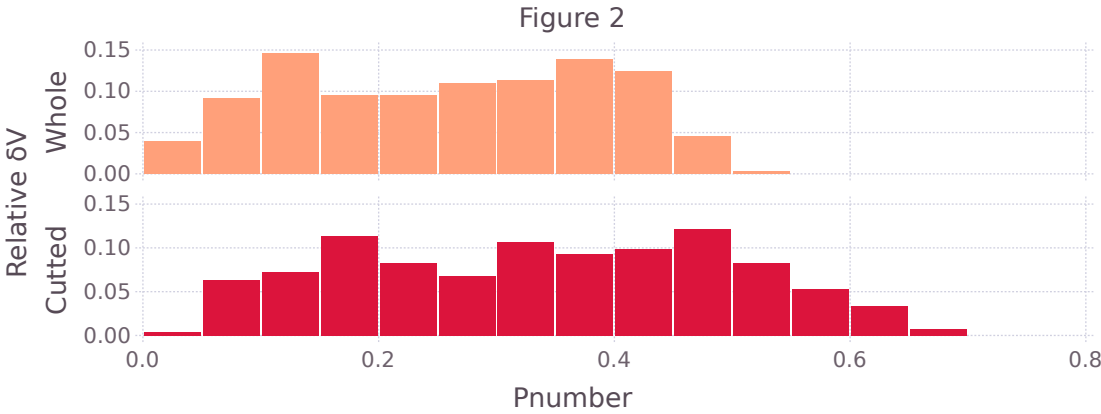


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4.6 256L

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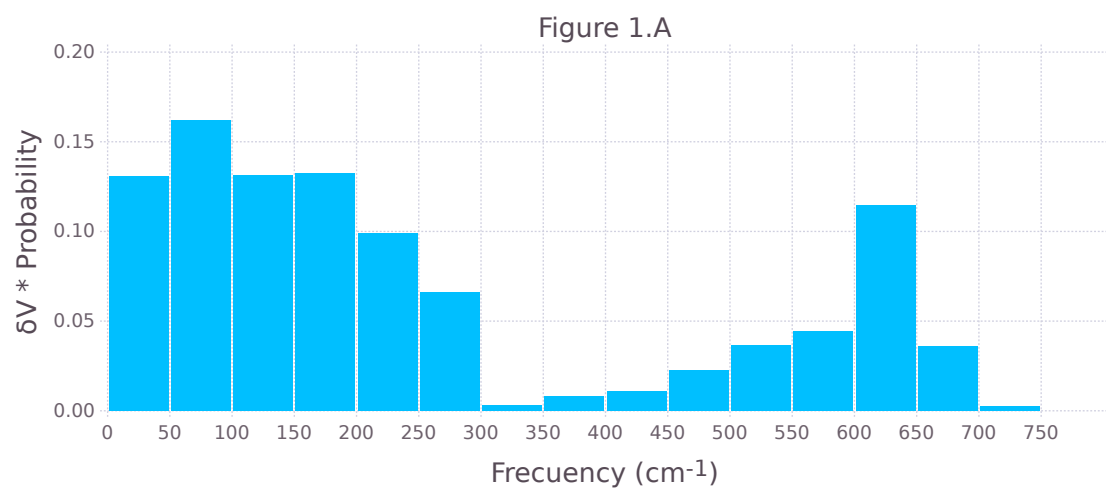


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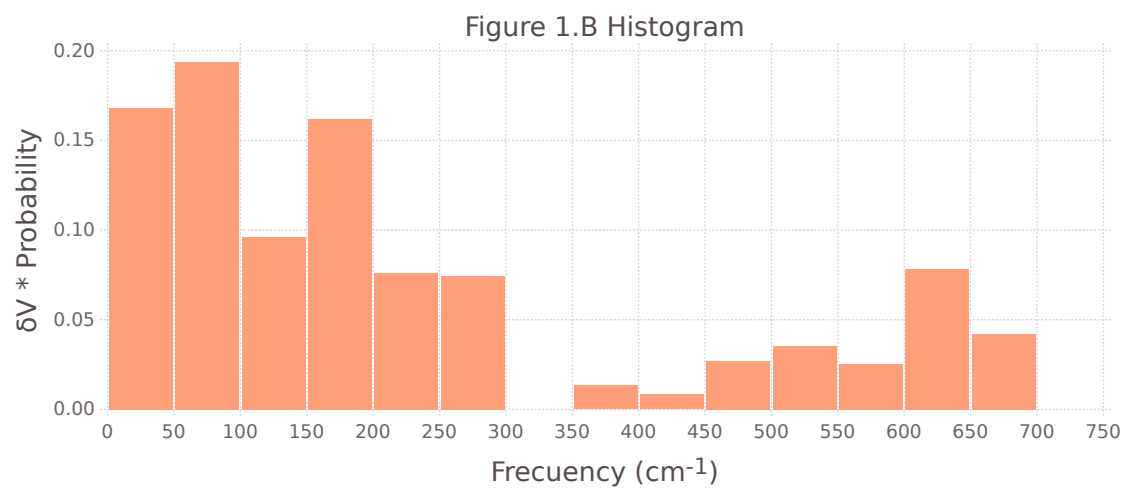


Figure 62. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

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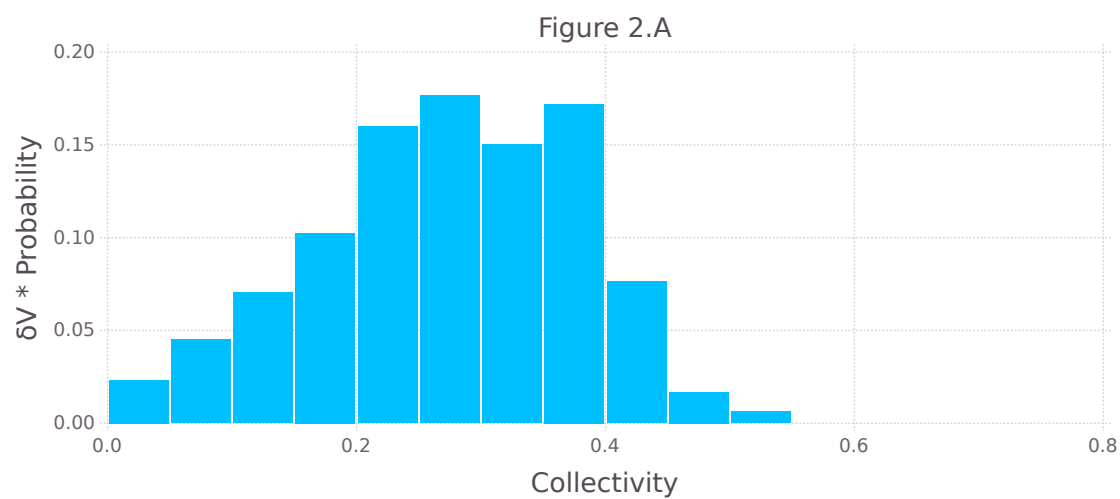


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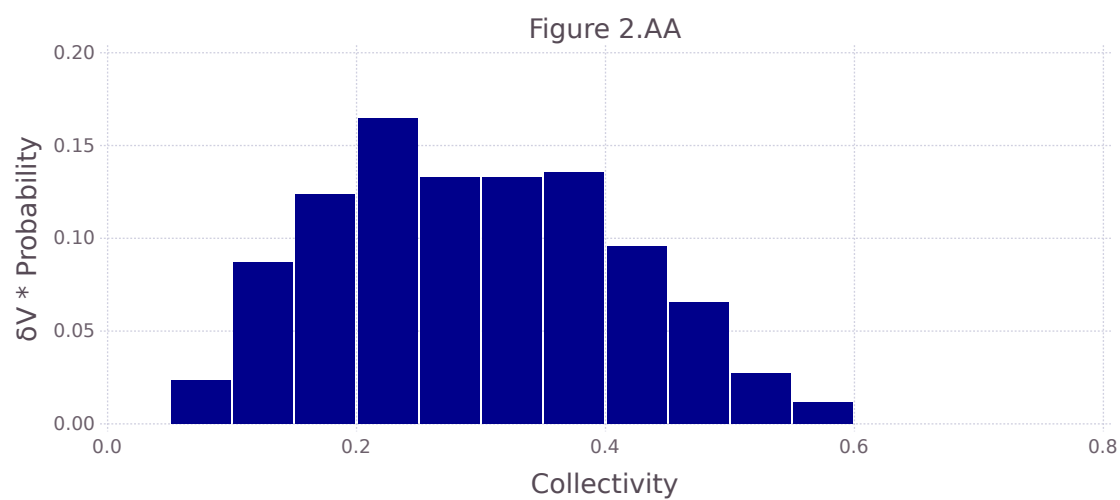


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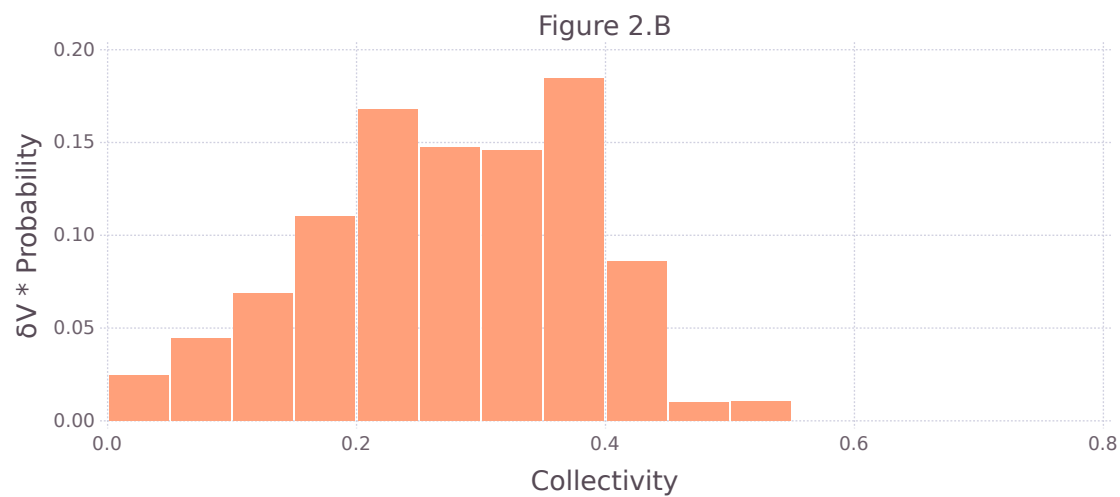


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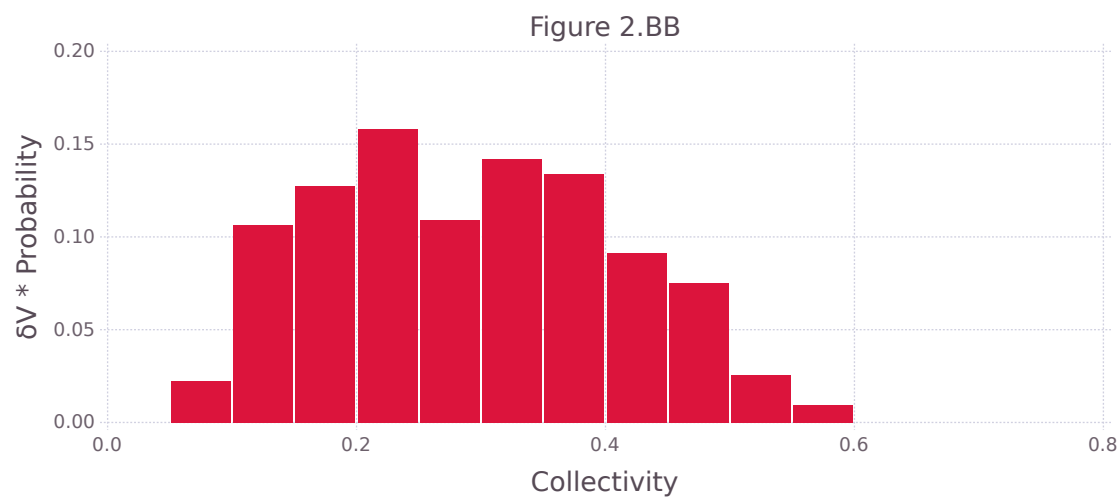


Figure 66. This is an inserted EPS graphic

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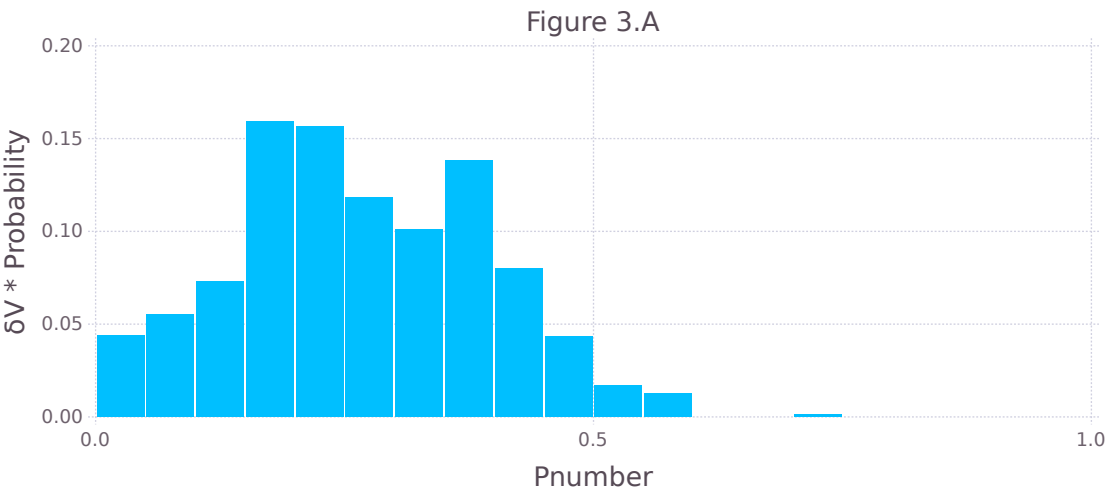


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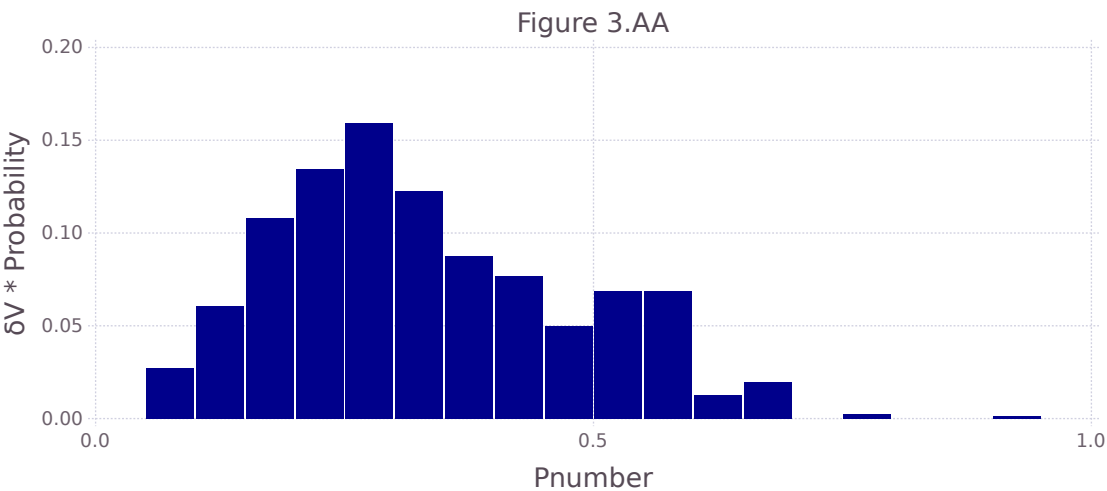


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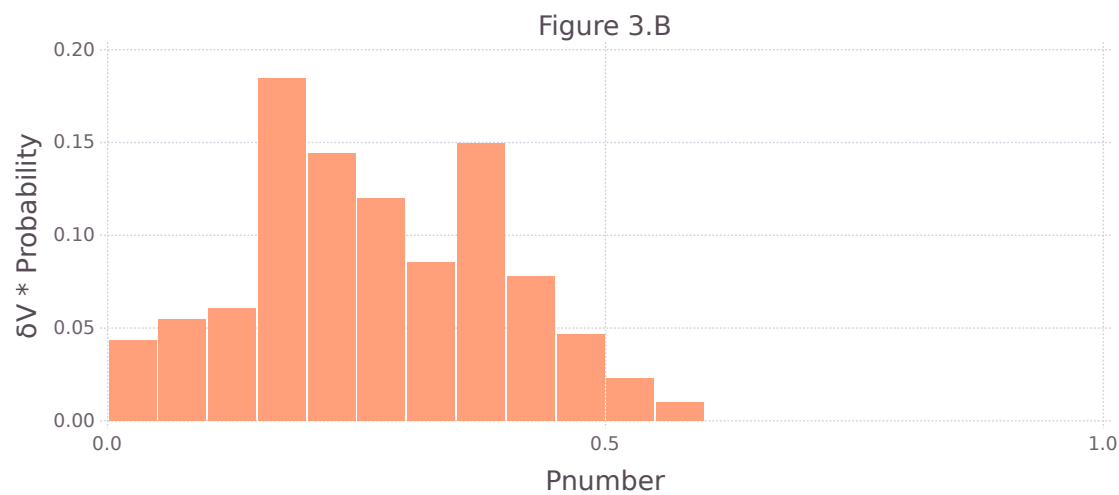


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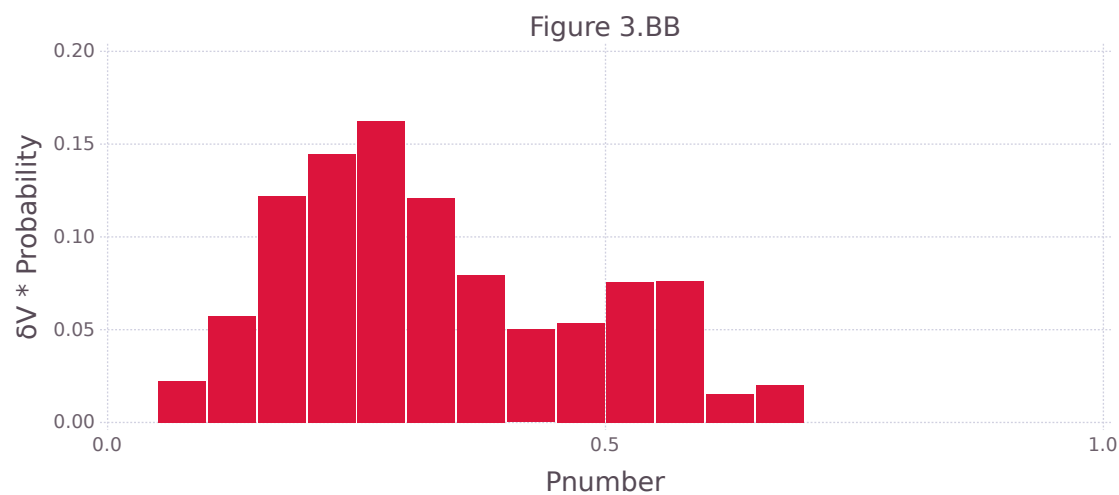


Figure 70. This is an inserted EPS graphic

VGV can be translated into cartesian coordinates and the module of the X, Y, Z coordinates obtained.

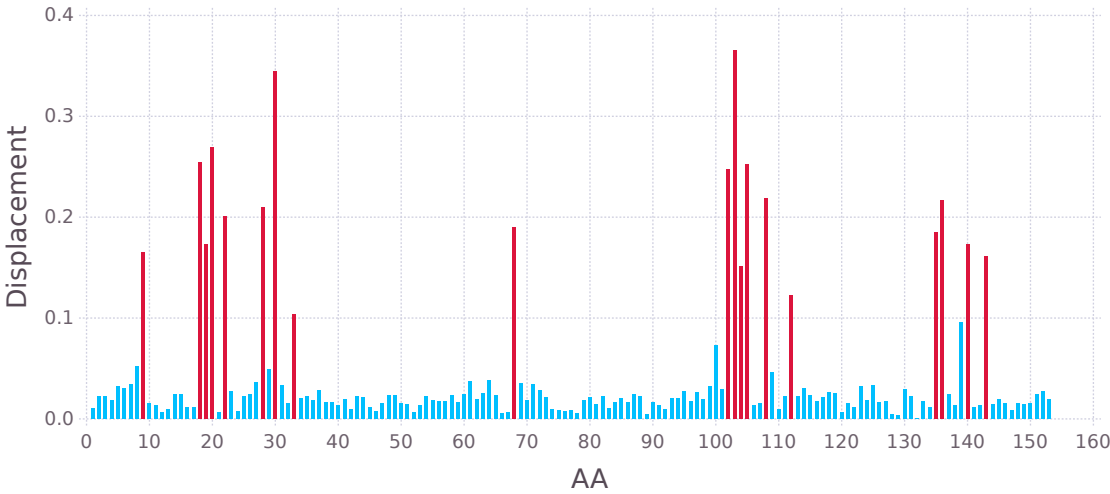


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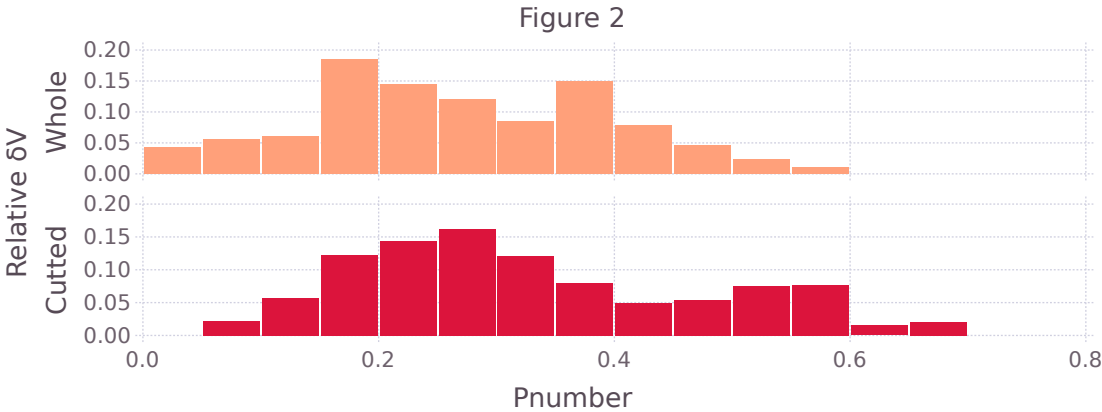


Figure 72. This is an inserted EPS graphic

5 Results HI PRECISION

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5.1 1HVR_APO

71

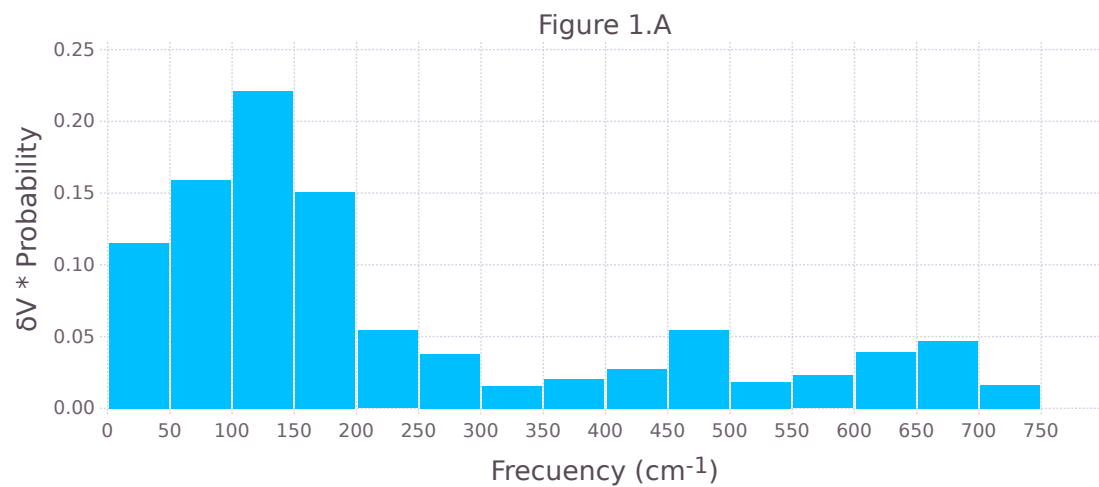


Figure 73. This is an inserted EPS graphic

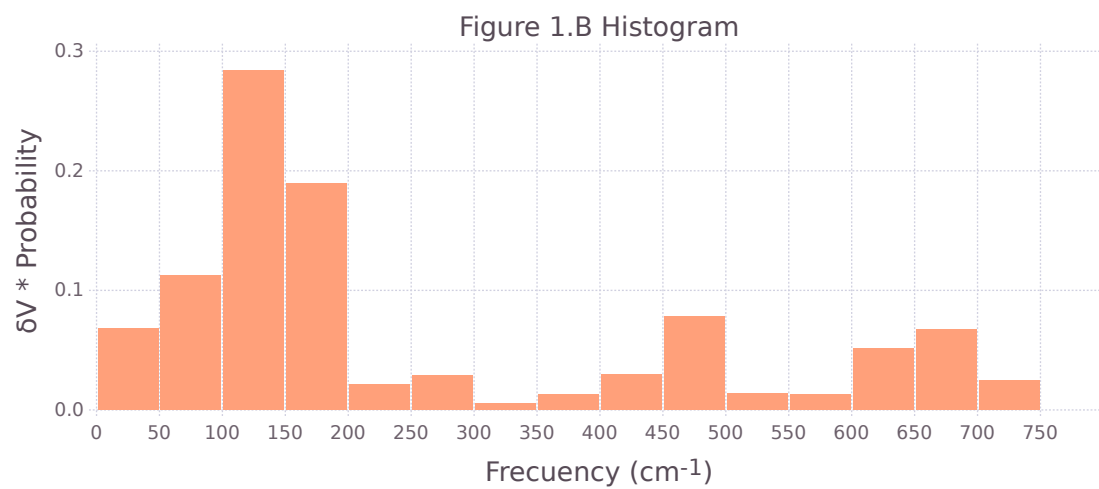


Figure 74. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

72

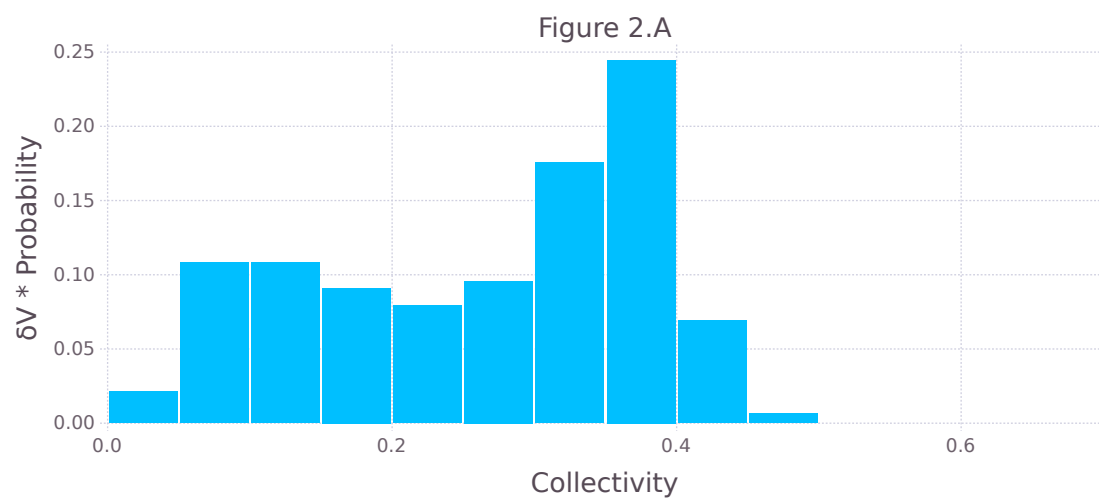


Figure 75. This is an inserted EPS graphic

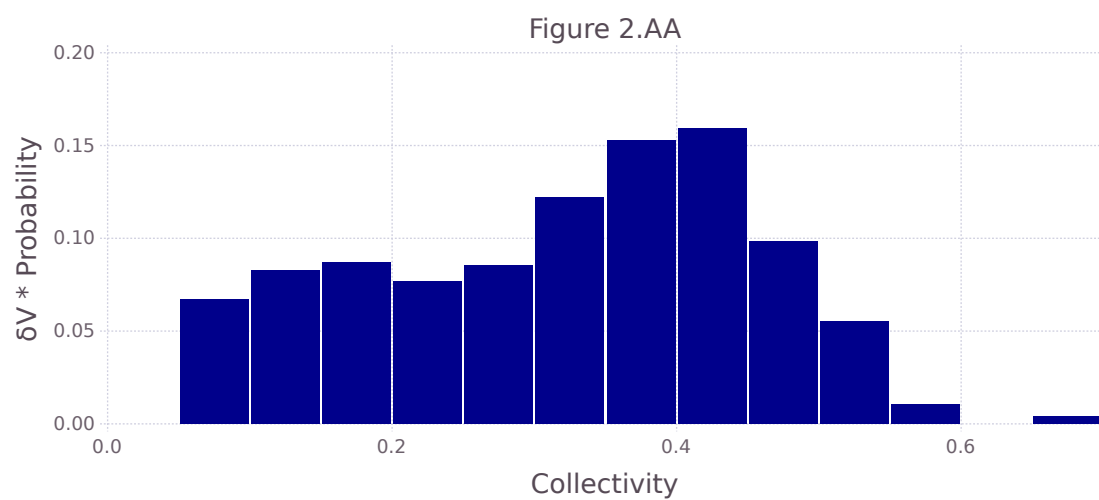


Figure 76. This is an inserted EPS graphic

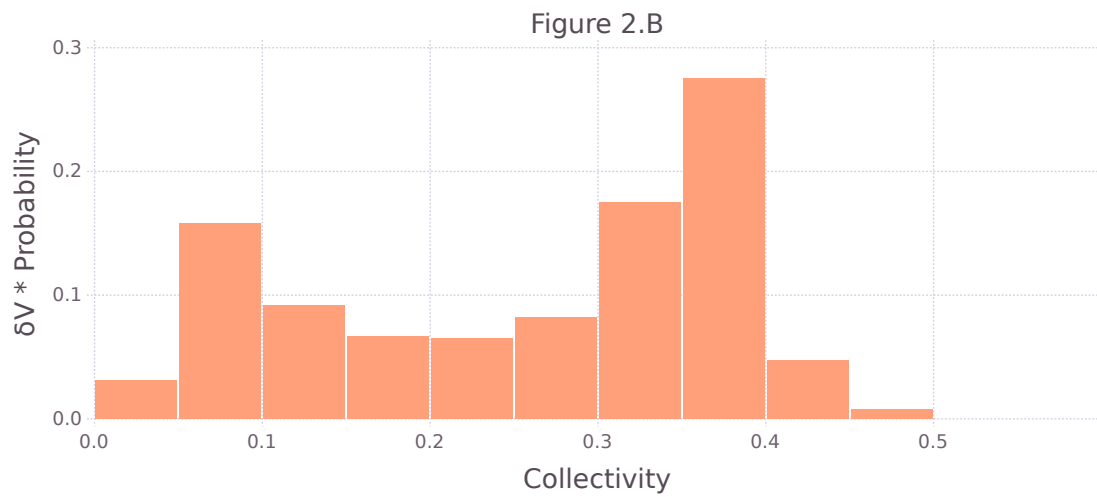


Figure 77. This is an inserted EPS graphic

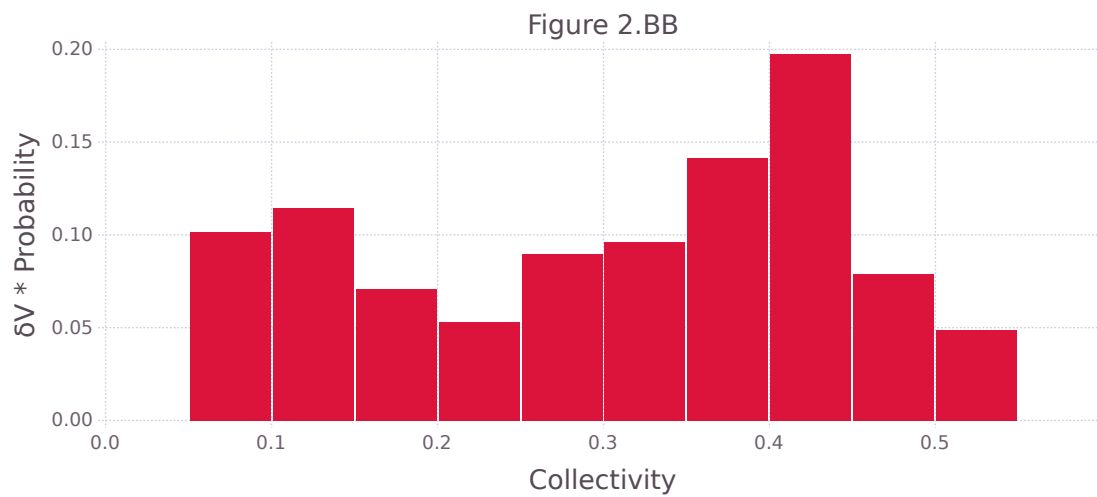


Figure 78. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with the **Participation Number**, as Fig.2 shows.

73

74

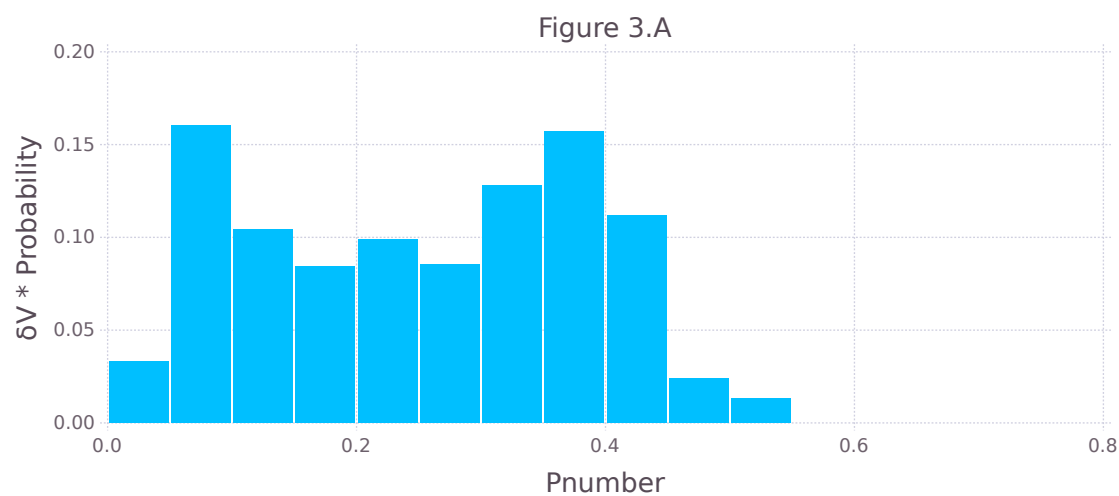


Figure 79. This is an inserted EPS graphic

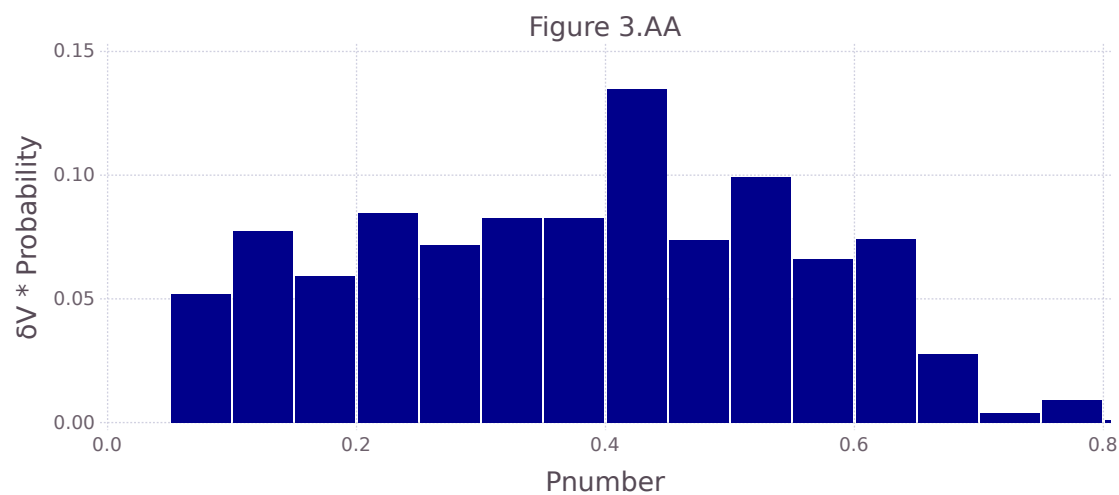


Figure 80. This is an inserted EPS graphic

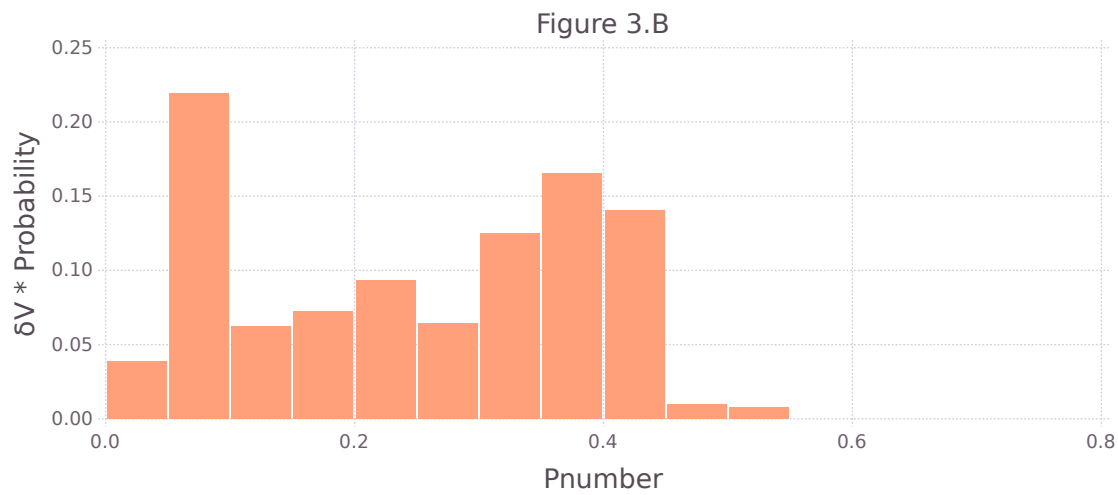


Figure 81. This is an inserted EPS graphic

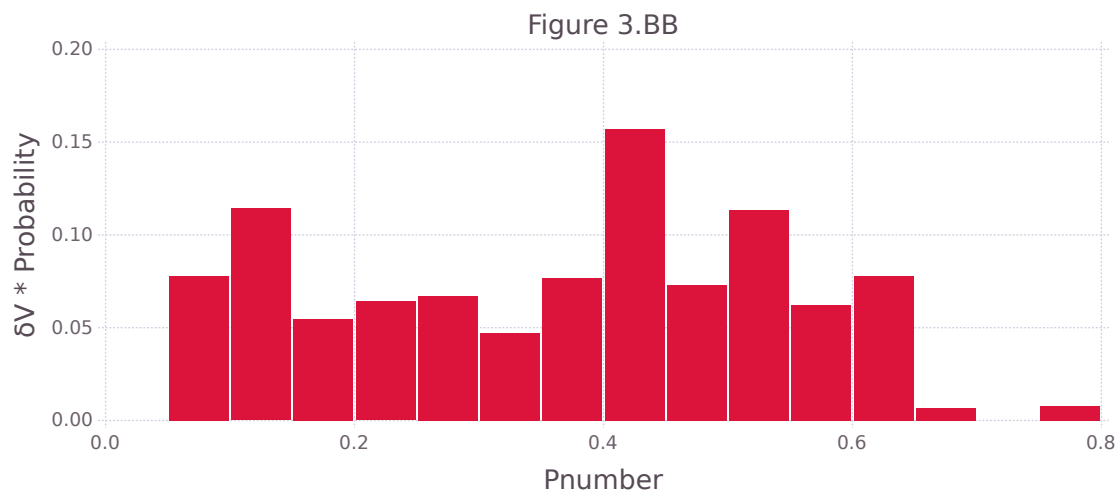


Figure 82. This is an inserted EPS graphic

VGV can be translated into cartesian coordinates and the module of the X, Y, Z coordinates obtained.

75

76

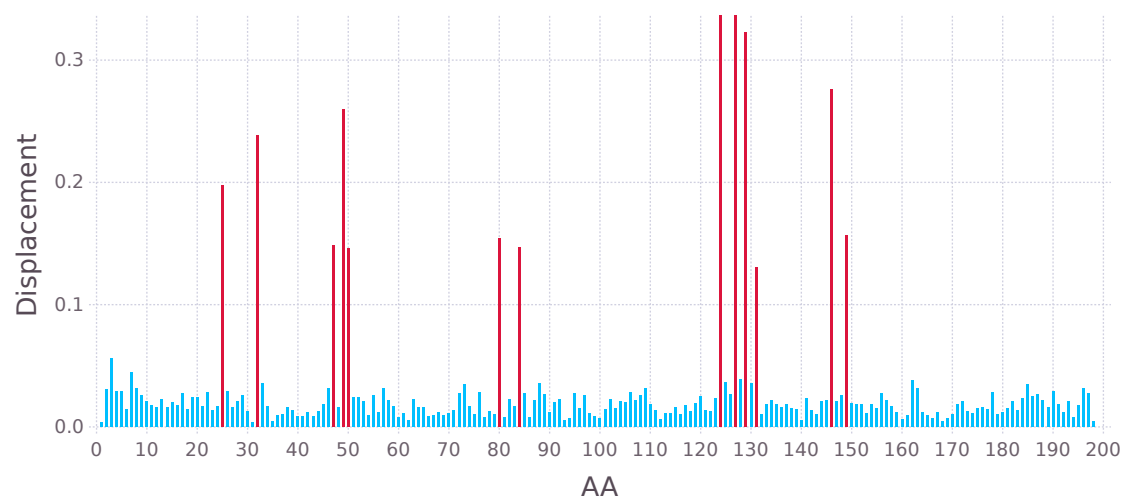


Figure 83. This is an inserted EPS graphic

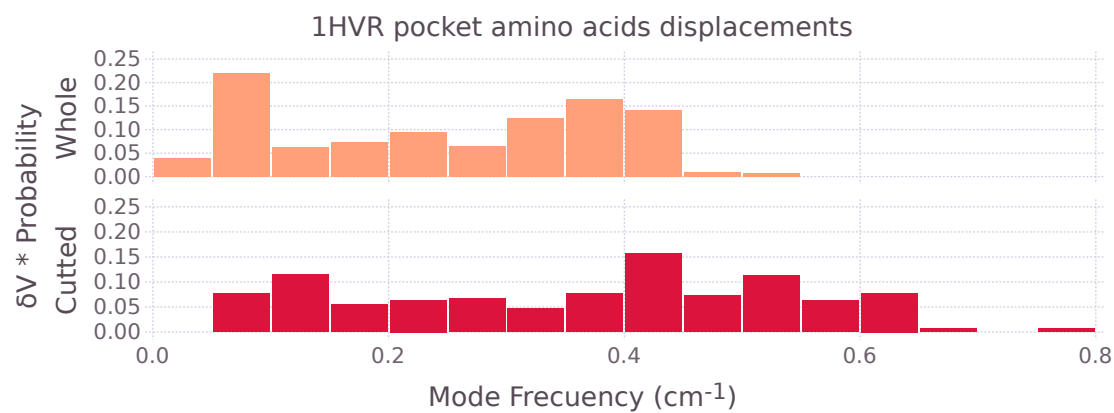
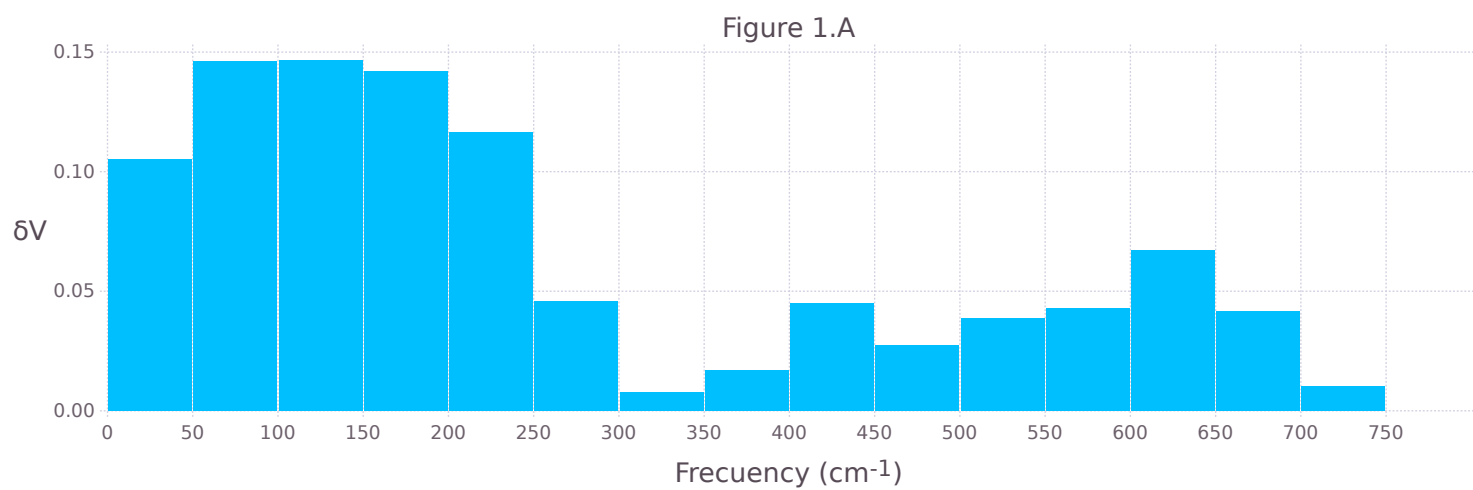
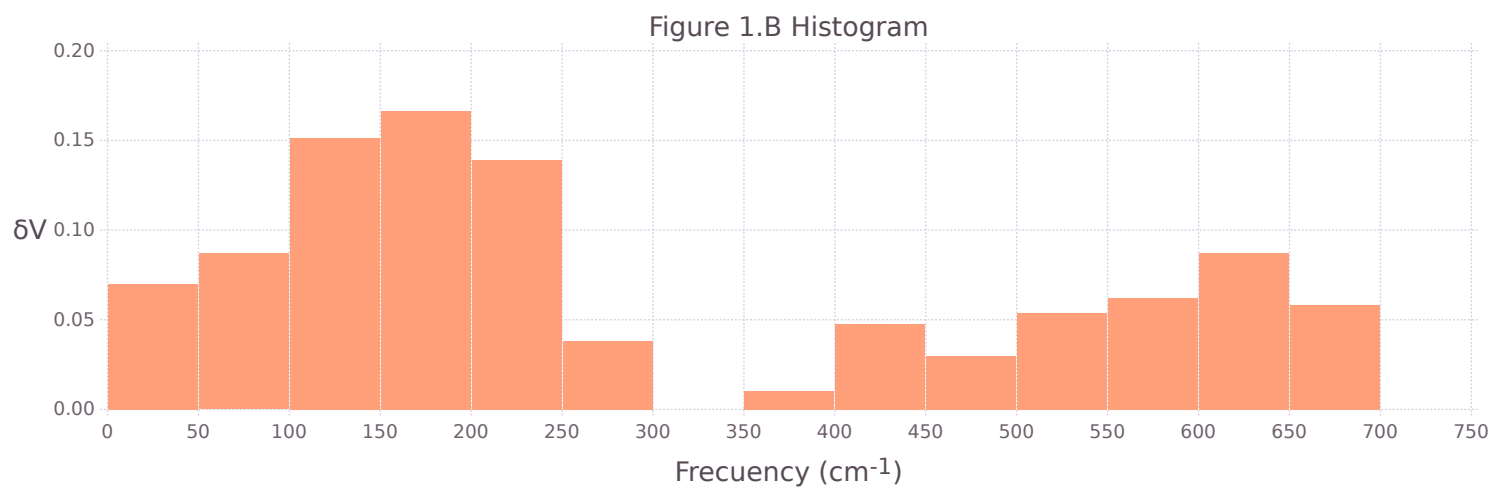


Figure 84. This is an inserted EPS graphic

5.2 1HVR_HOLO

77

**Figure 85.** This is an inserted EPS graphic**Figure 86.** This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

78

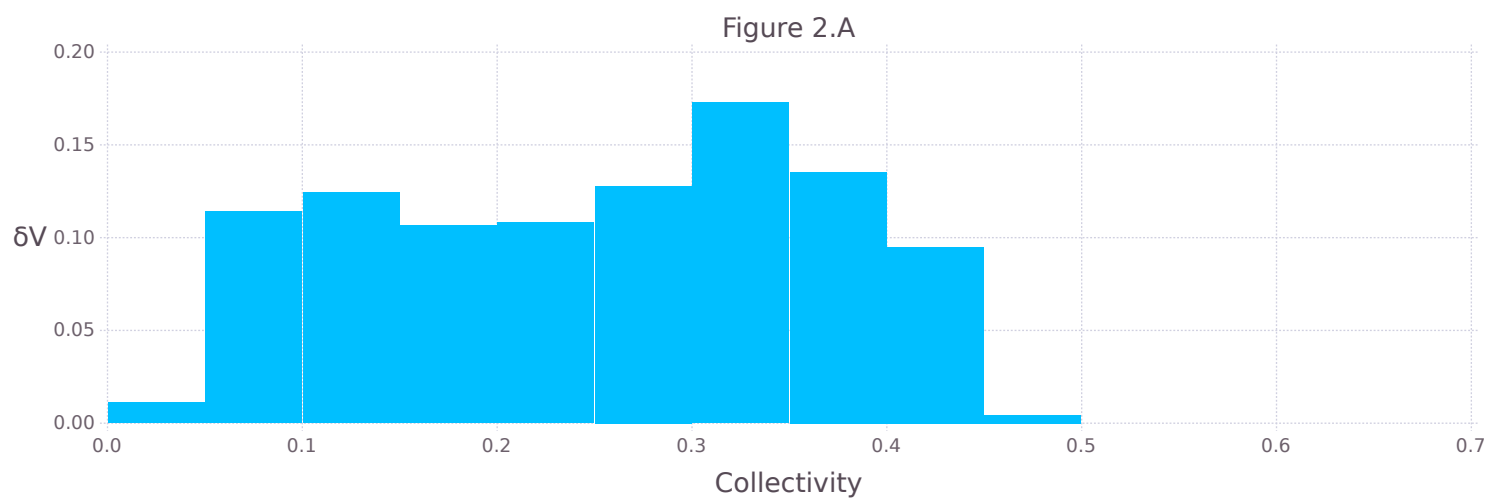


Figure 87. This is an inserted EPS graphic

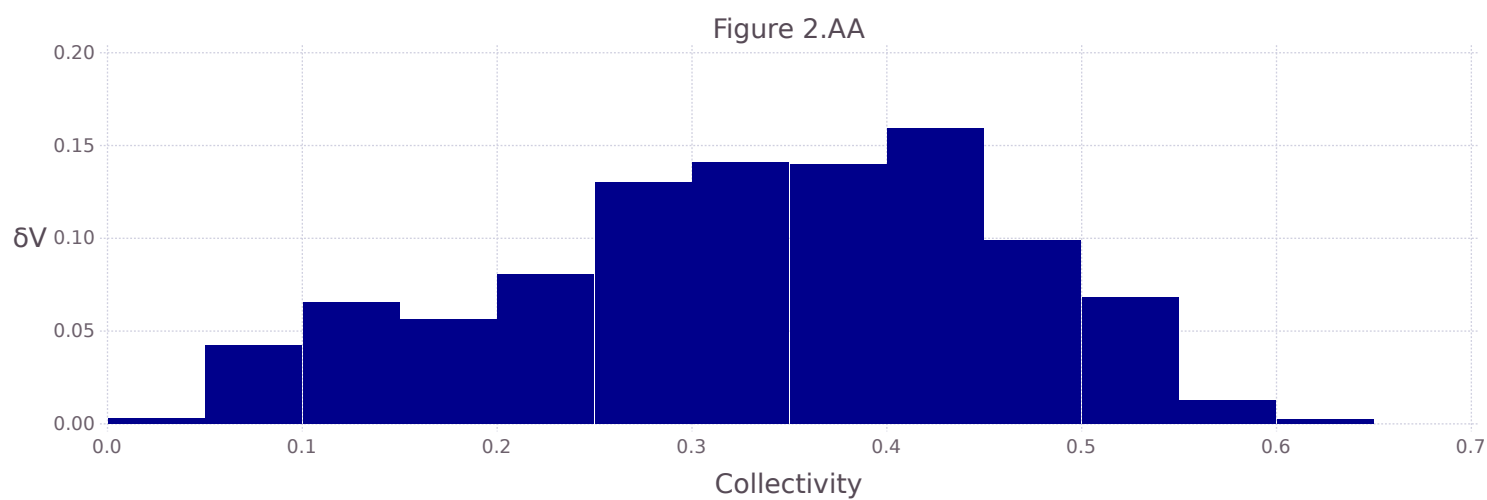


Figure 88. This is an inserted EPS graphic

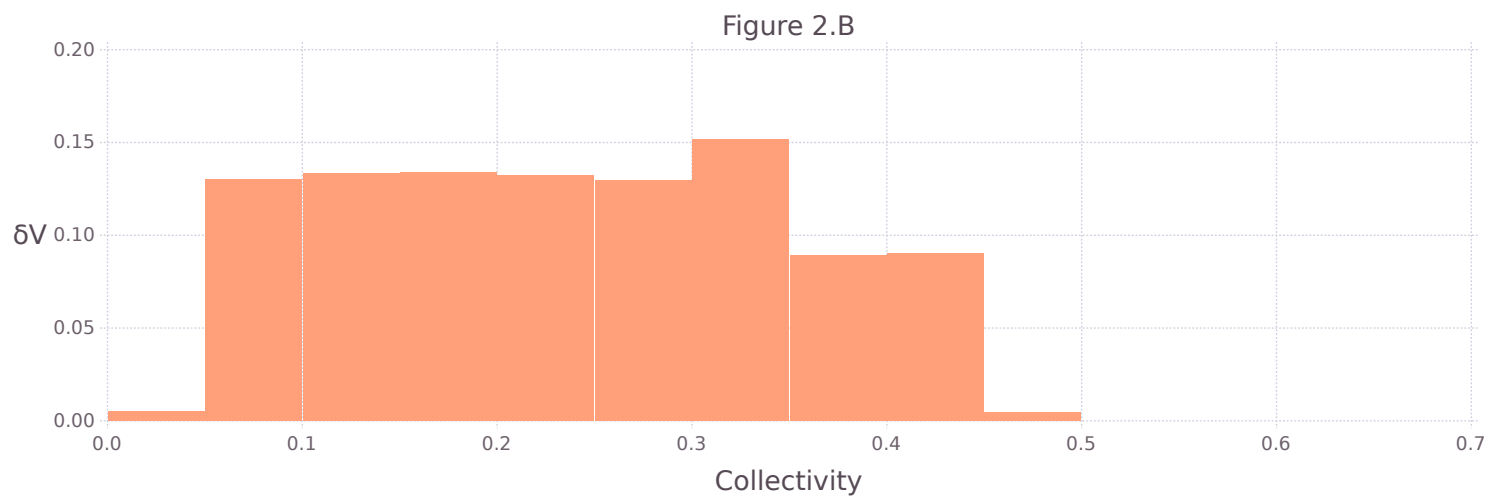


Figure 89. This is an inserted EPS graphic

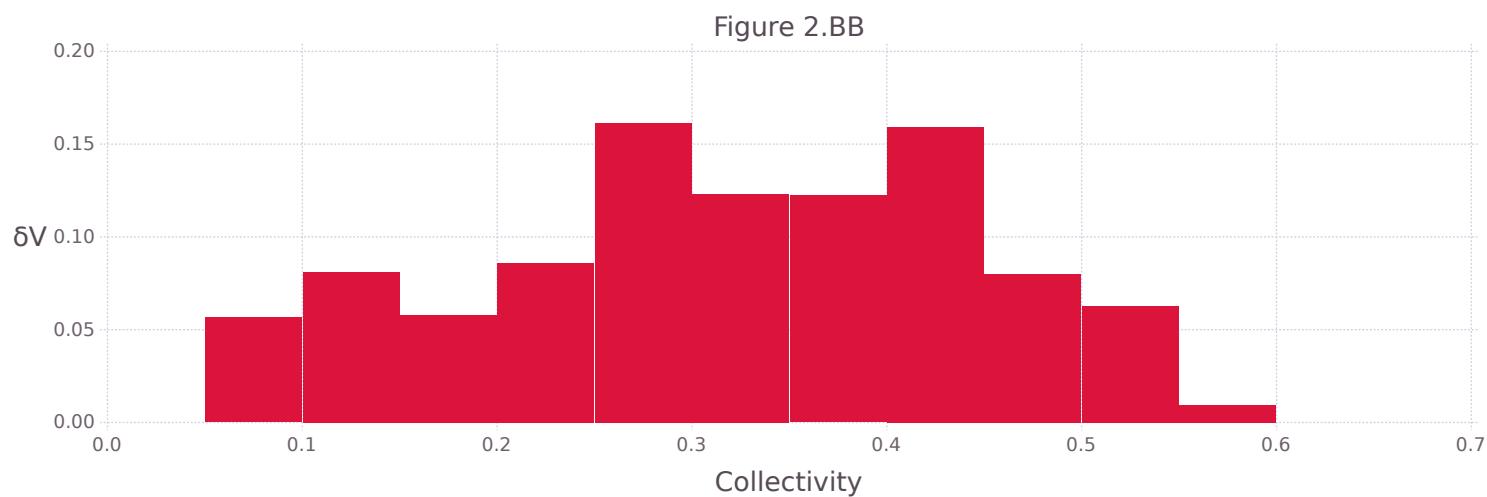


Figure 90. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with the **Participation Number**, as Fig.2 shows.

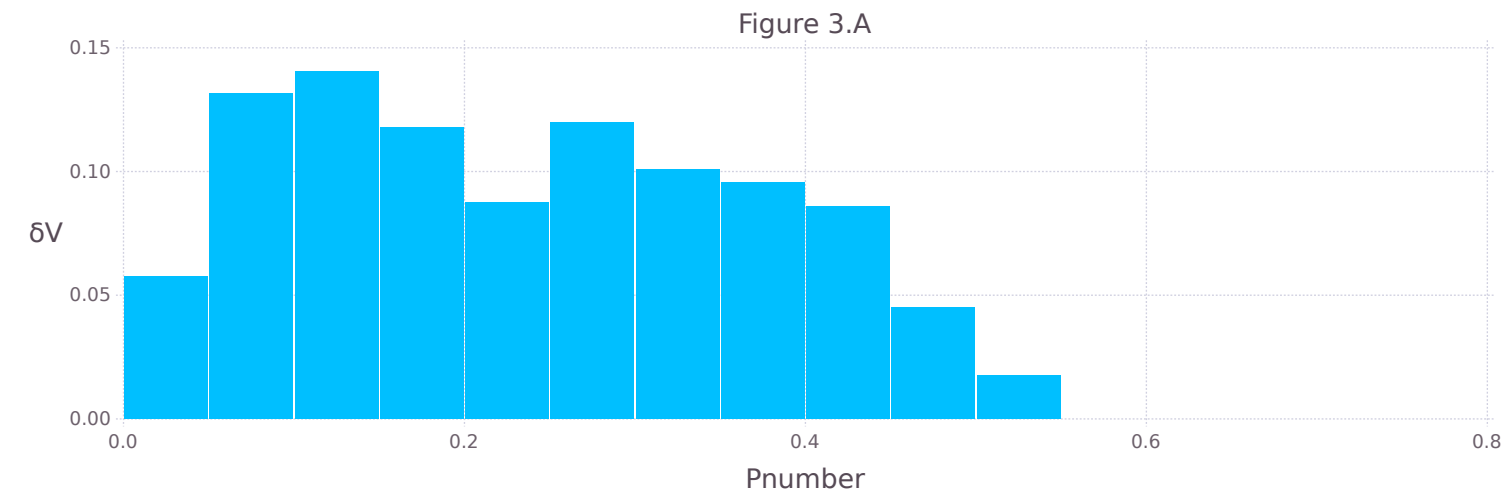


Figure 91. This is an inserted EPS graphic

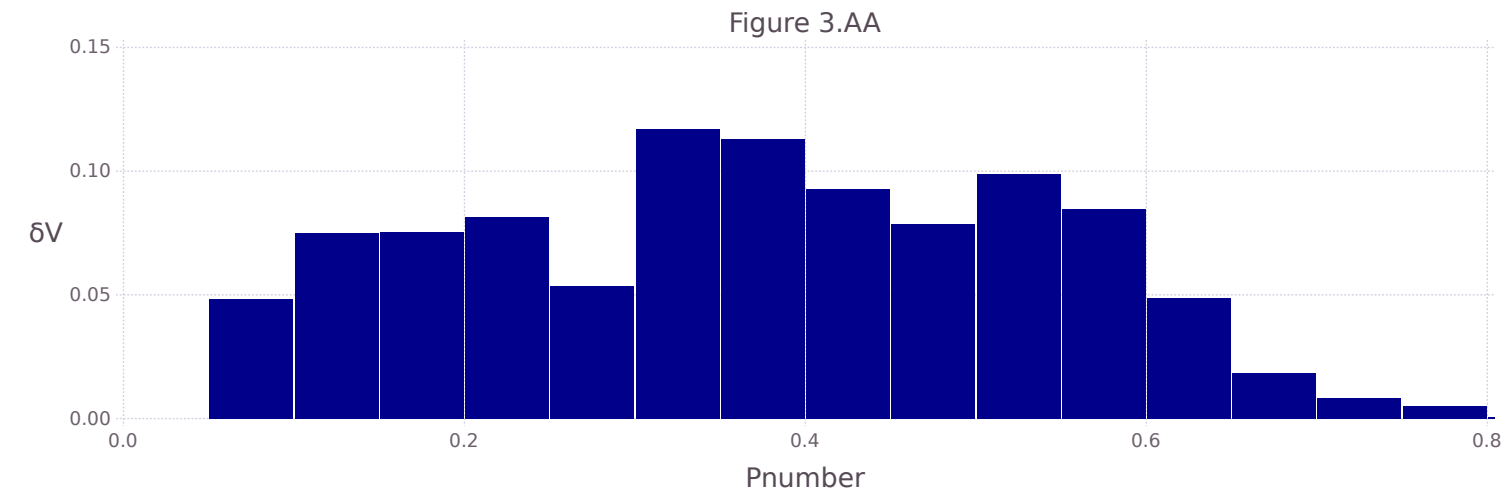


Figure 92. This is an inserted EPS graphic

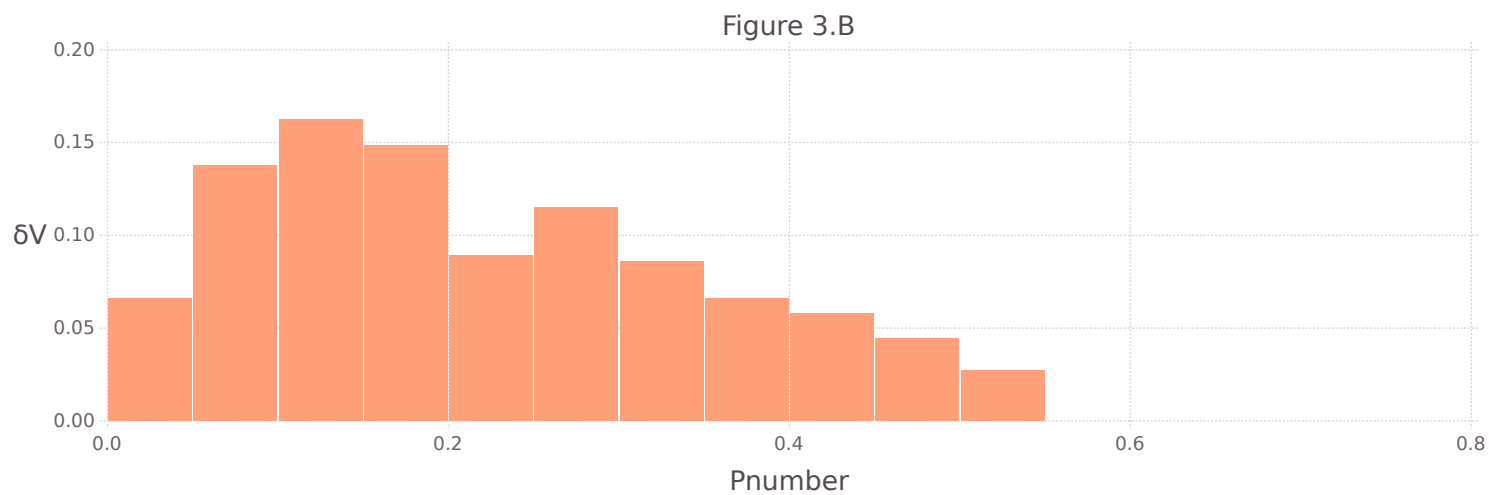


Figure 93. This is an inserted EPS graphic

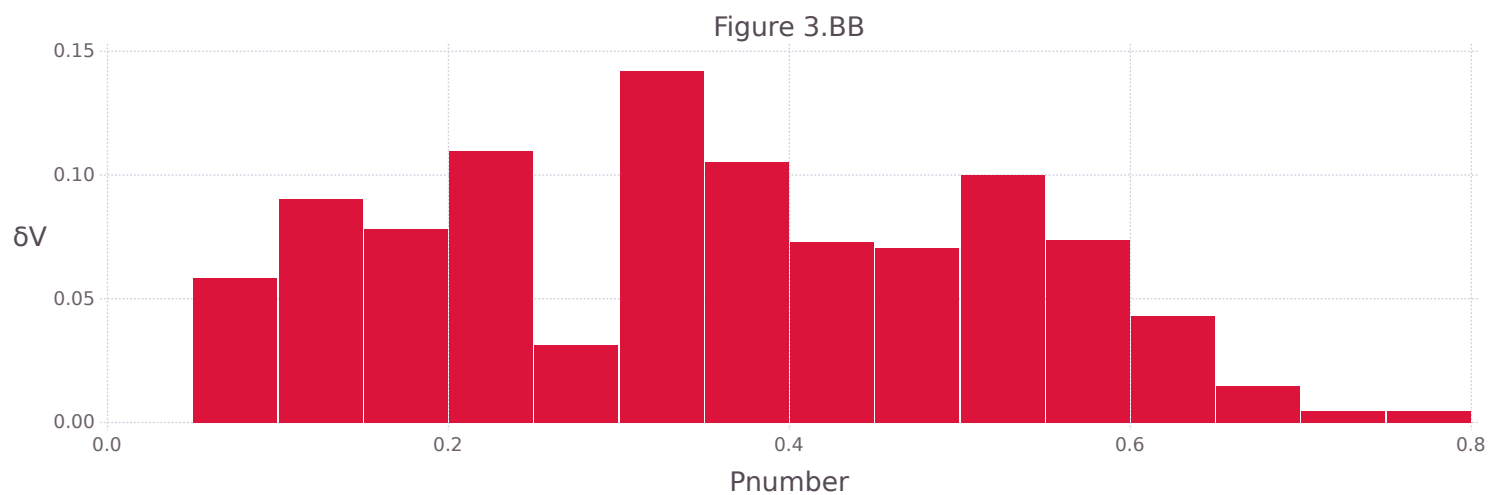


Figure 94. This is an inserted EPS graphic

VG_V can be translated into cartesian coordinates and the module of the X, Y, Z coordinates obtained.

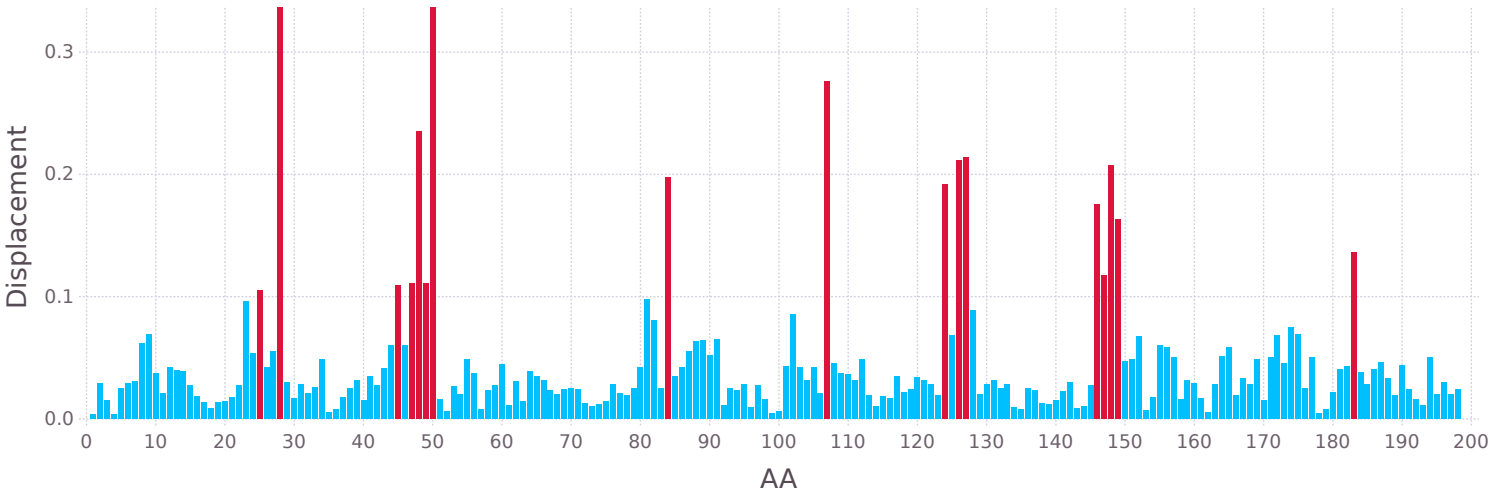


Figure 95. This is an inserted EPS graphic

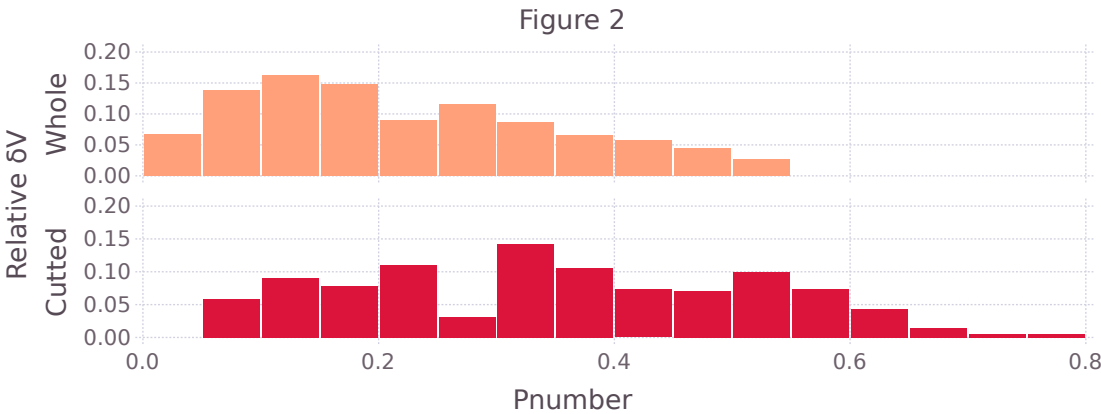


Figure 96. This is an inserted EPS graphic

5.3 1XKK

83

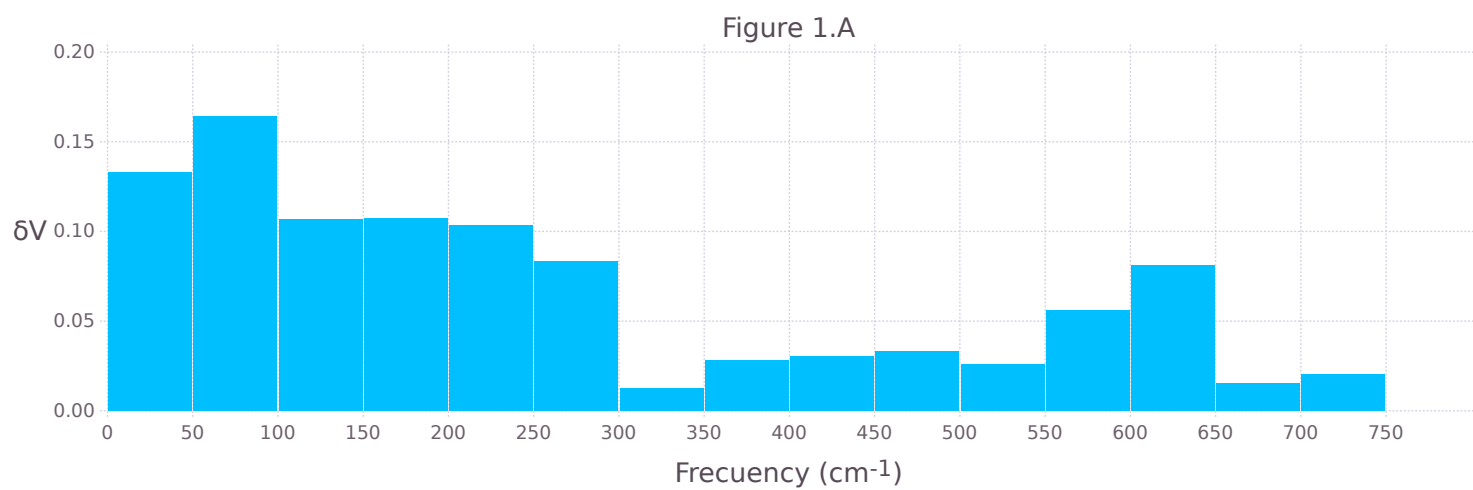


Figure 97. This is an inserted EPS graphic

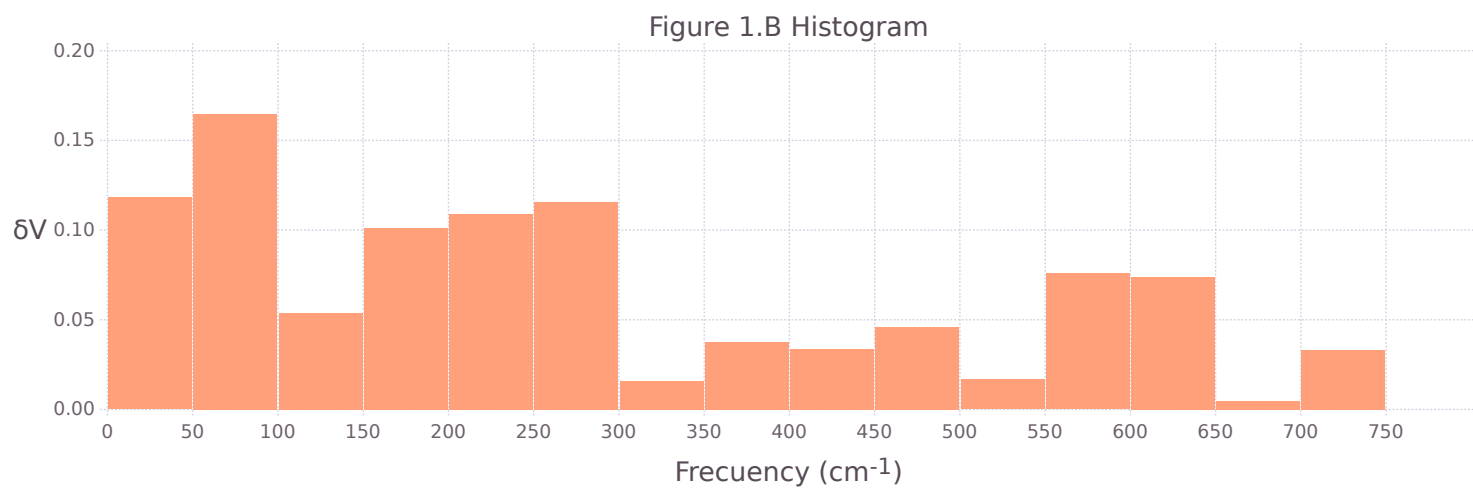


Figure 98. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

84

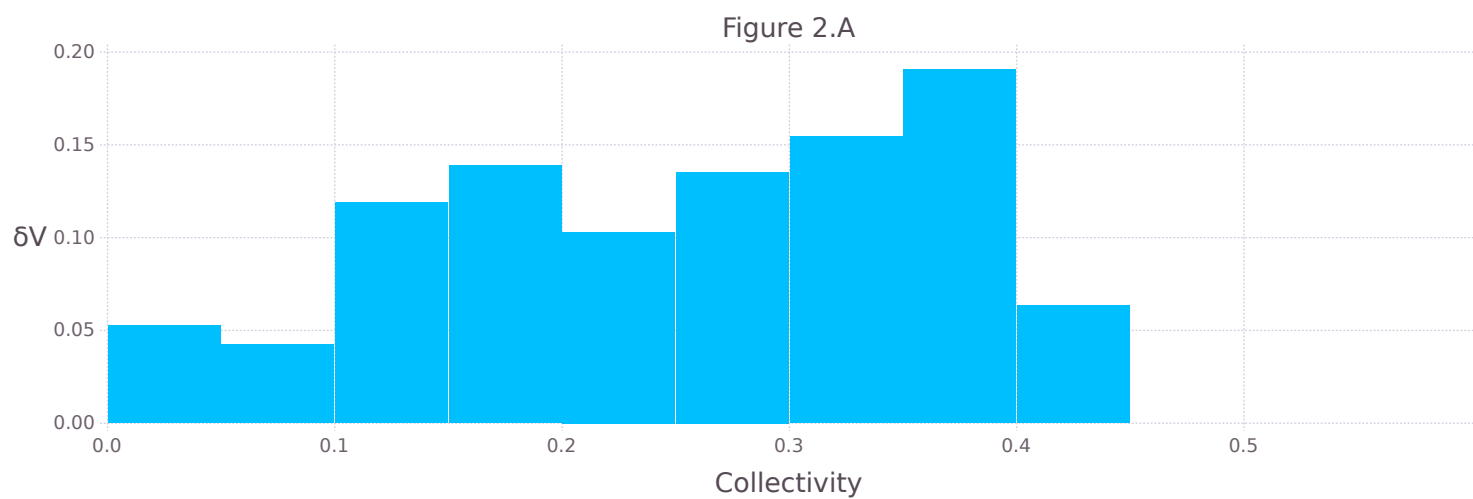


Figure 99. This is an inserted EPS graphic

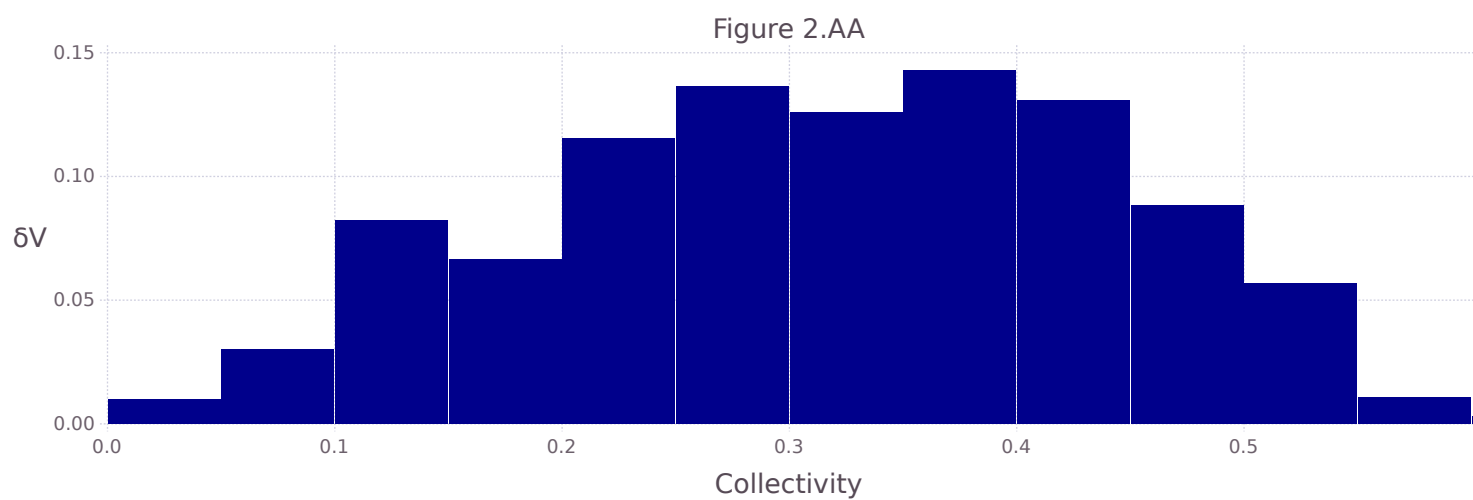


Figure 100. This is an inserted EPS graphic

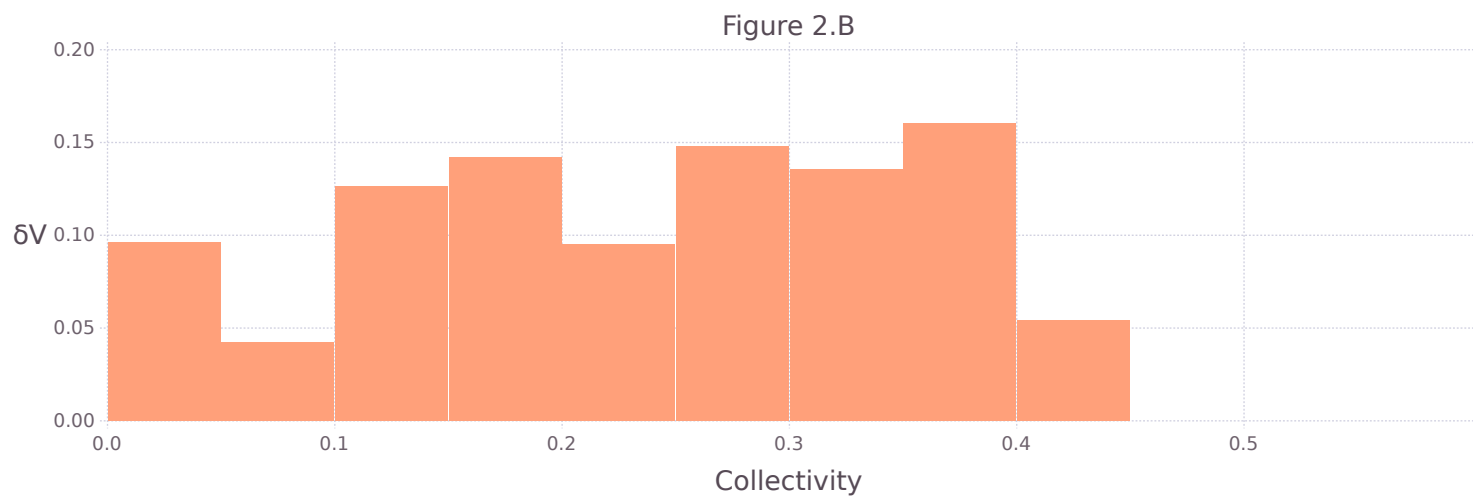


Figure 101. This is an inserted EPS graphic

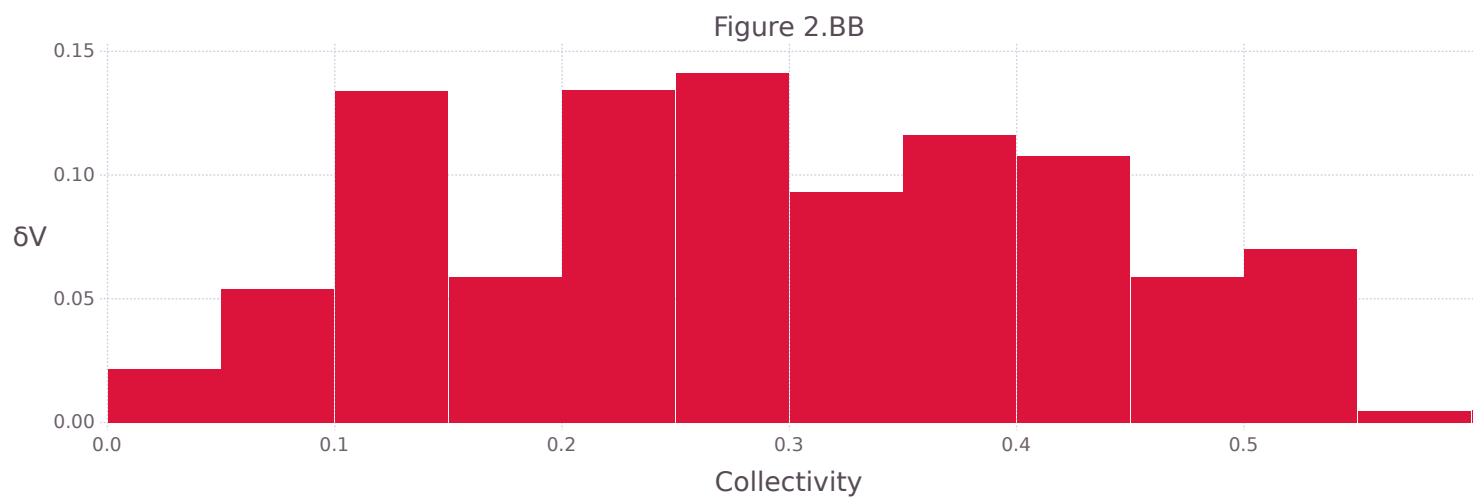


Figure 102. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with the **Participation Number**, as Fig.2 shows.

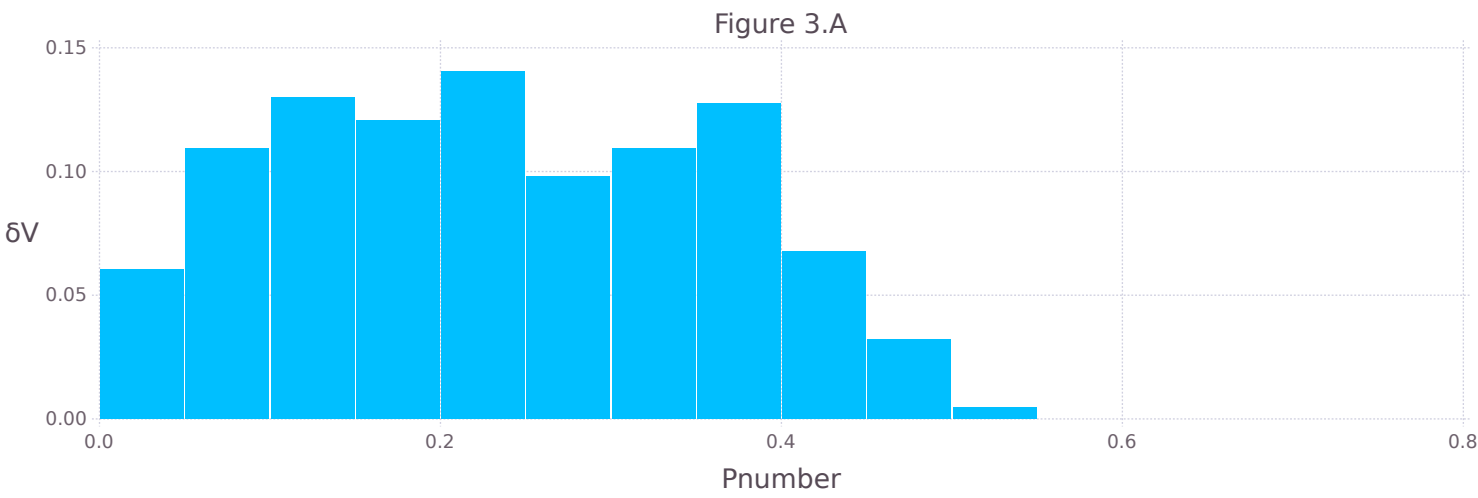


Figure 103. This is an inserted EPS graphic

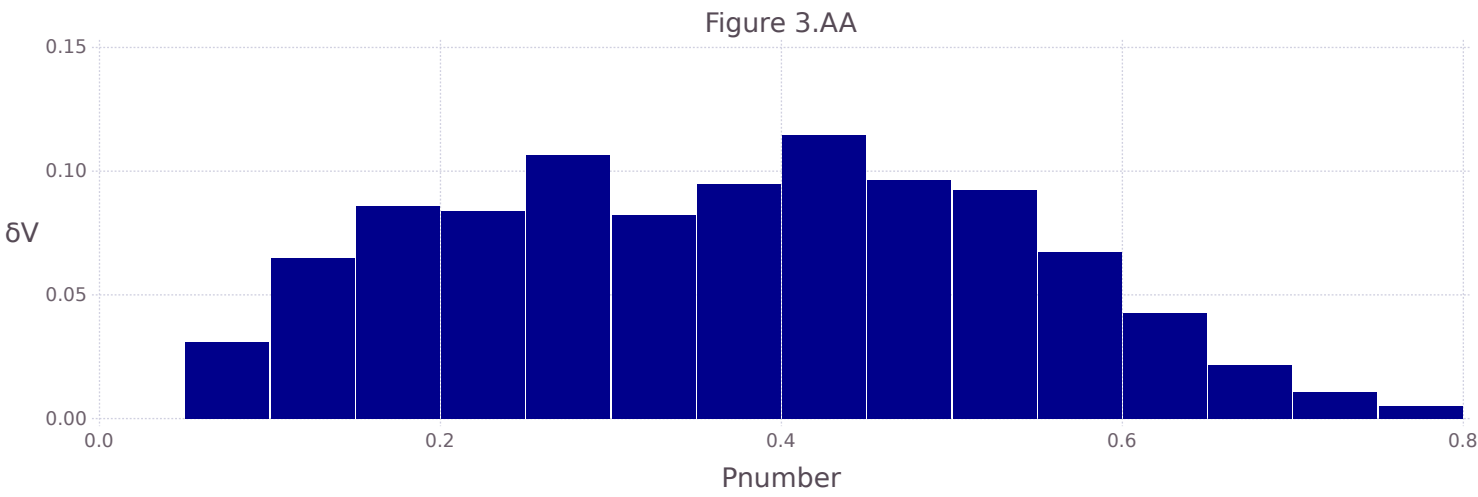


Figure 104. This is an inserted EPS graphic

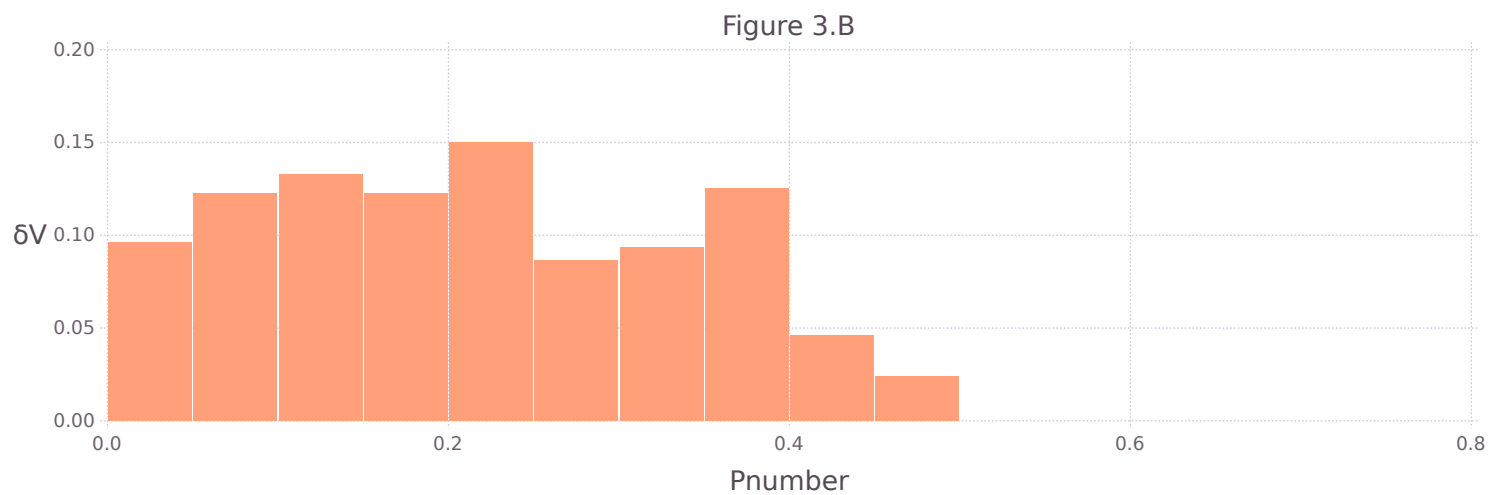


Figure 105. This is an inserted EPS graphic

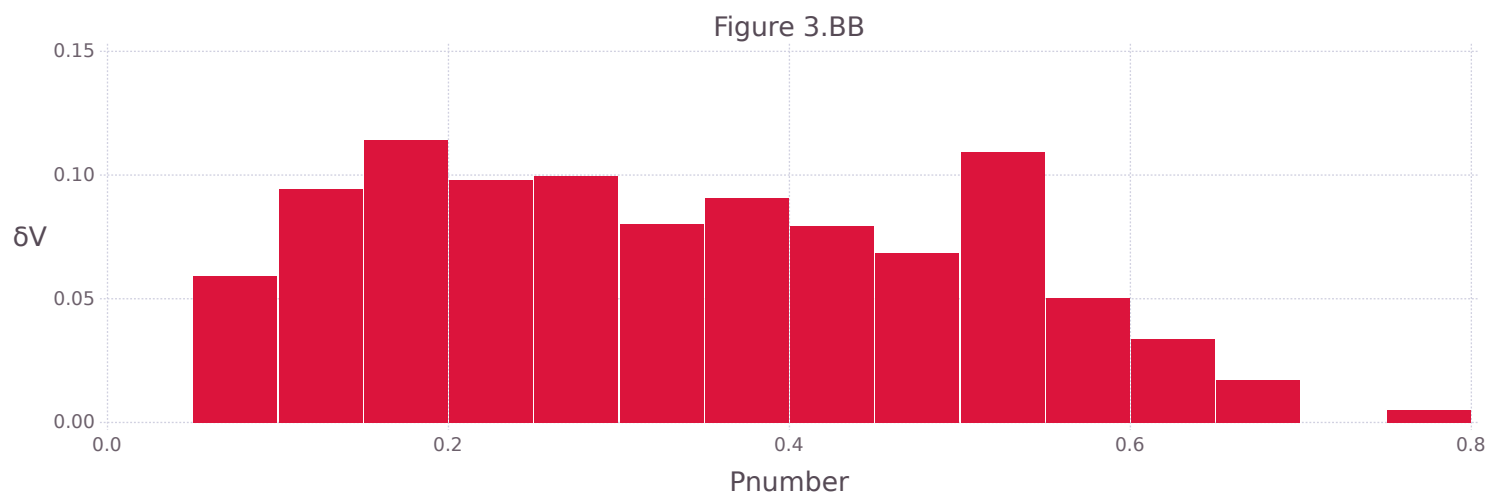


Figure 106. This is an inserted EPS graphic

VG_V can be translated into cartesian coordinates and the module of the *X,Y,Z* coordinates obtained.

87
88

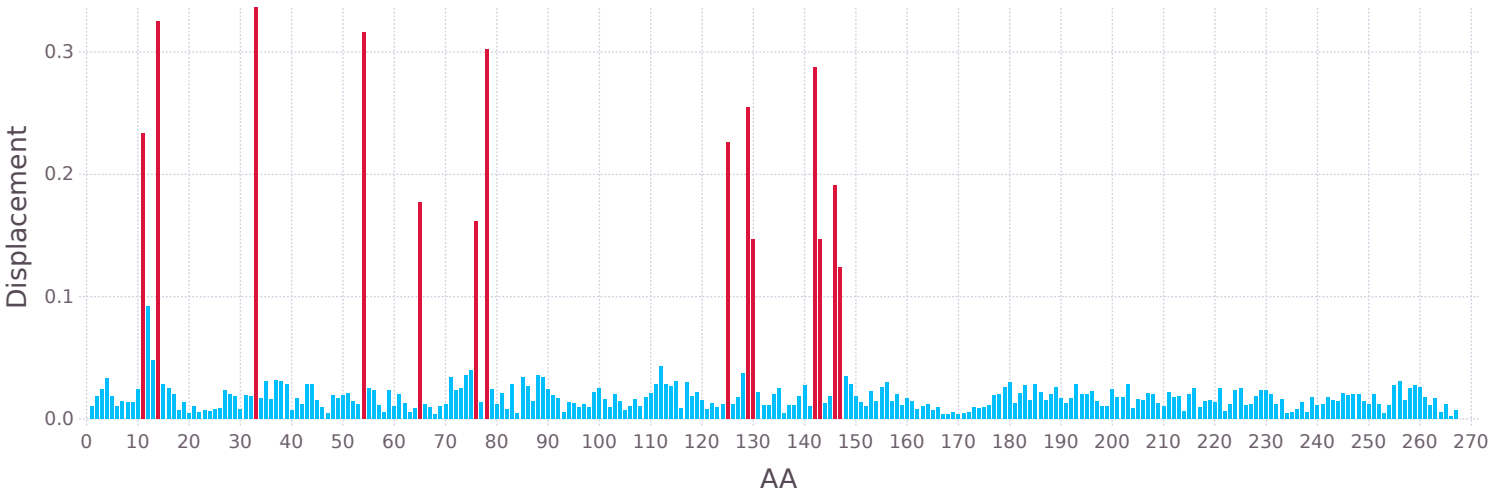


Figure 107. This is an inserted EPS graphic

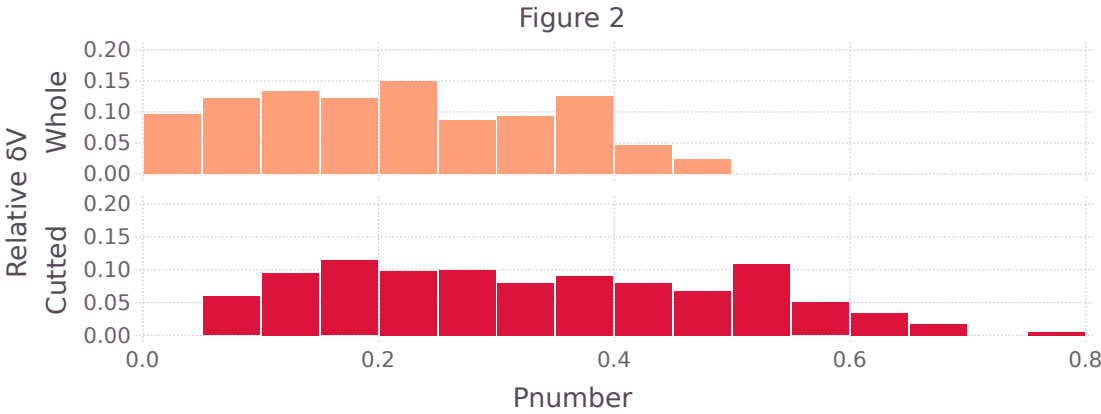


Figure 108. This is an inserted EPS graphic

5.4 1M14

89

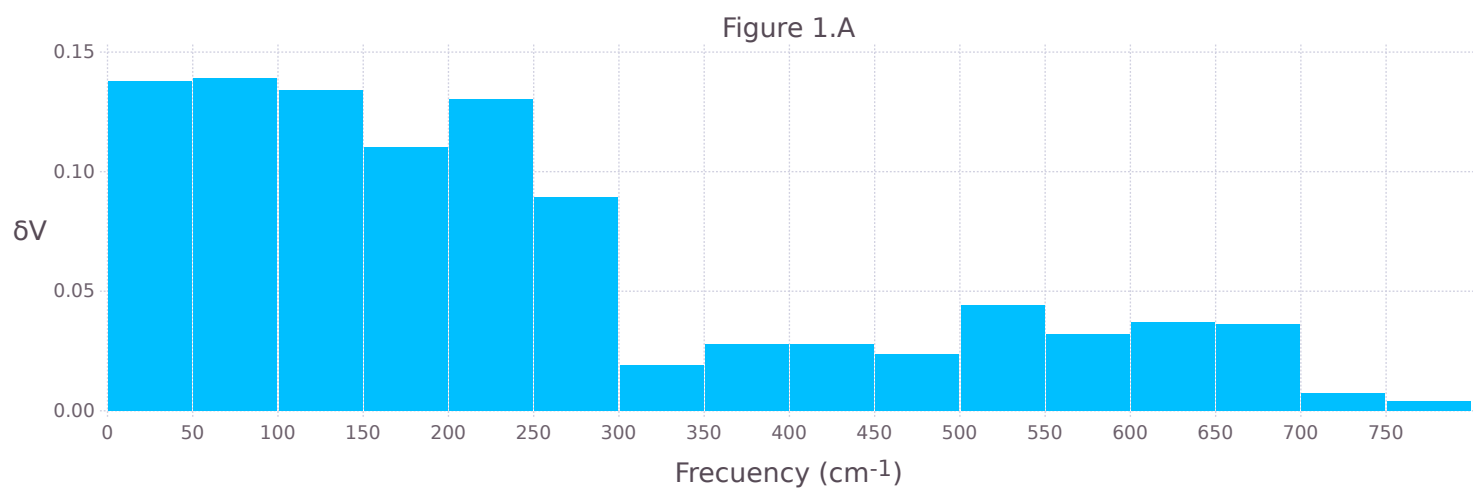


Figure 109. This is an inserted EPS graphic

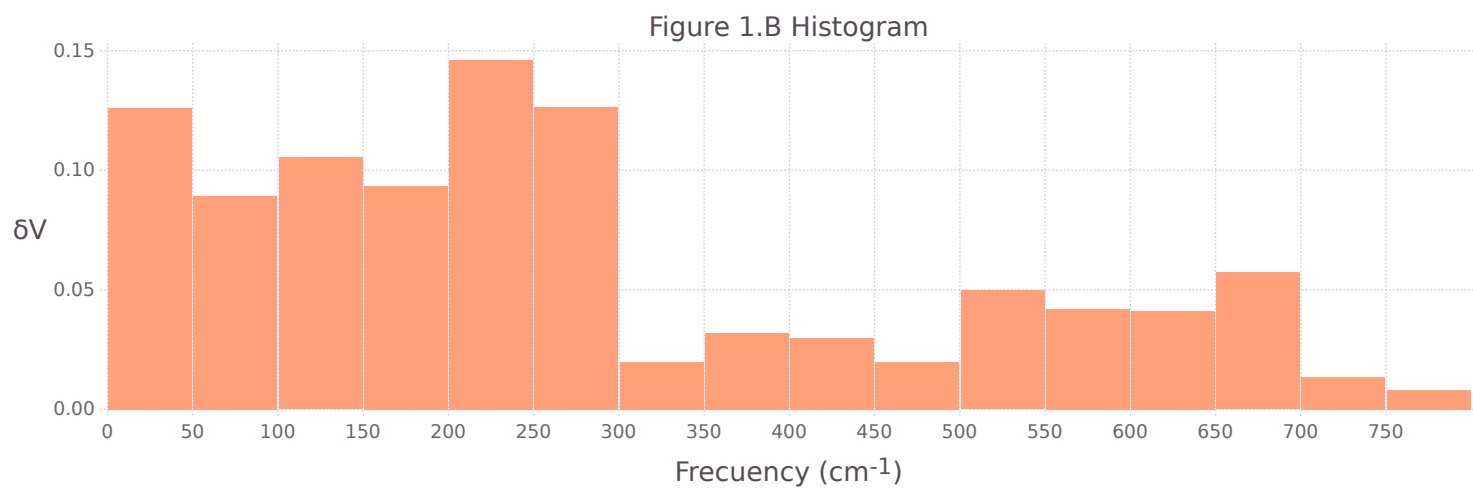


Figure 110. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

90

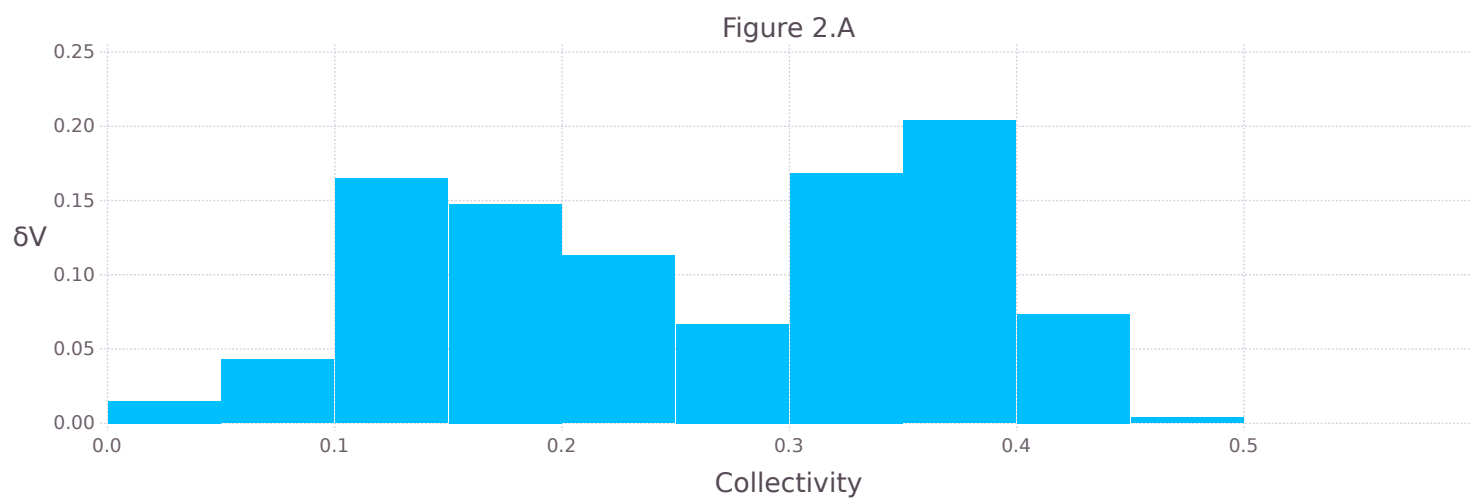


Figure 111. This is an inserted EPS graphic

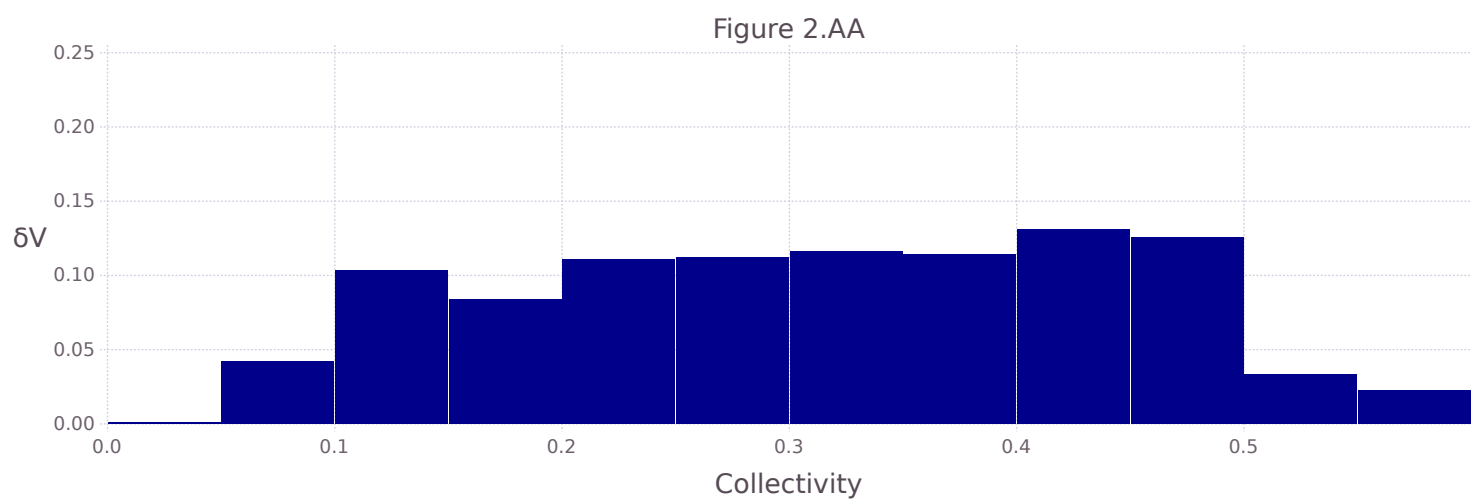


Figure 112. This is an inserted EPS graphic

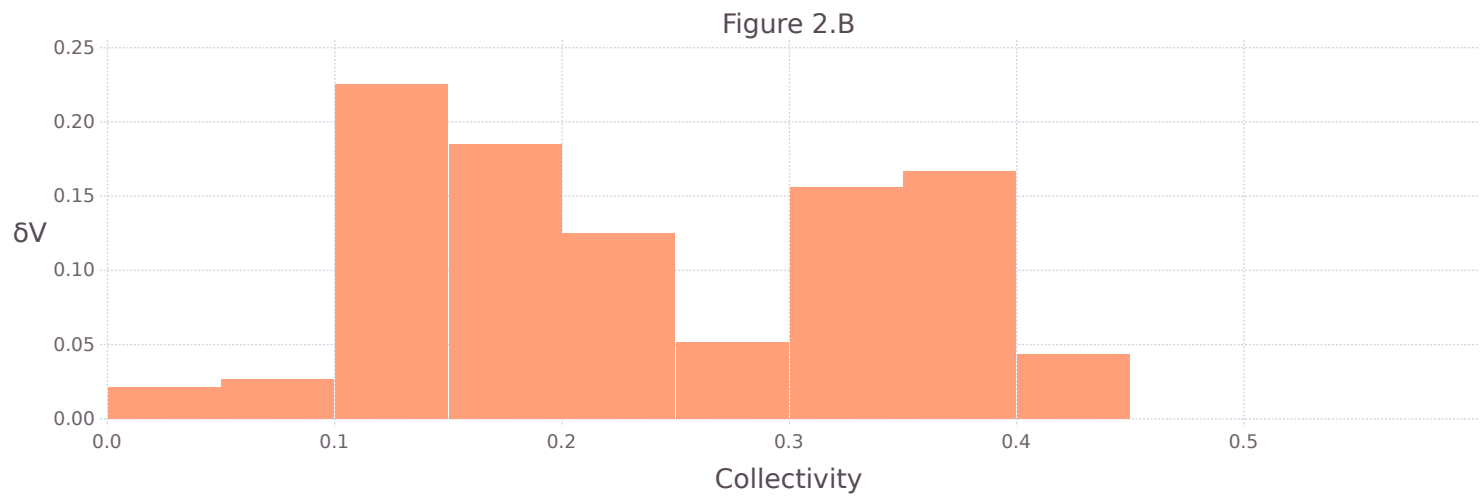


Figure 113. This is an inserted EPS graphic

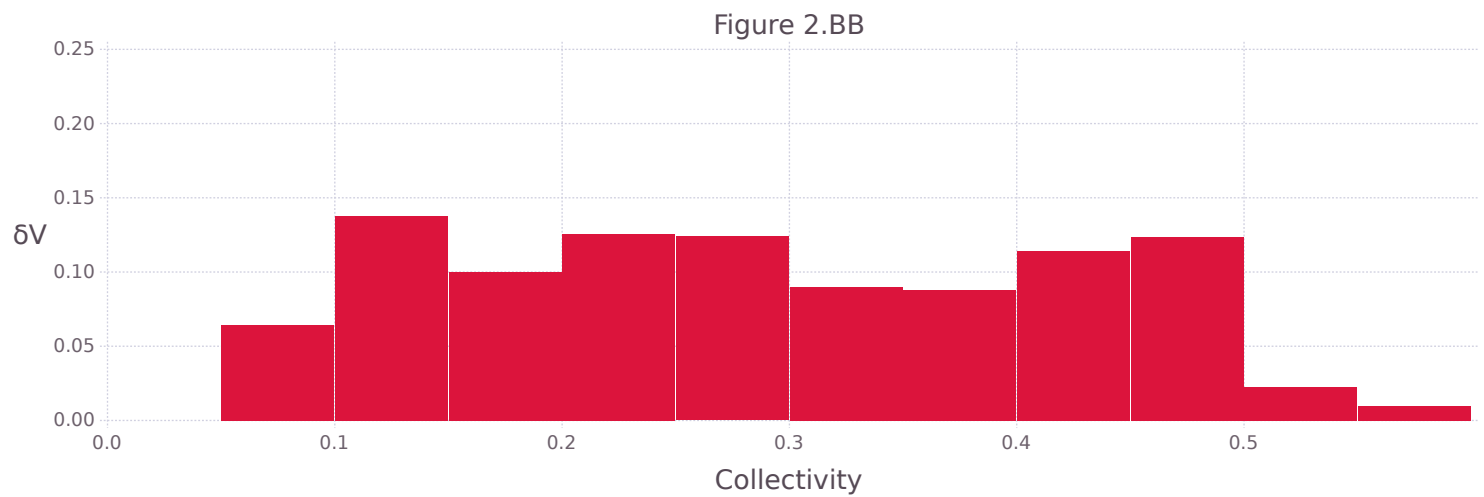


Figure 114. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with the **Participation Number**, as Fig.2 shows.

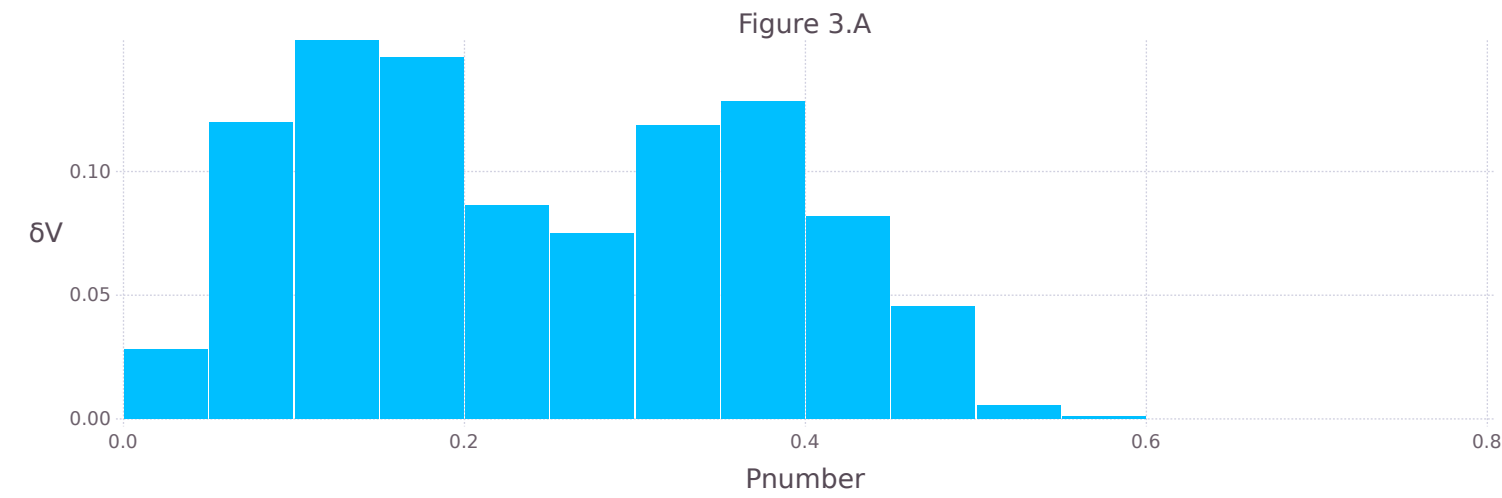


Figure 115. This is an inserted EPS graphic

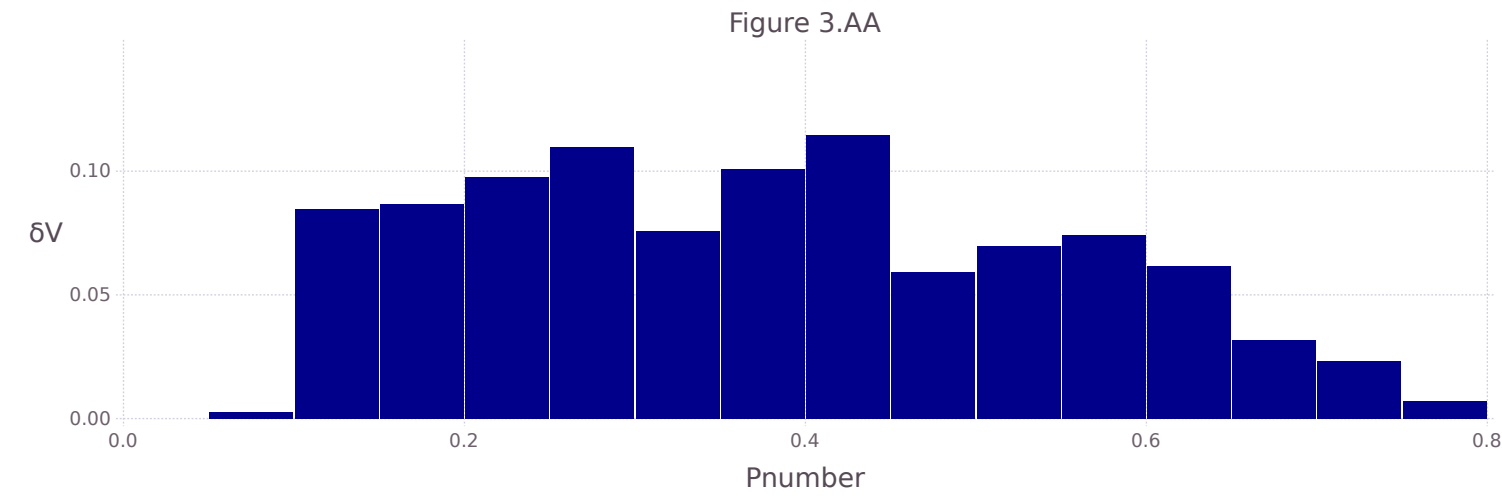


Figure 116. This is an inserted EPS graphic

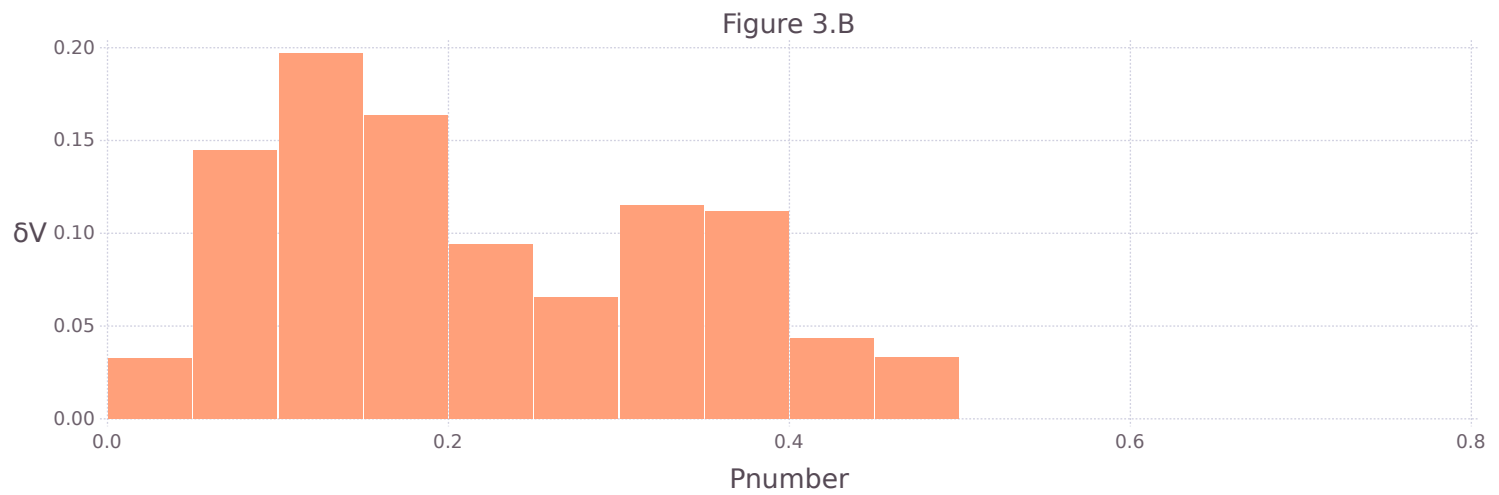


Figure 117. This is an inserted EPS graphic

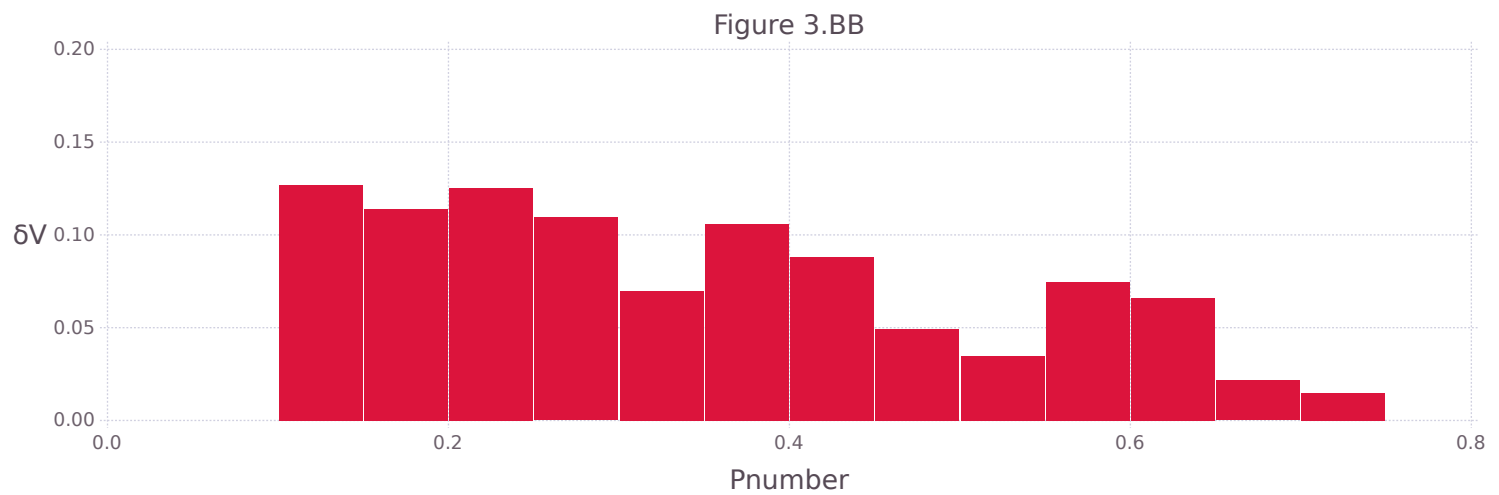


Figure 118. This is an inserted EPS graphic

VGV can be translated into cartesian coordinates and the module of the X, Y, Z coordinates obtained.

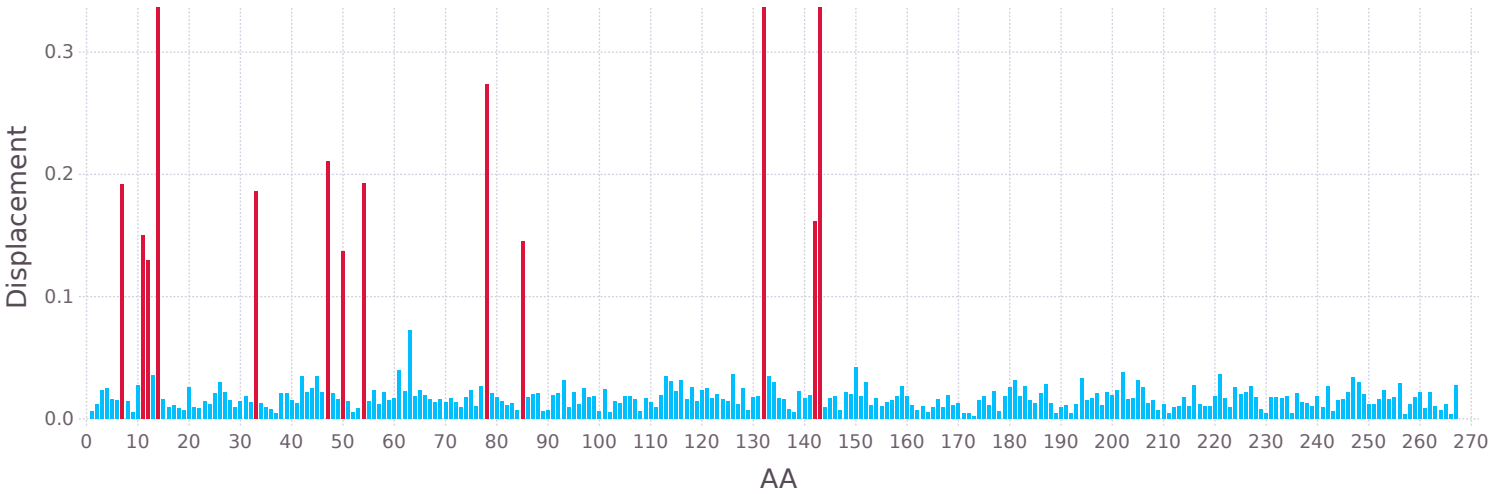


Figure 119. This is an inserted EPS graphic

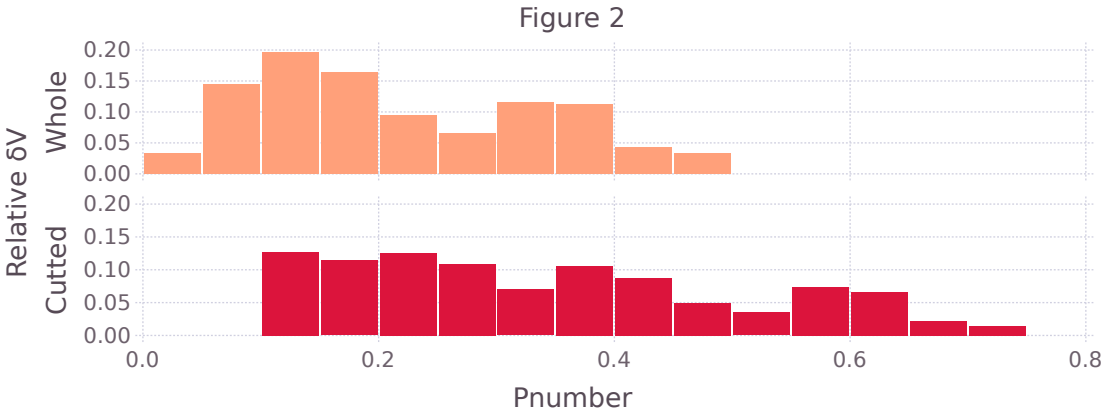


Figure 120. This is an inserted EPS graphic

5.5 1PRN

95

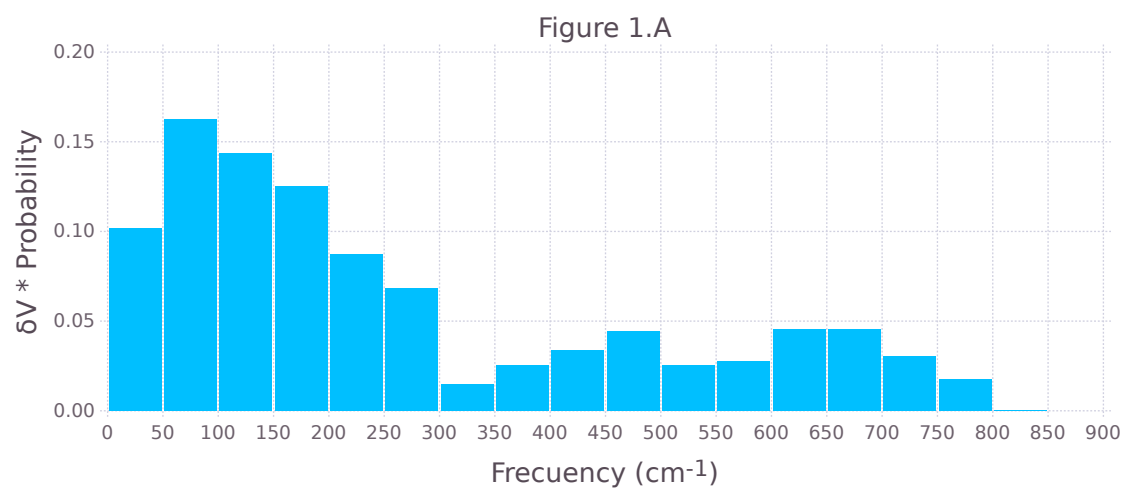


Figure 121. This is an inserted EPS graphic

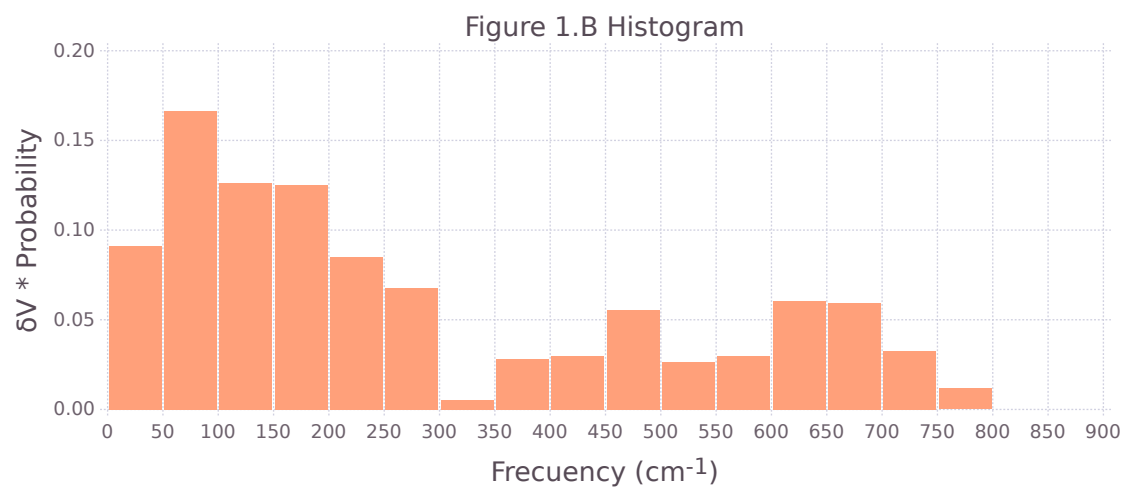


Figure 122. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

96

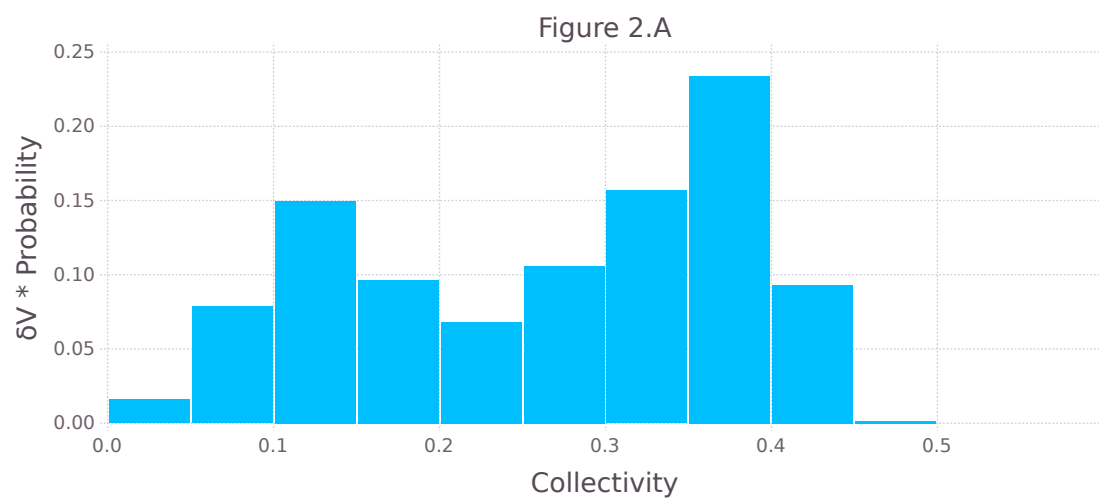


Figure 123. This is an inserted EPS graphic

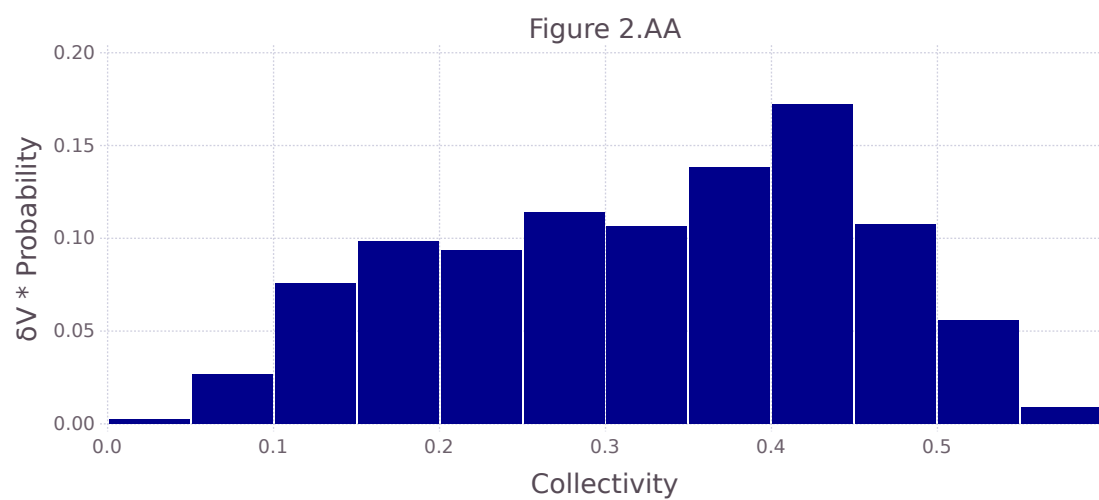


Figure 124. This is an inserted EPS graphic

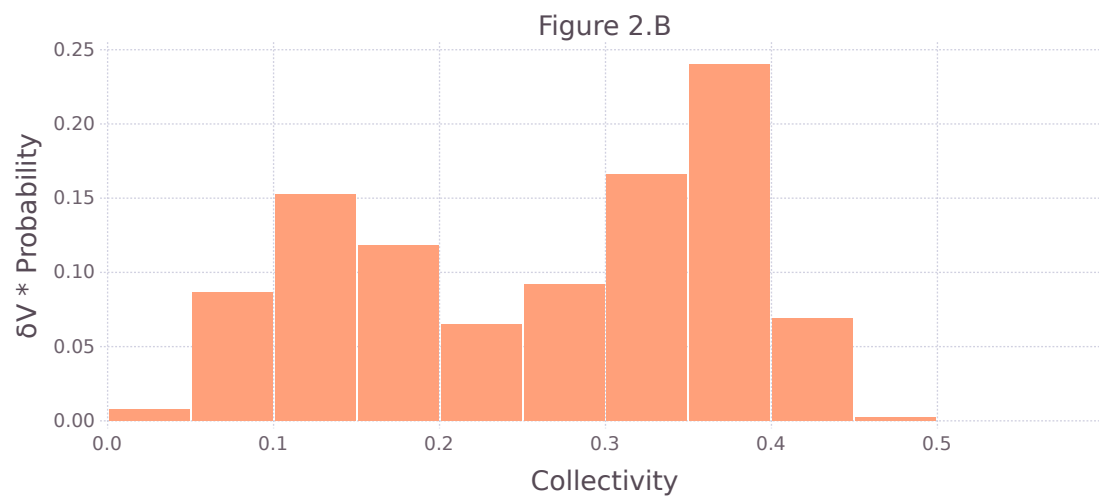


Figure 125. This is an inserted EPS graphic

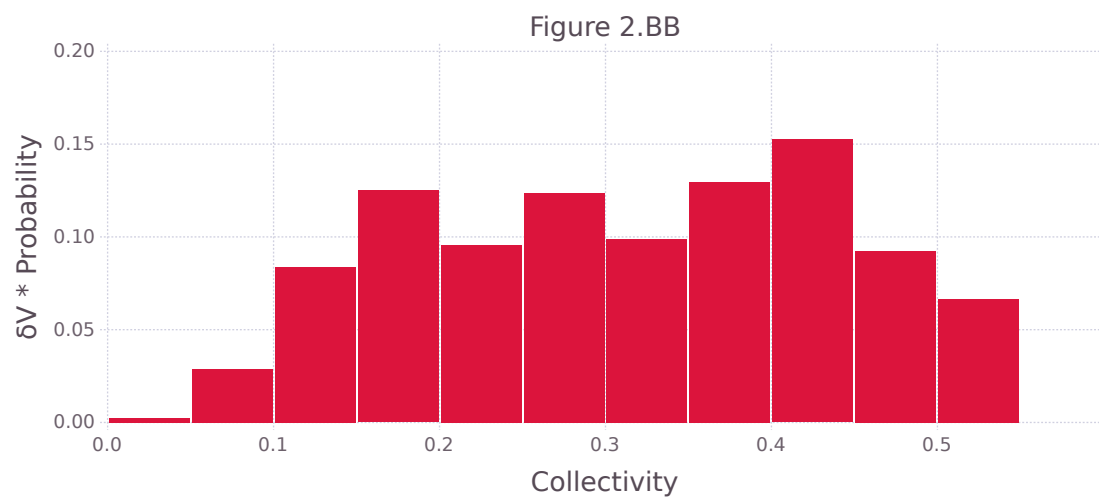


Figure 126. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with the **Participation Number**, as Fig.2 shows.

97
98

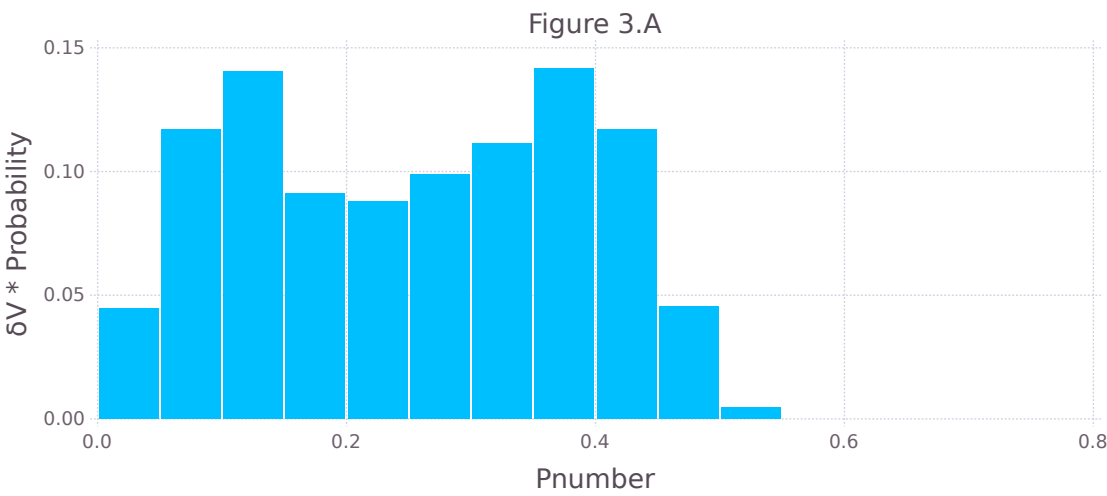


Figure 127. This is an inserted EPS graphic

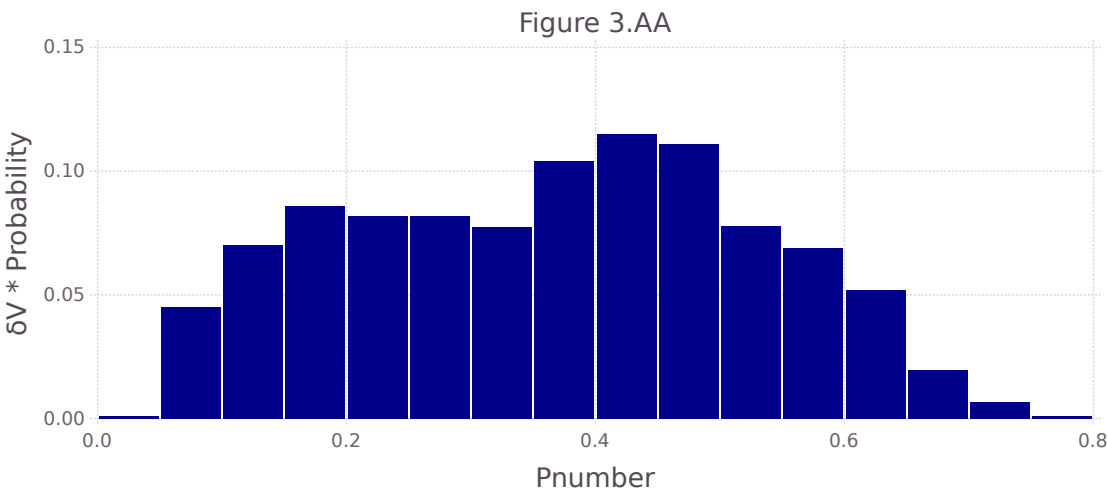


Figure 128. This is an inserted EPS graphic

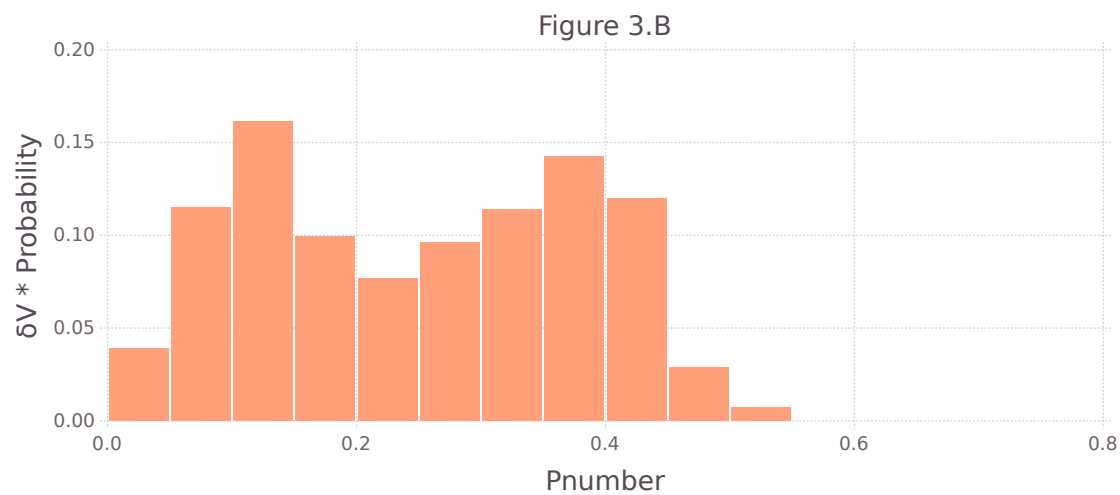


Figure 129. This is an inserted EPS graphic

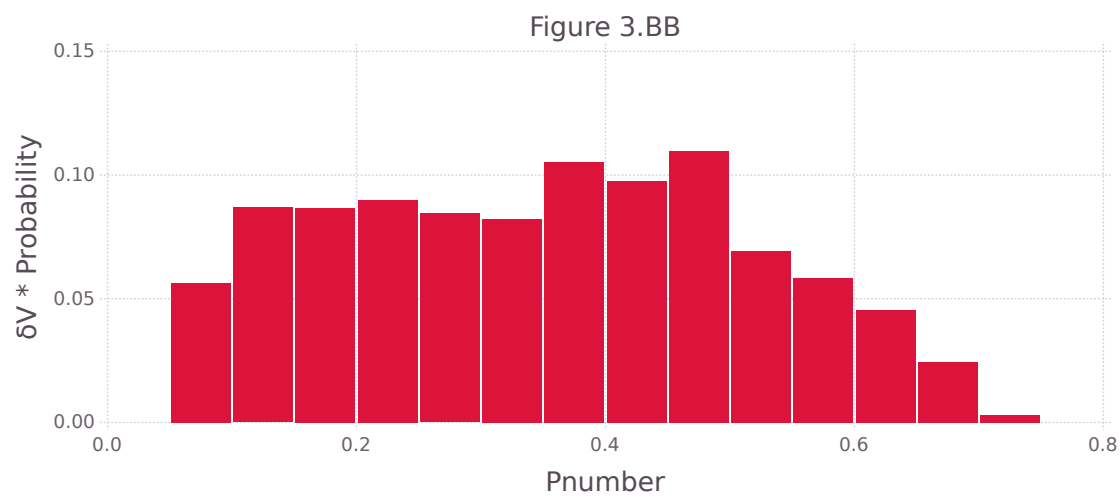


Figure 130. This is an inserted EPS graphic

VG_V can be translated into cartesian coordinates and the module of the X, Y, Z coordinates obtained.

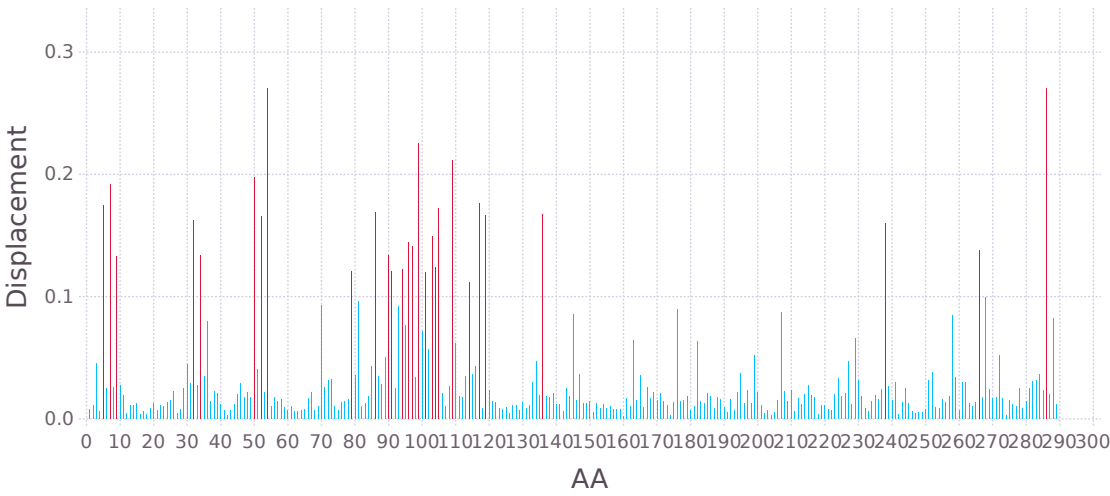


Figure 131. This is an inserted EPS graphic

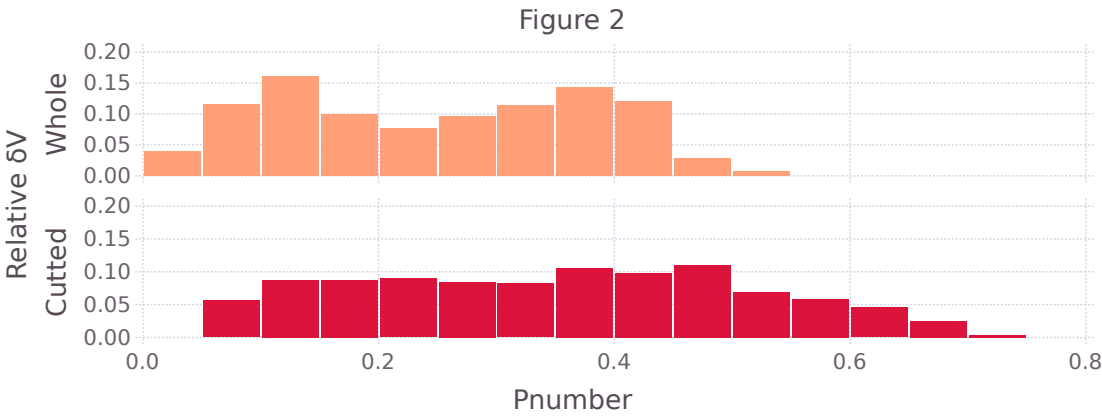


Figure 132. This is an inserted EPS graphic

5.6 256L

101

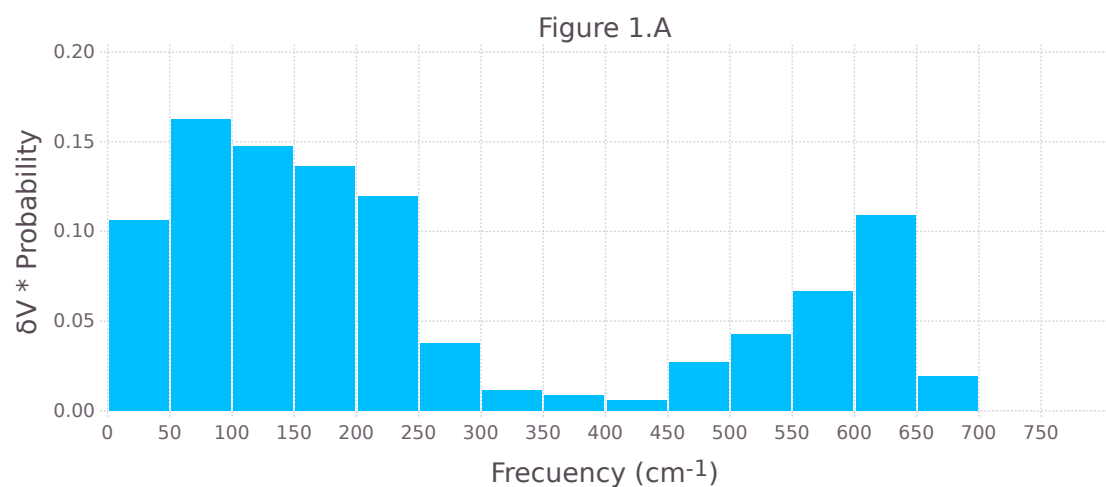


Figure 133. This is an inserted EPS graphic

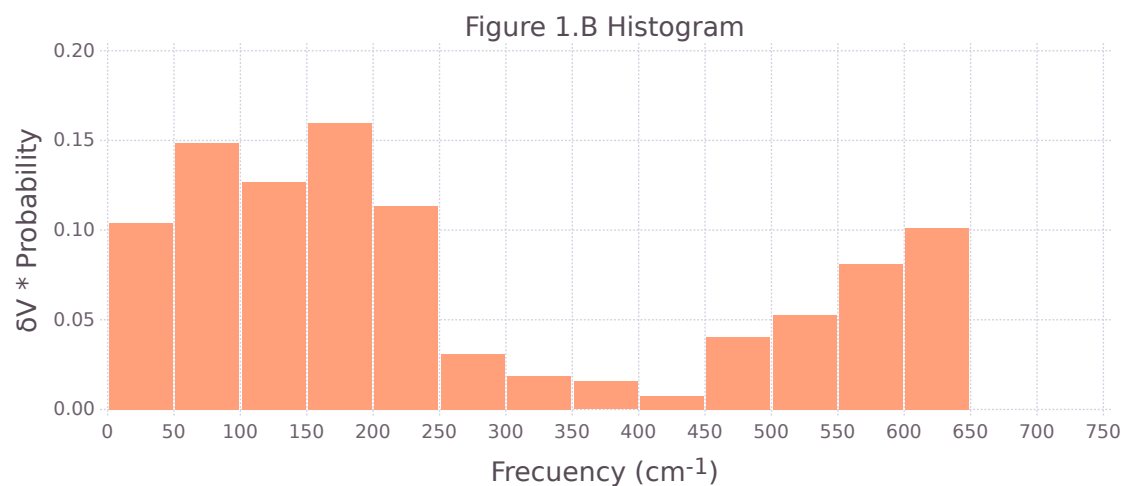


Figure 134. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

102

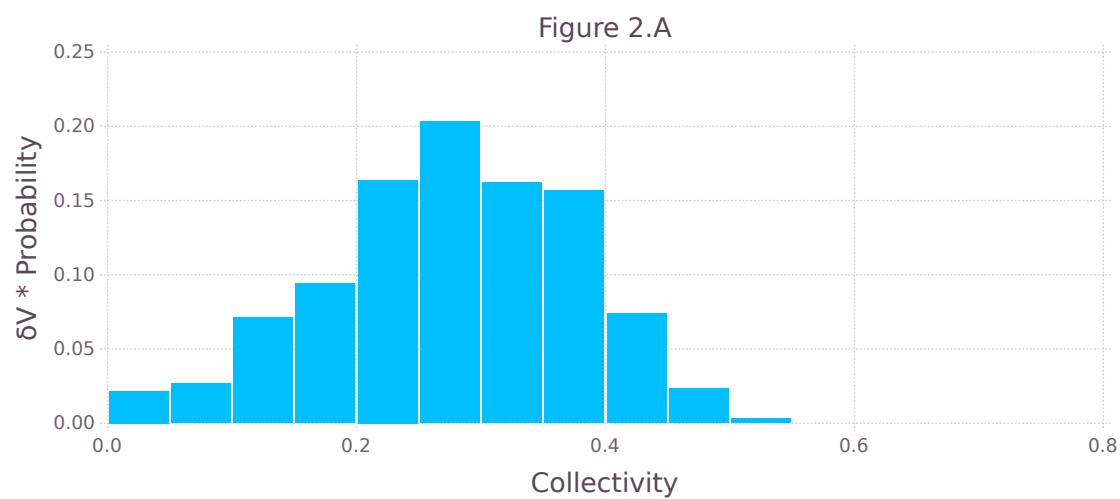


Figure 135. This is an inserted EPS graphic

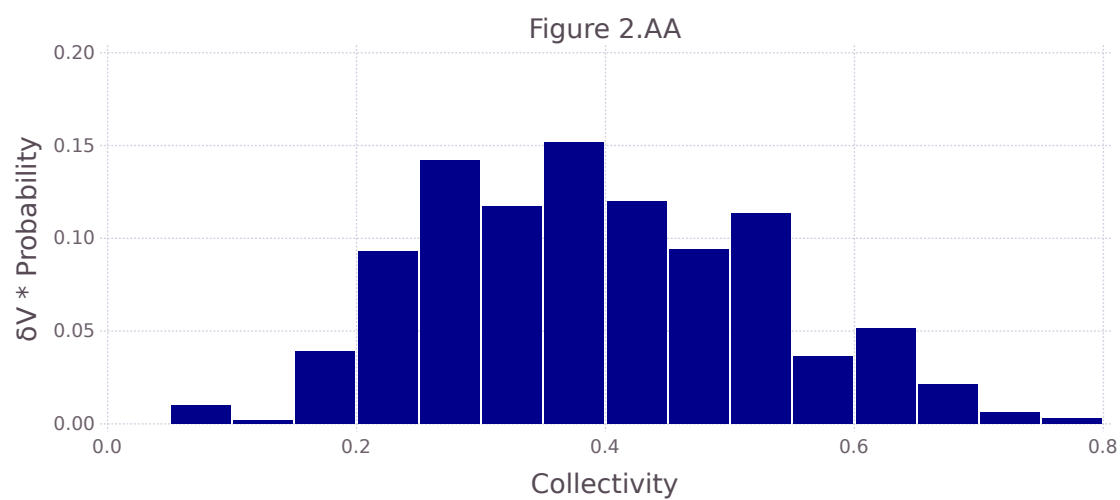


Figure 136. This is an inserted EPS graphic

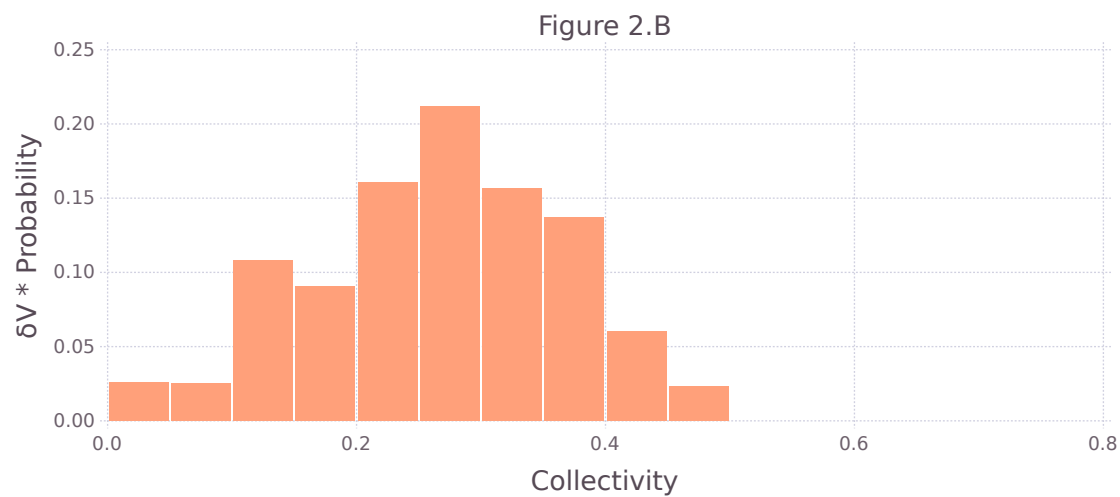


Figure 137. This is an inserted EPS graphic

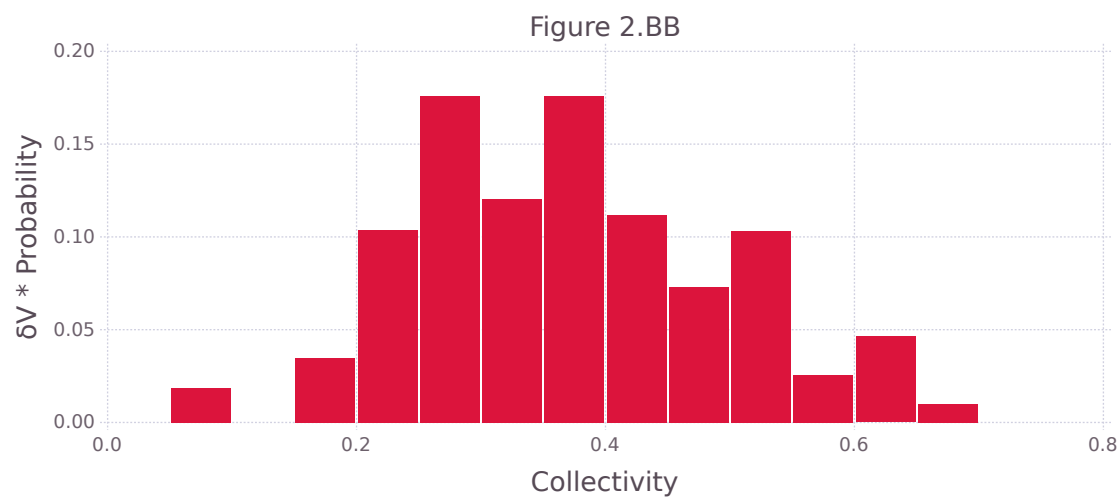


Figure 138. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with the **Participation Number**, as Fig.2 shows.

103
104

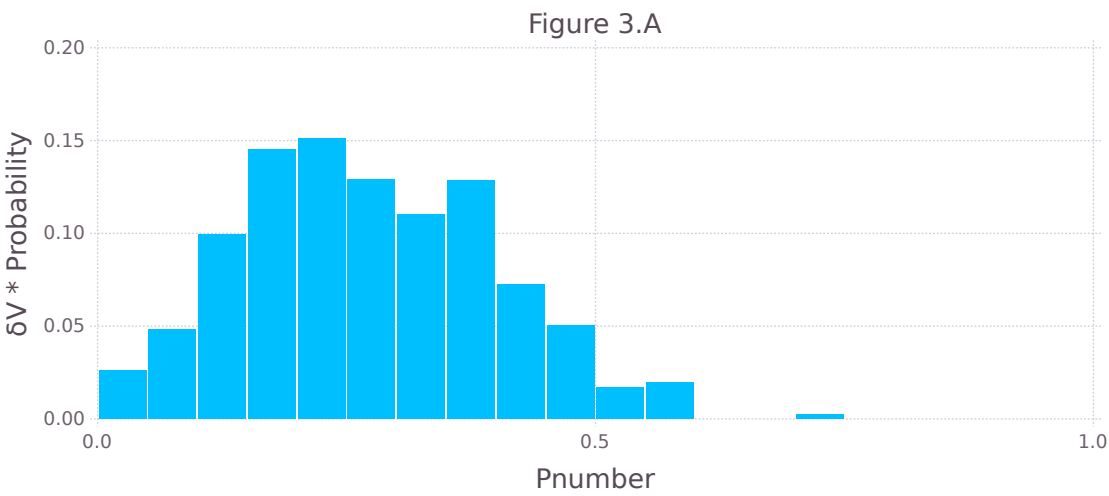


Figure 139. This is an inserted EPS graphic

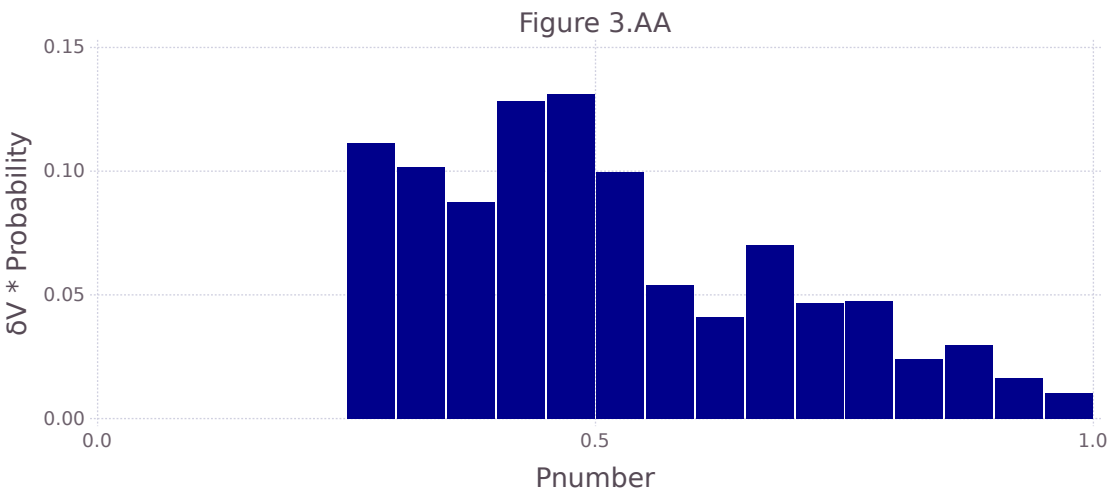


Figure 140. This is an inserted EPS graphic

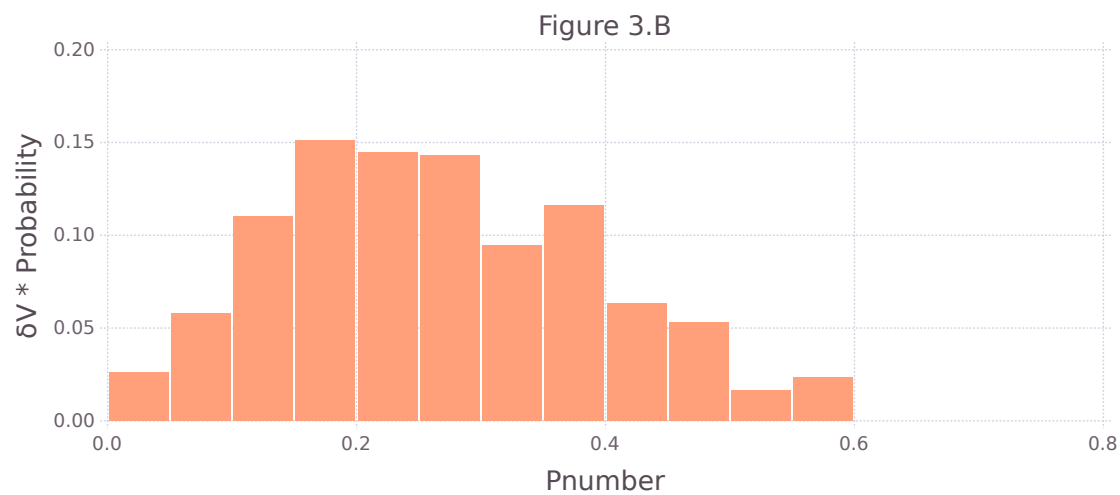


Figure 141. This is an inserted EPS graphic

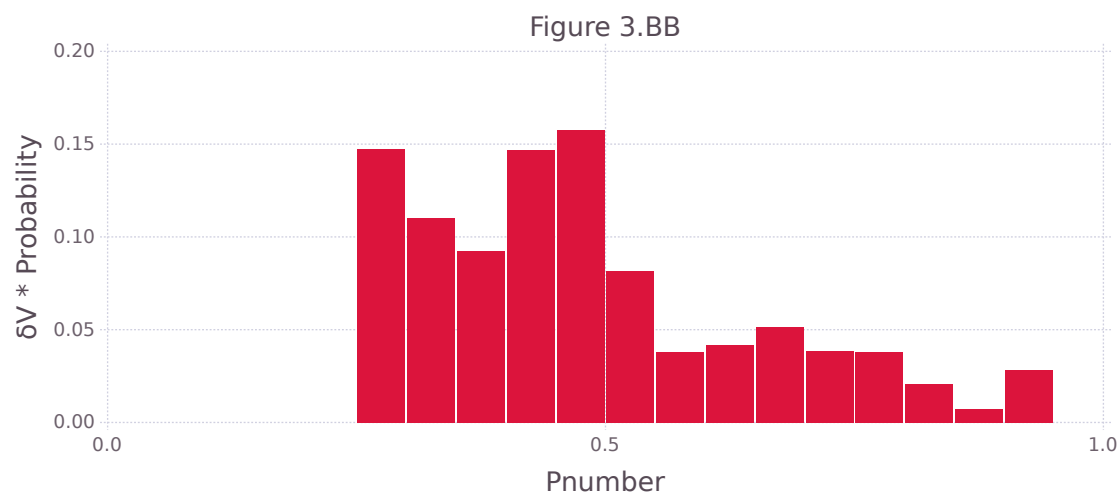


Figure 142. This is an inserted EPS graphic

VG_V can be translated into cartesian coordinates and the module of the X, Y, Z coordinates obtained.

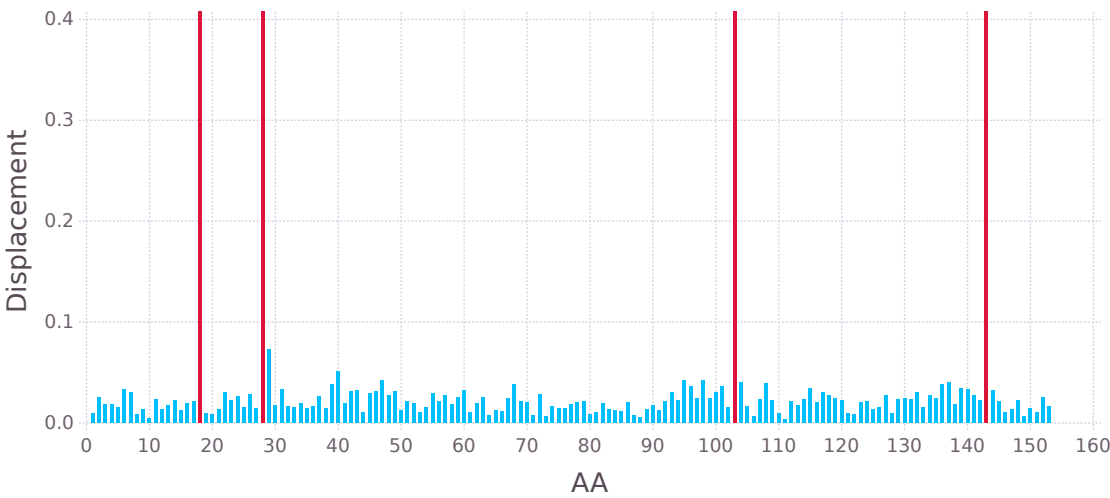


Figure 143. This is an inserted EPS graphic

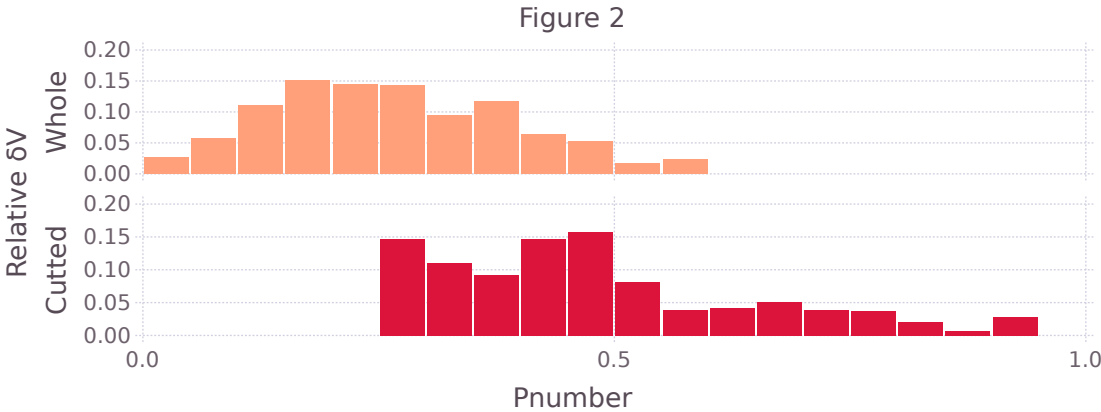


Figure 144. This is an inserted EPS graphic

6 Results VERY HI PRECISION

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6.1 1HVR_APO

108

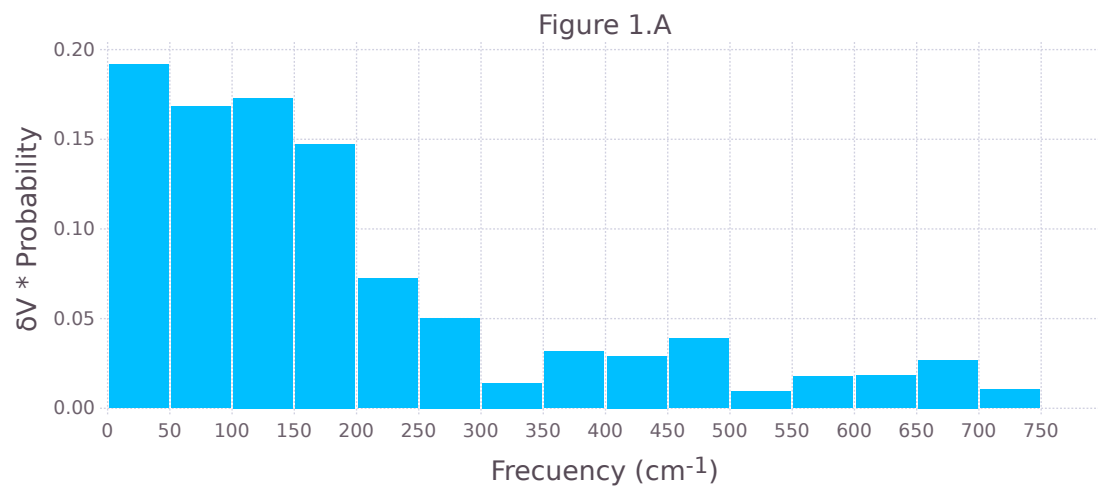


Figure 145. This is an inserted EPS graphic

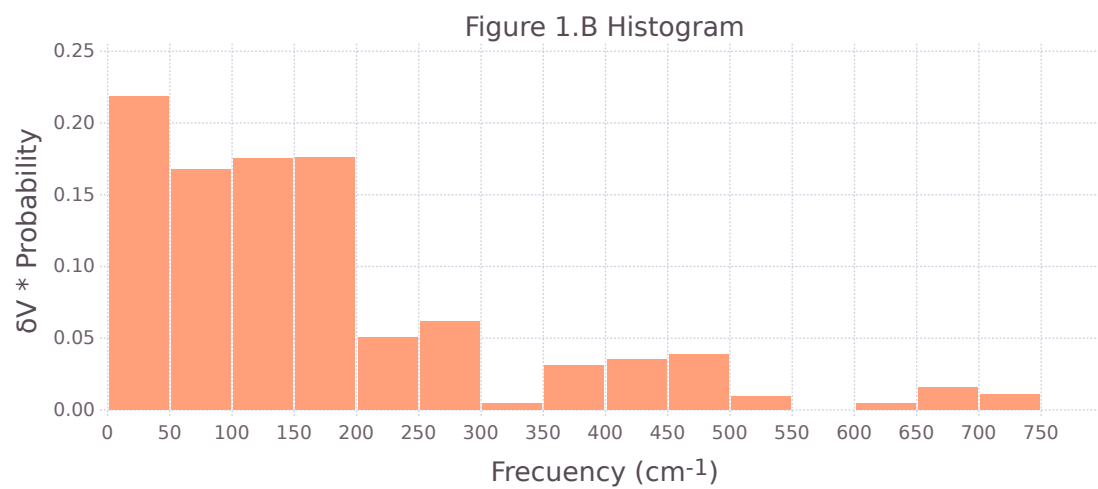


Figure 146. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

109

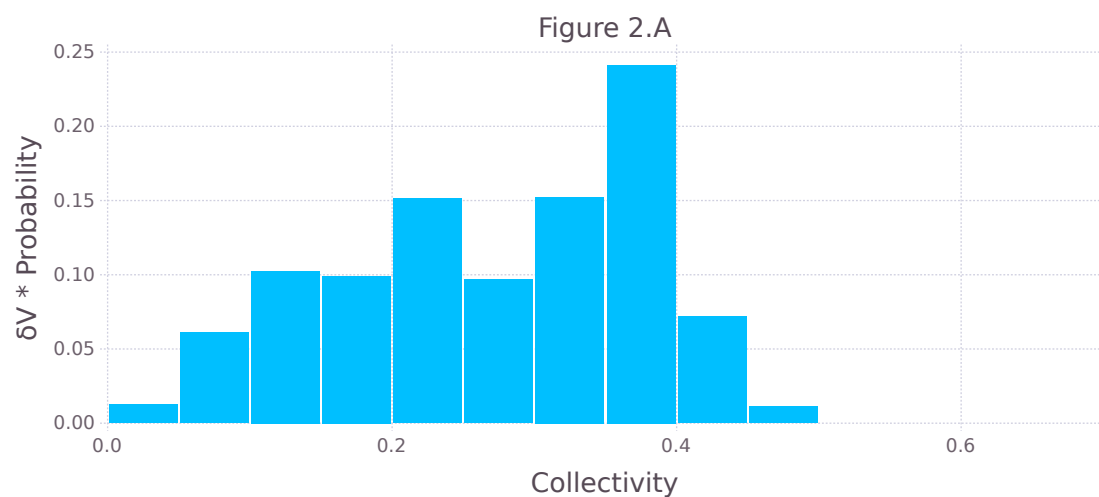


Figure 147. This is an inserted EPS graphic

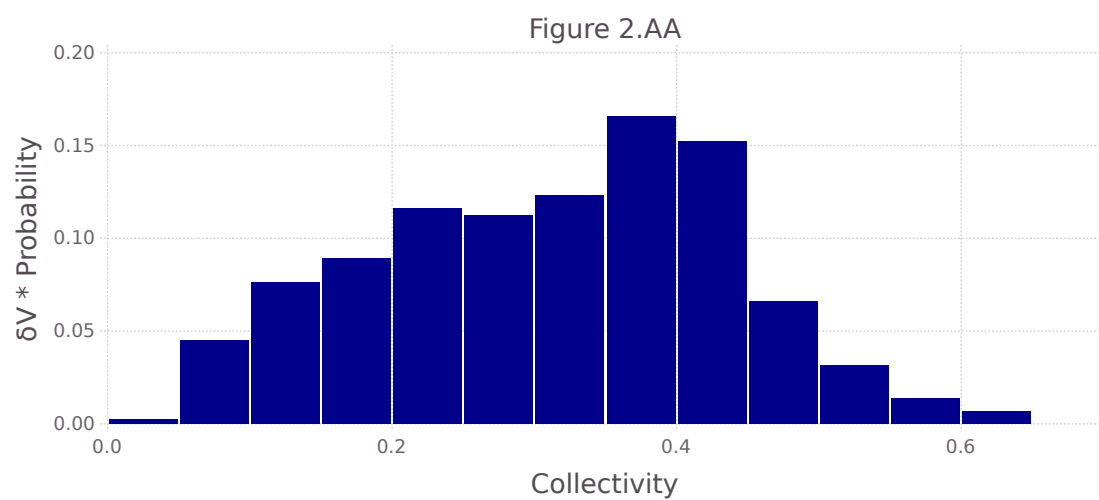


Figure 148. This is an inserted EPS graphic

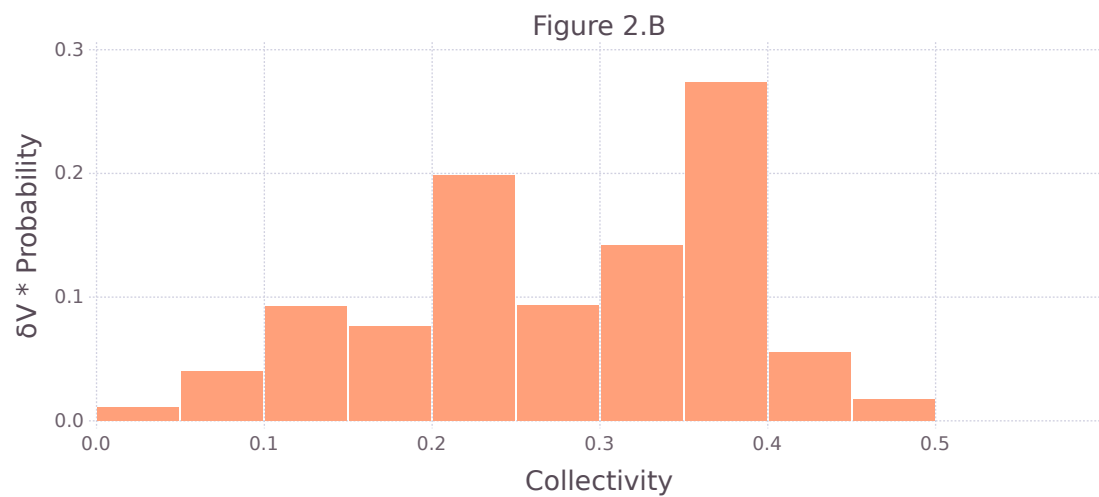


Figure 149. This is an inserted EPS graphic

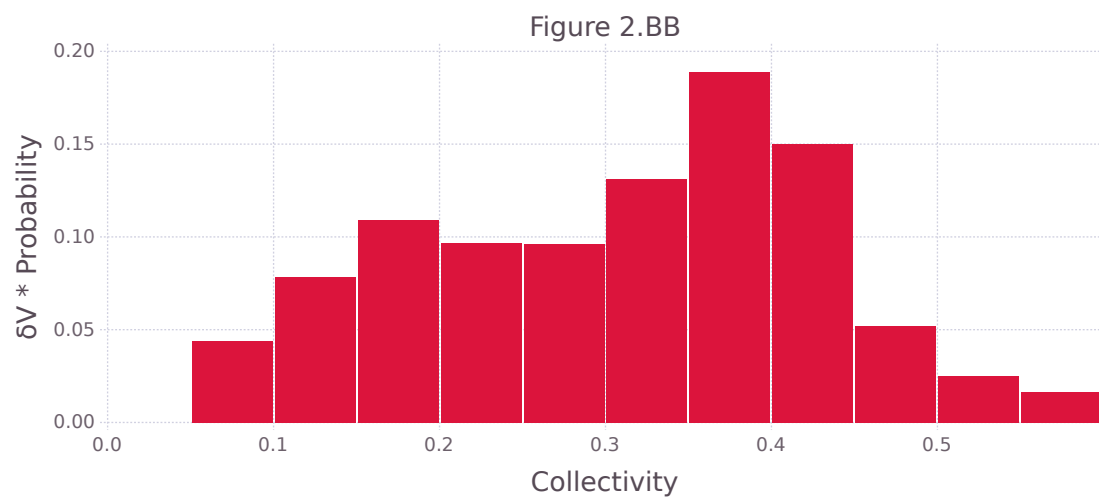


Figure 150. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with the **Participation Number**, as Fig.2 shows.

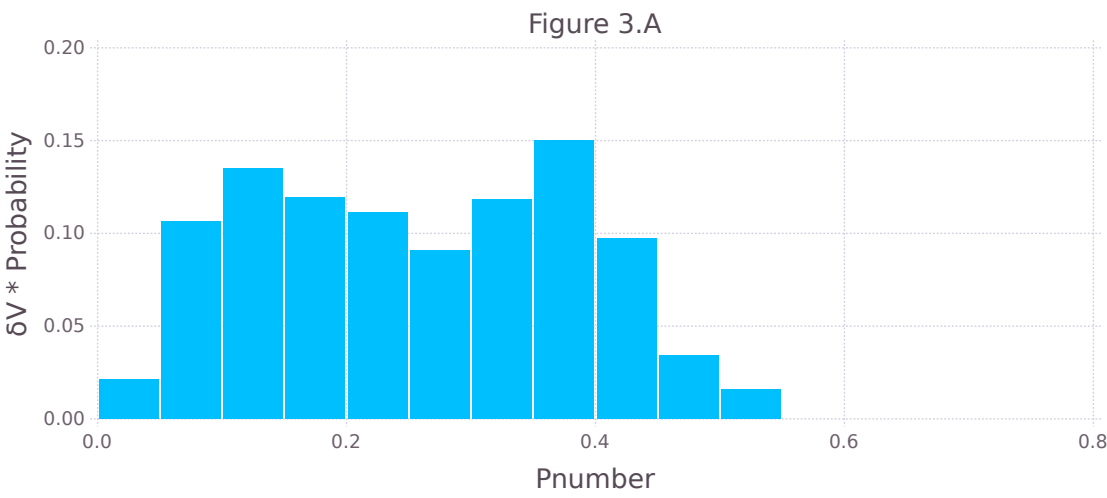


Figure 151. This is an inserted EPS graphic

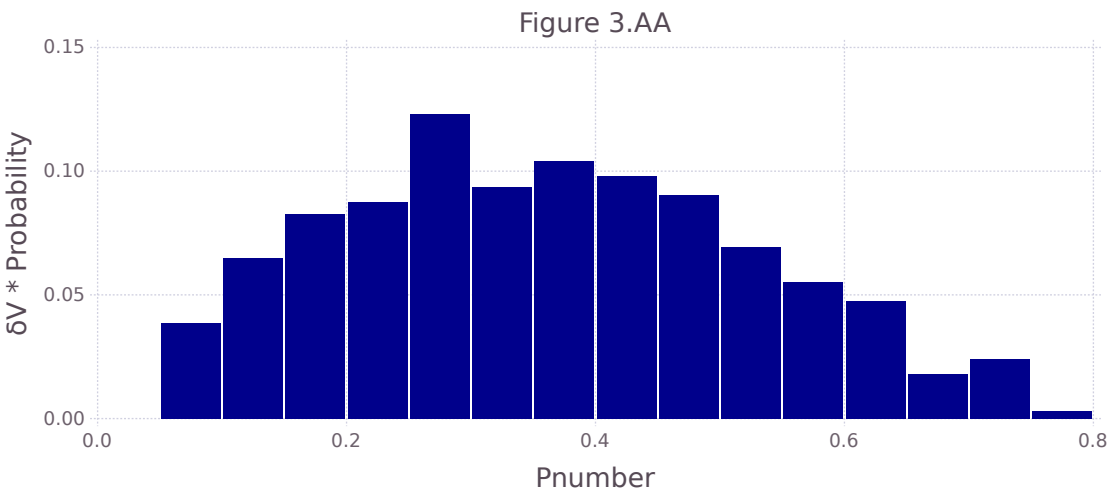


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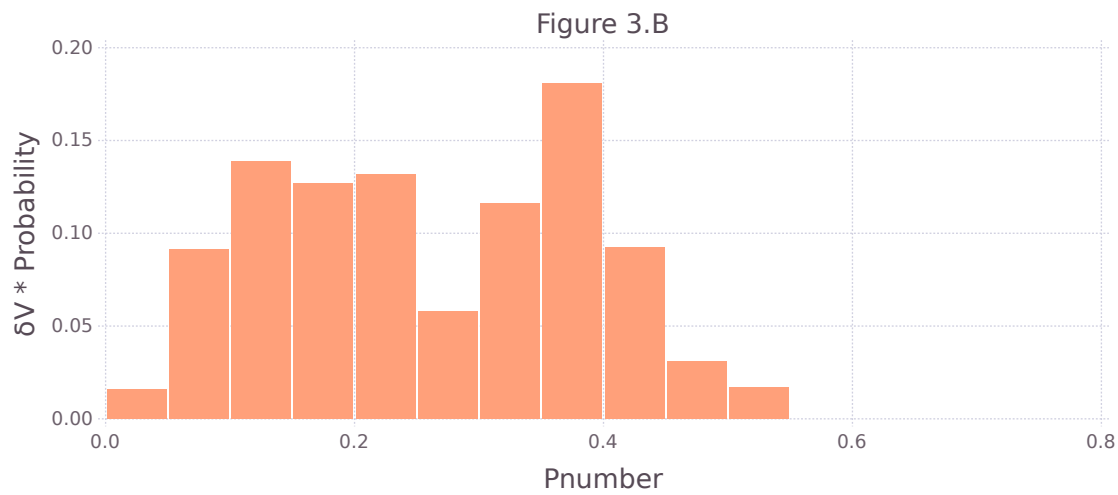


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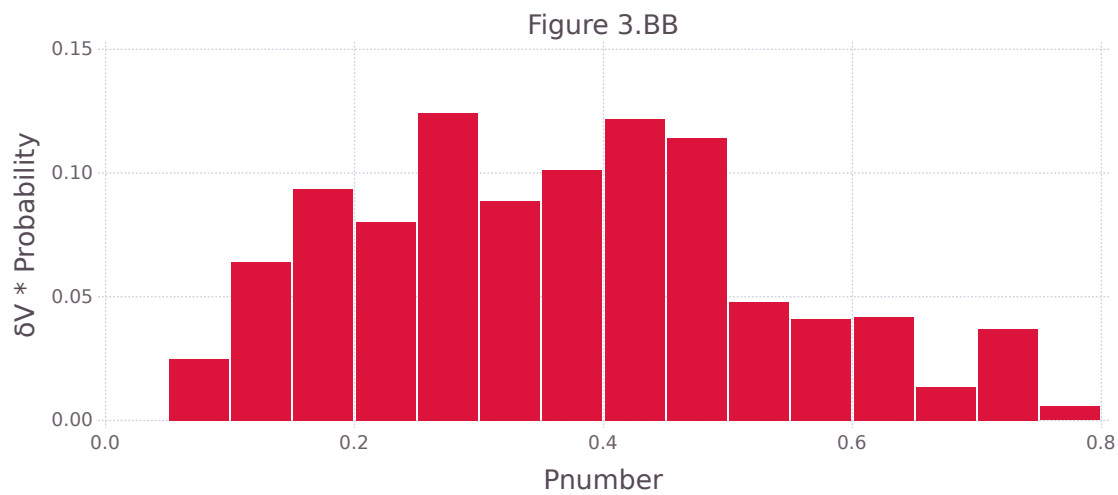


Figure 154. This is an inserted EPS graphic

VG_V can be translated into cartesian coordinates and the module of the X,Y,Z coordinates obtained.

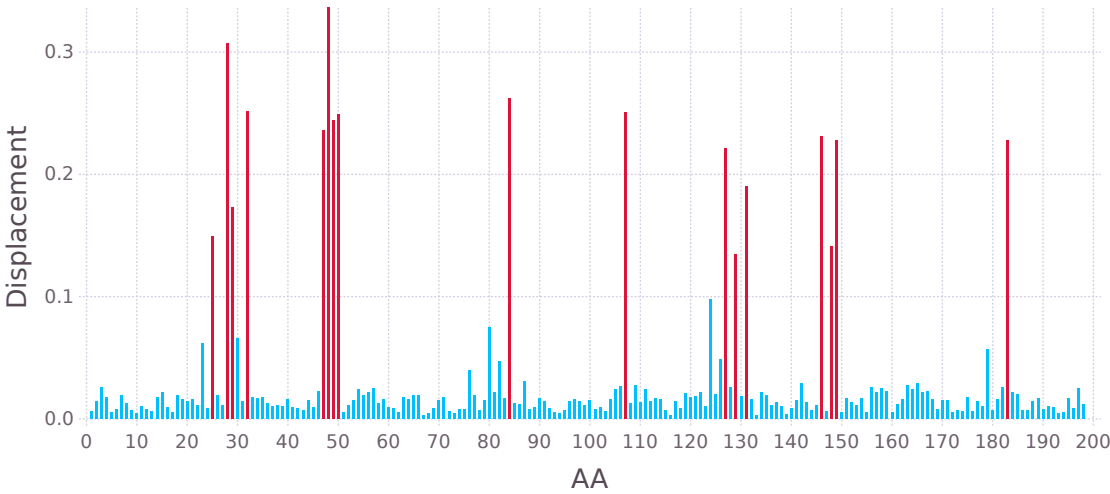


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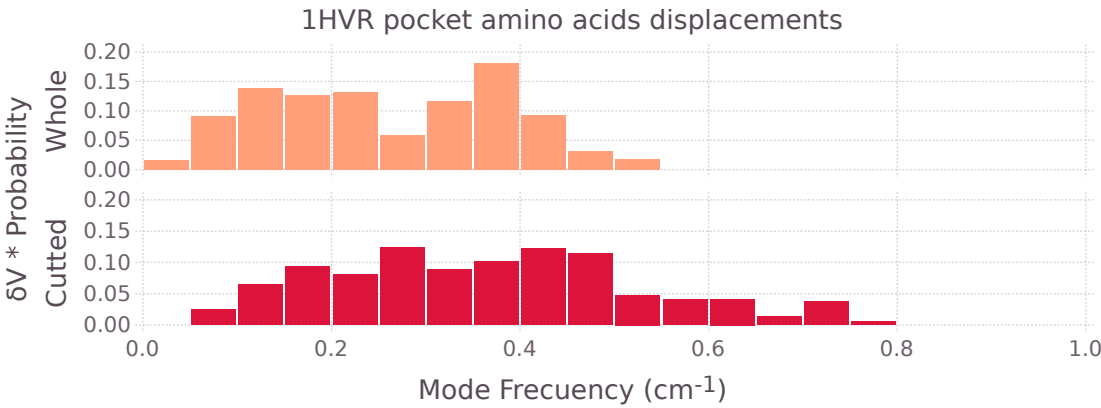


Figure 156. This is an inserted EPS graphic

6.2 1HVR_HOLO

114

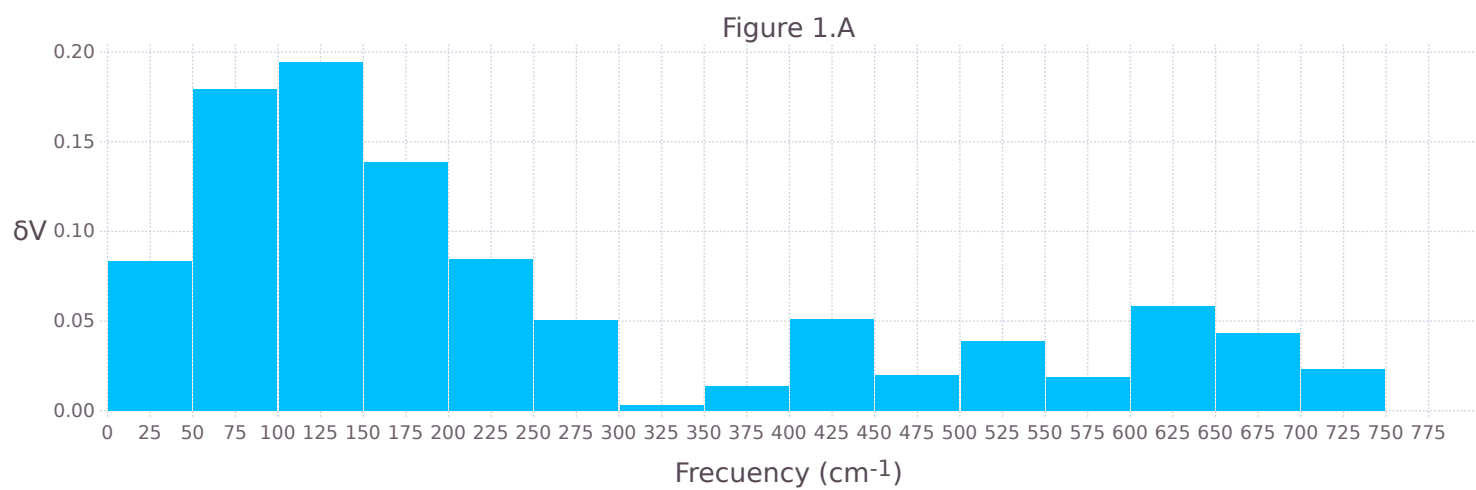


Figure 157. This is an inserted EPS graphic

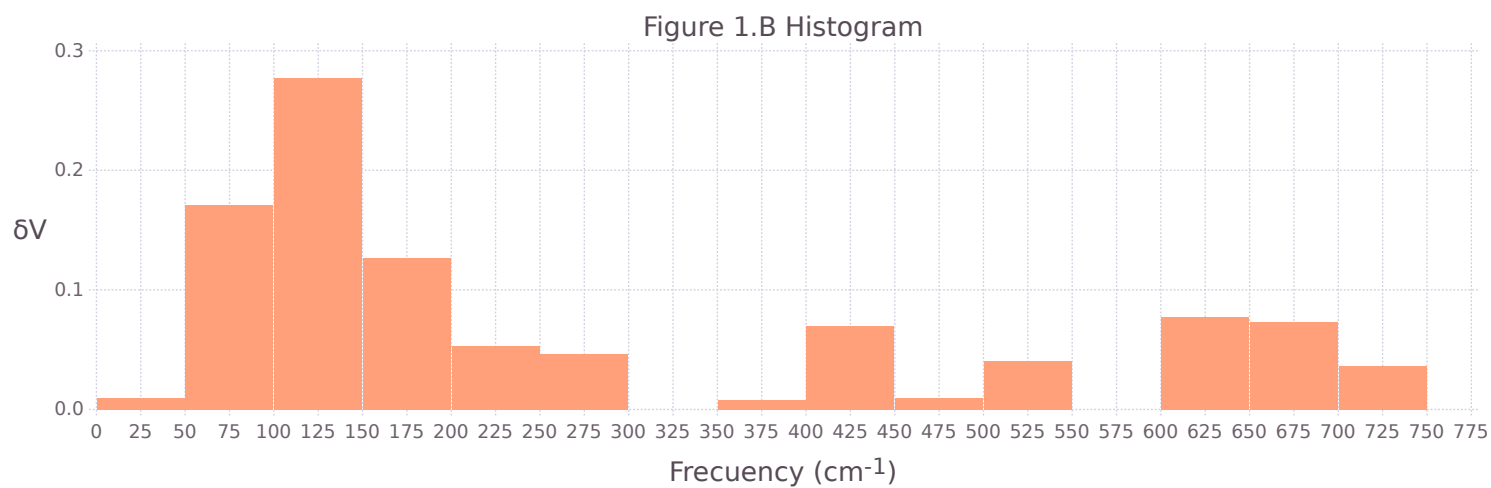


Figure 158. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

115

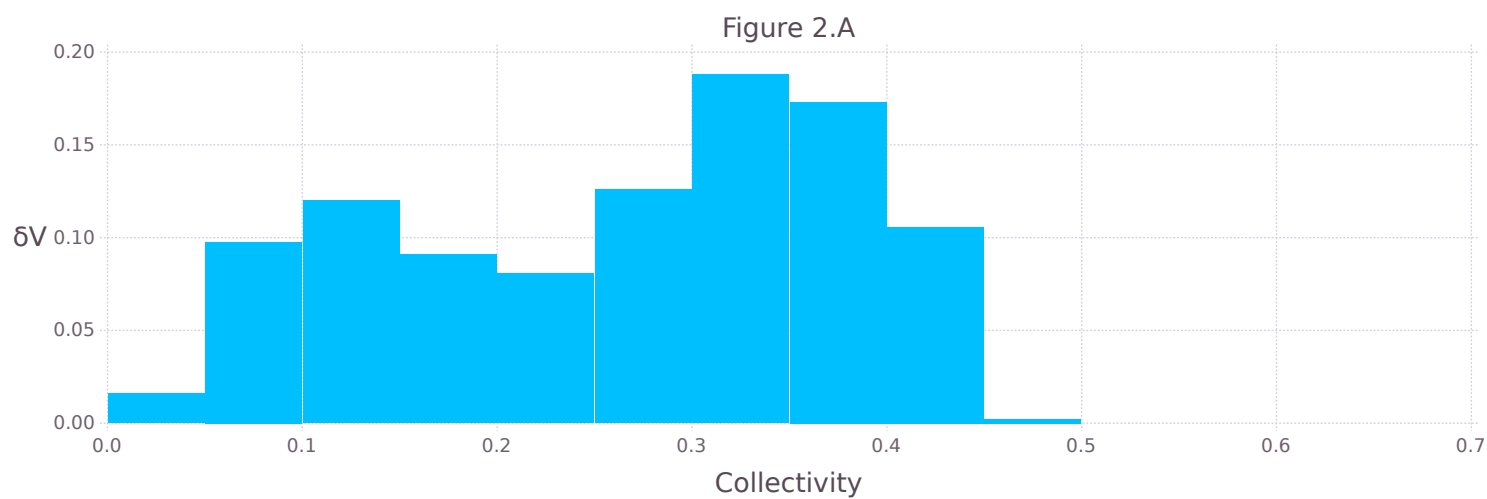


Figure 159. This is an inserted EPS graphic

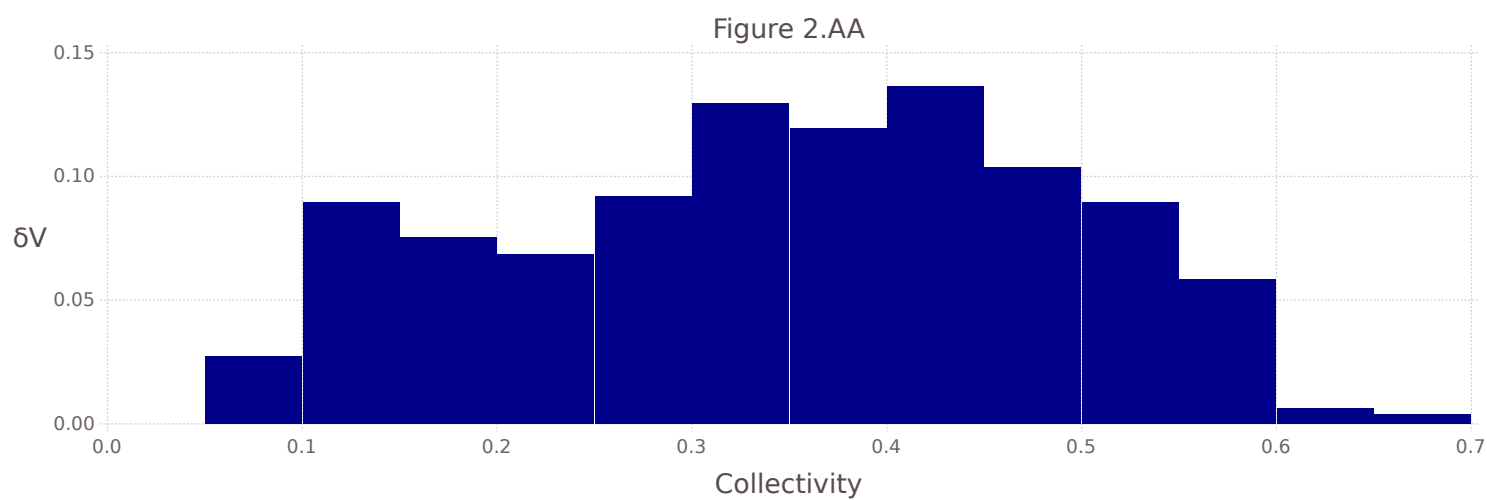


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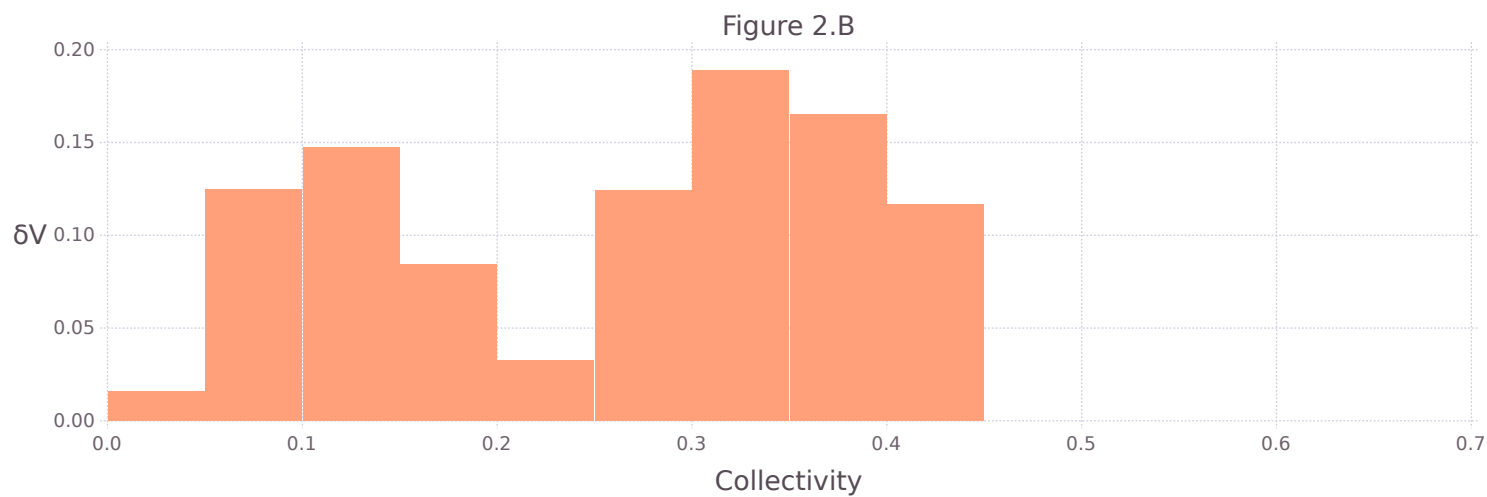


Figure 161. This is an inserted EPS graphic

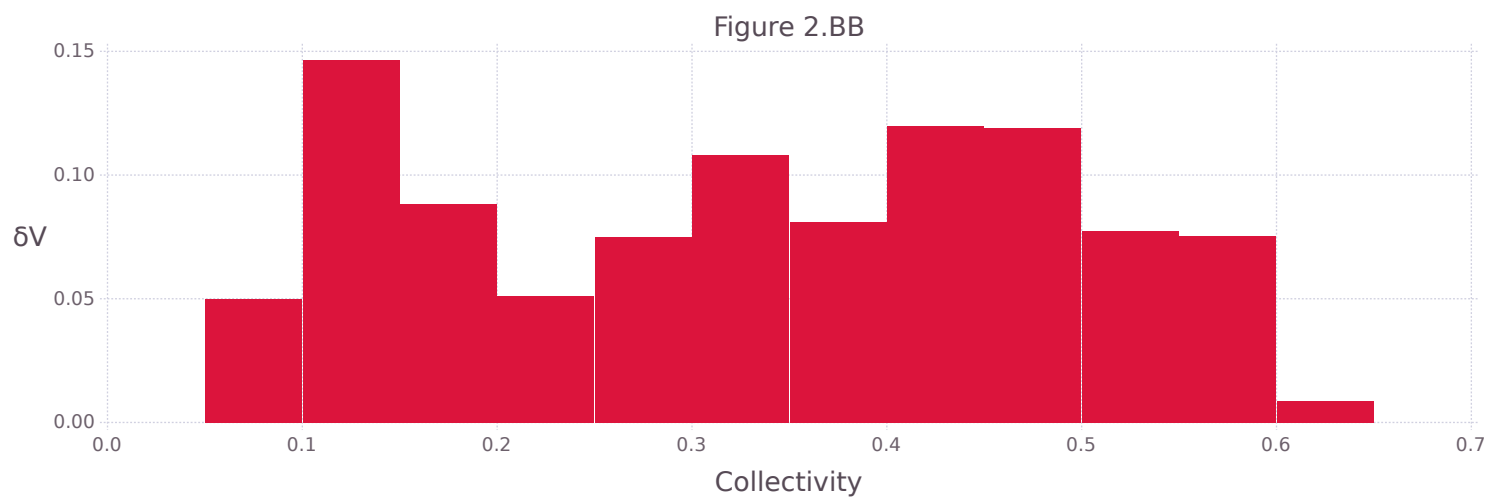


Figure 162. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with the **Participation Number**, as Fig.2 shows.

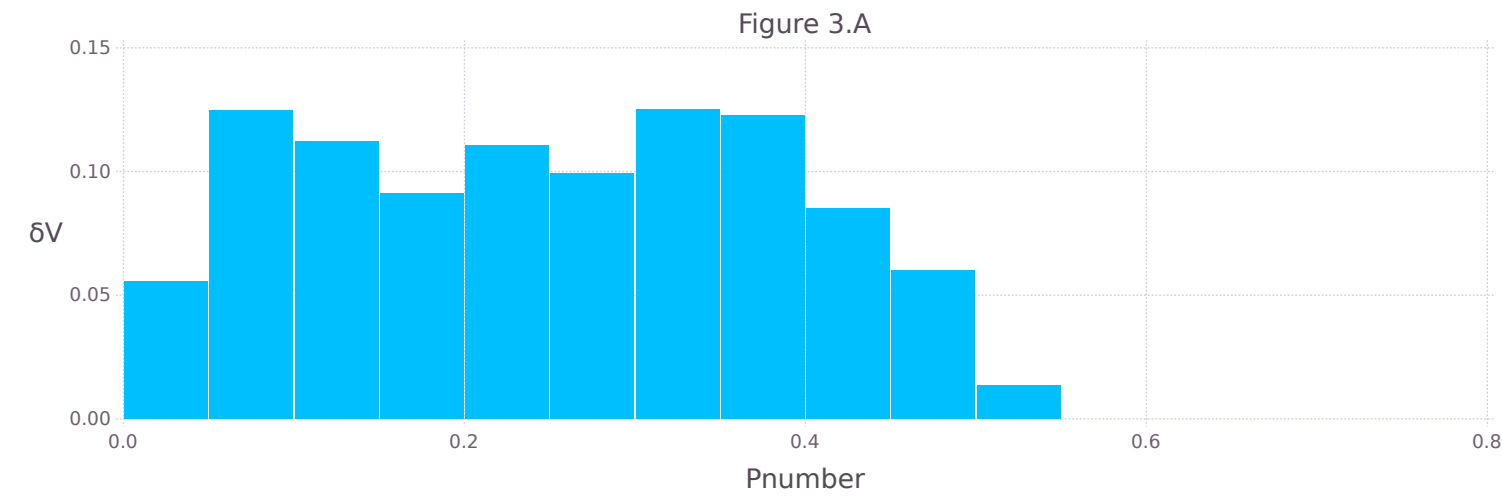


Figure 163. This is an inserted EPS graphic

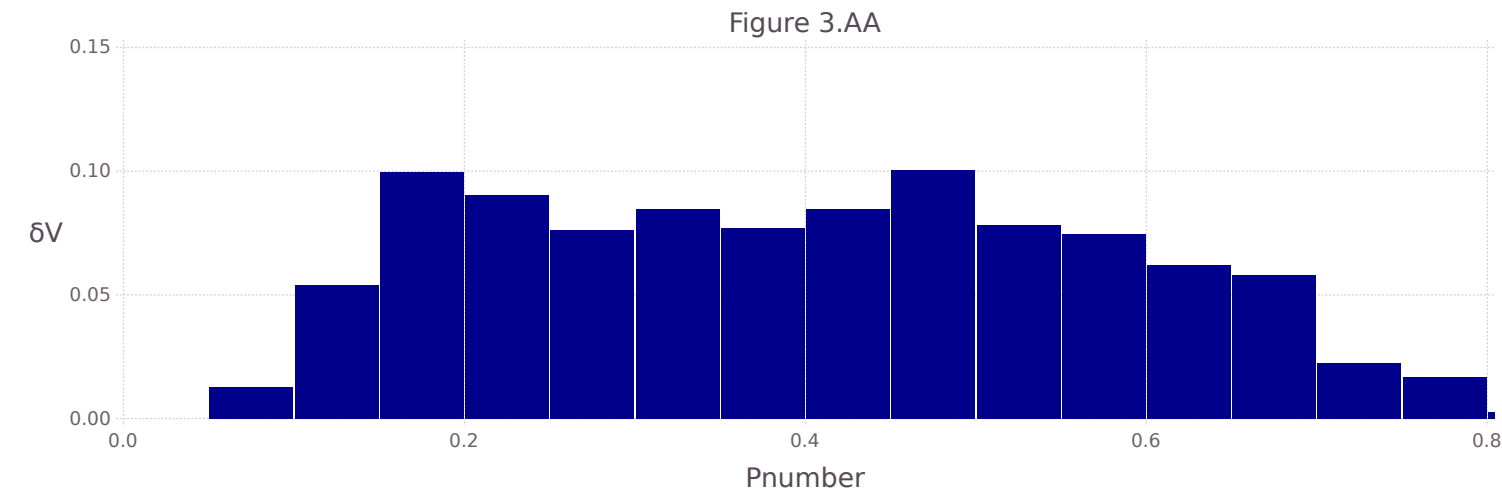


Figure 164. This is an inserted EPS graphic

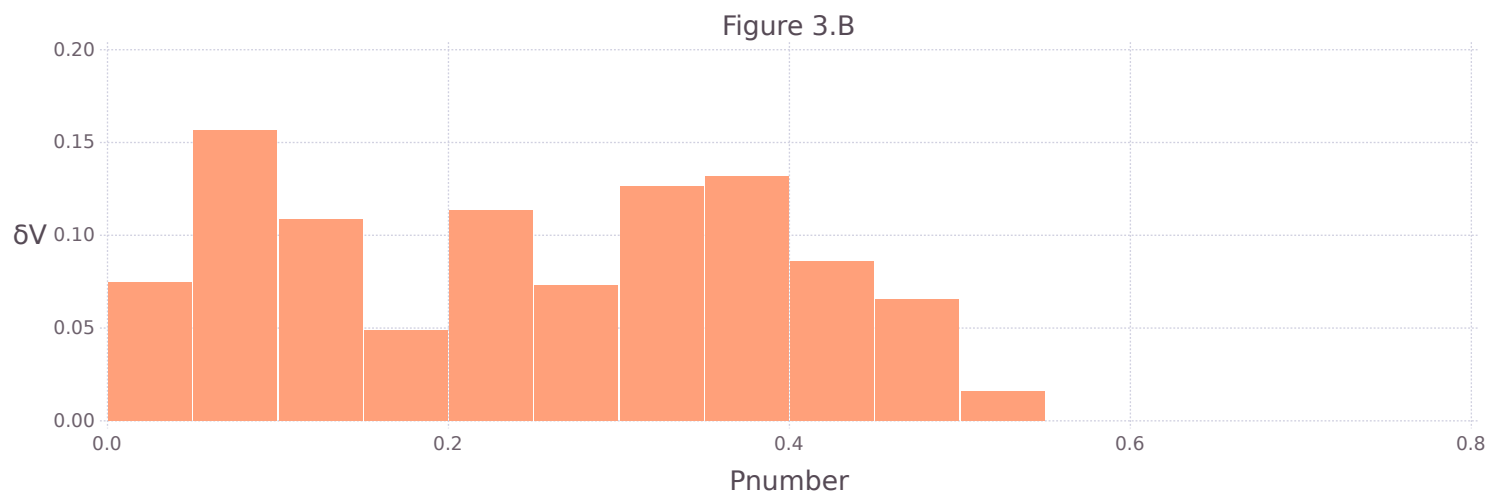


Figure 165. This is an inserted EPS graphic

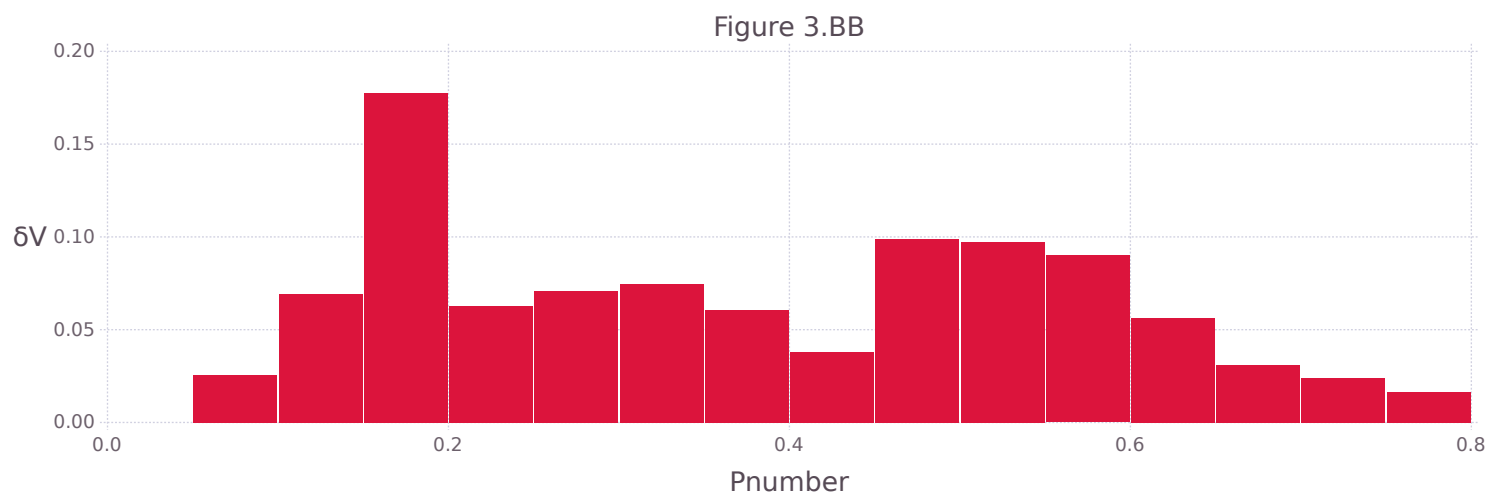


Figure 166. This is an inserted EPS graphic

VG_V can be translated into cartesian coordinates and the module of the X, Y, Z coordinates obtained.

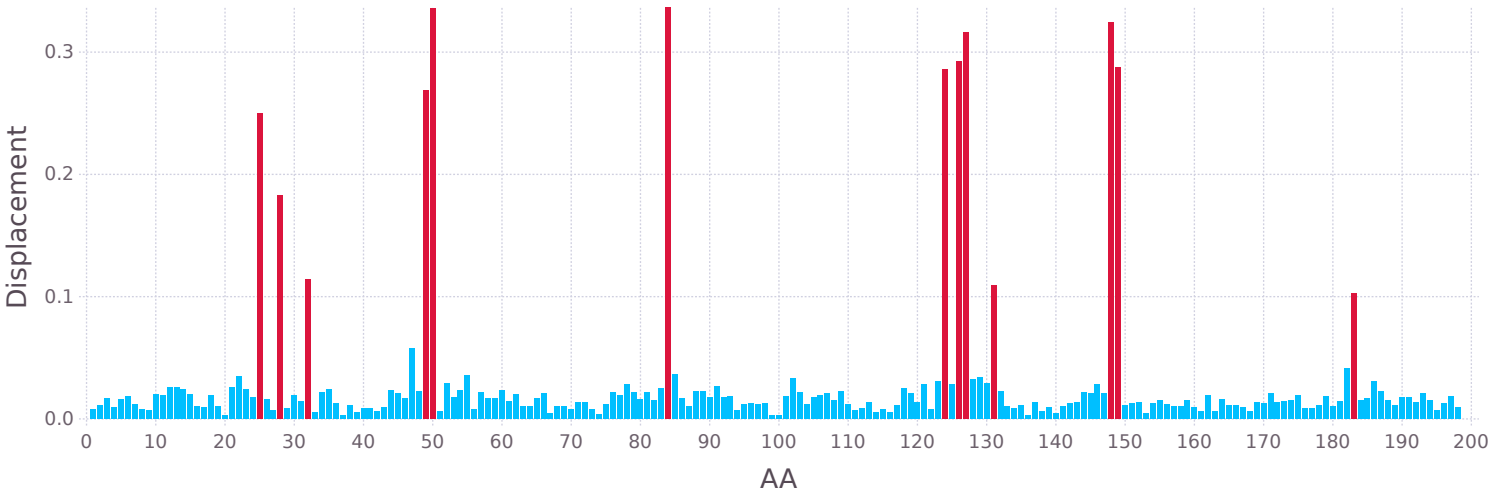


Figure 167. This is an inserted EPS graphic

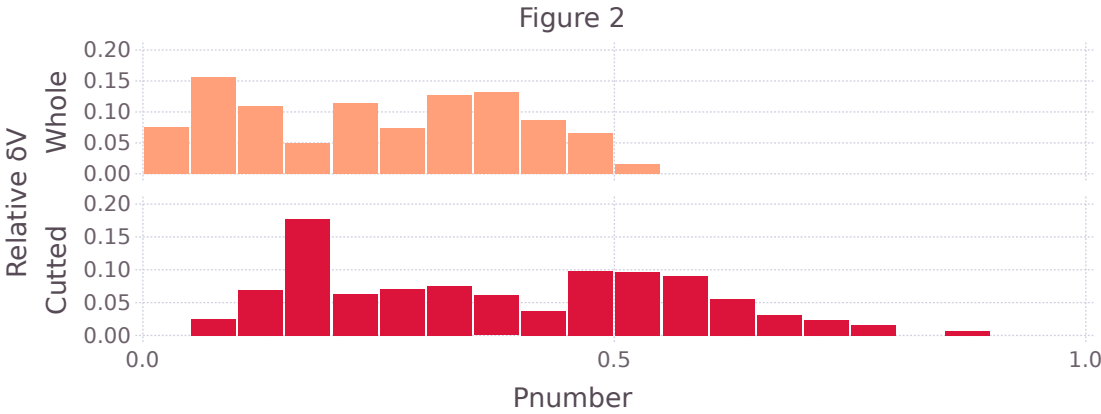


Figure 168. This is an inserted EPS graphic

6.3 1XKK

120

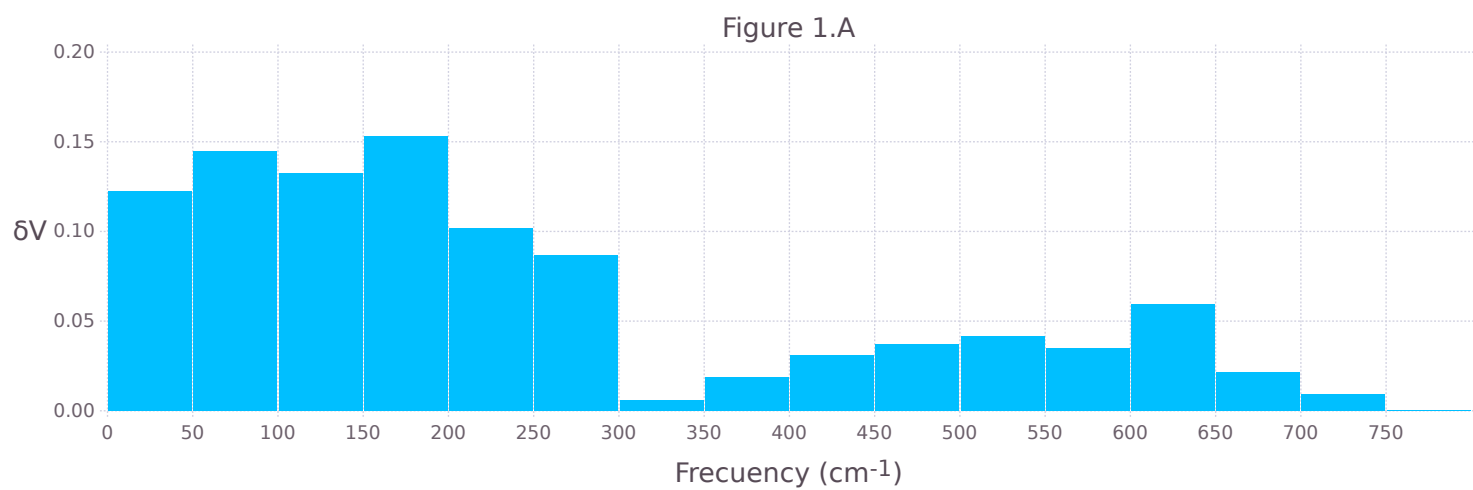


Figure 169. This is an inserted EPS graphic

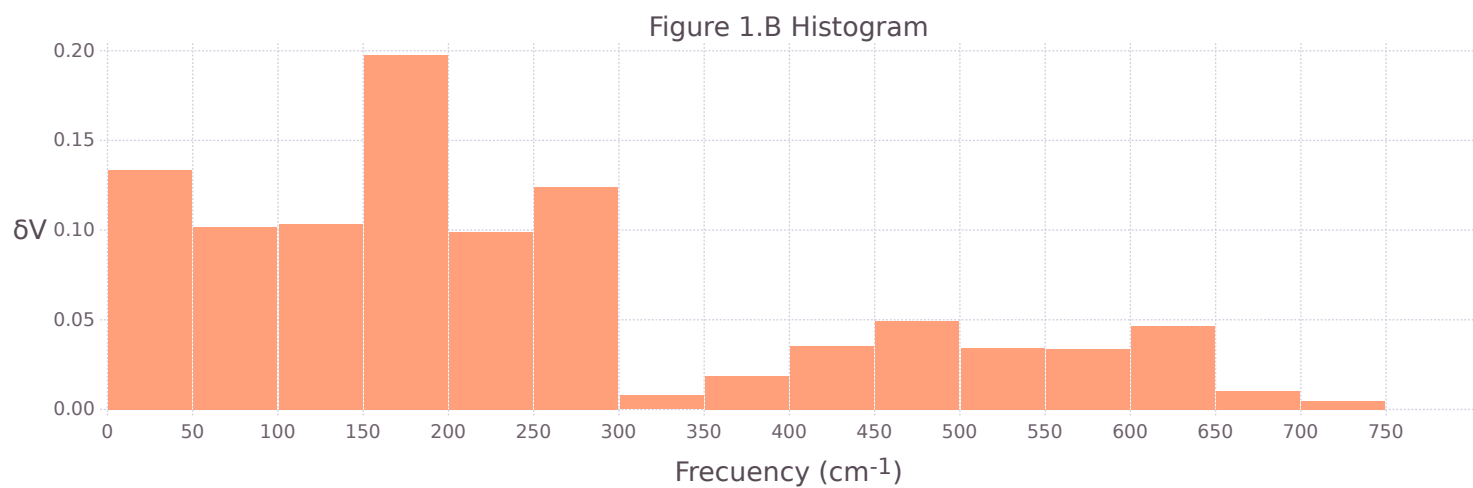


Figure 170. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

121

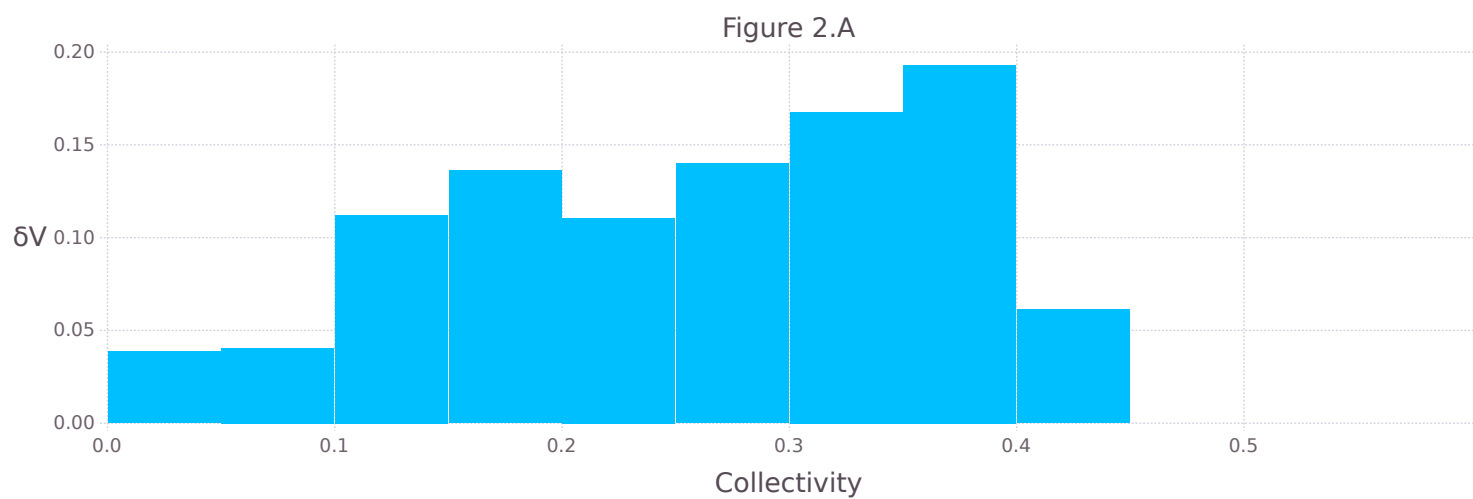


Figure 171. This is an inserted EPS graphic

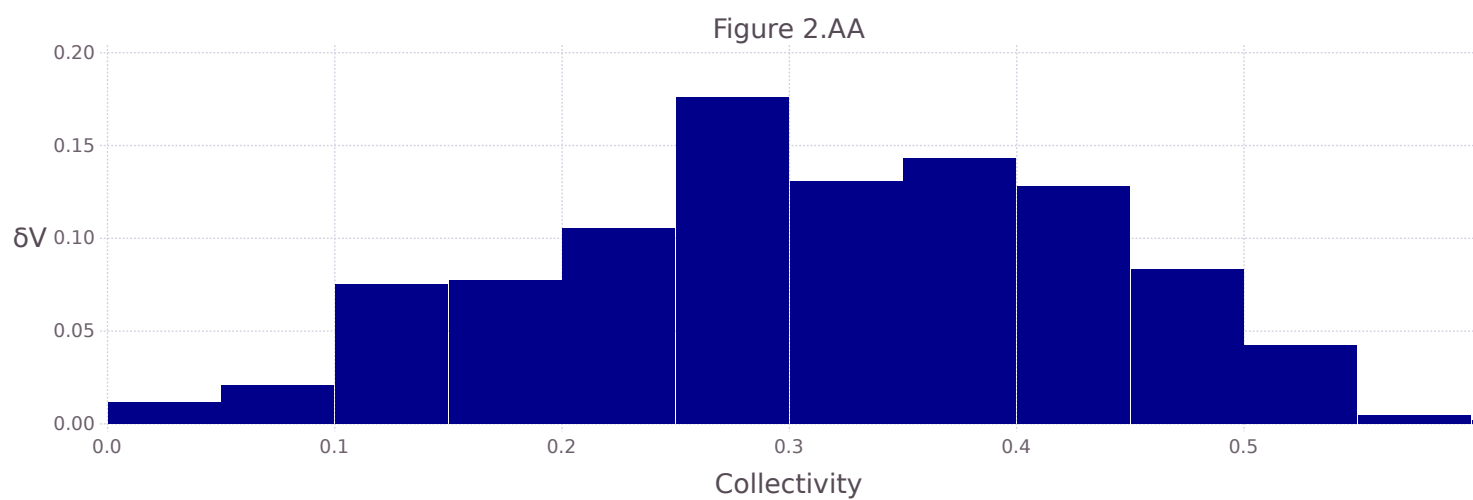


Figure 172. This is an inserted EPS graphic

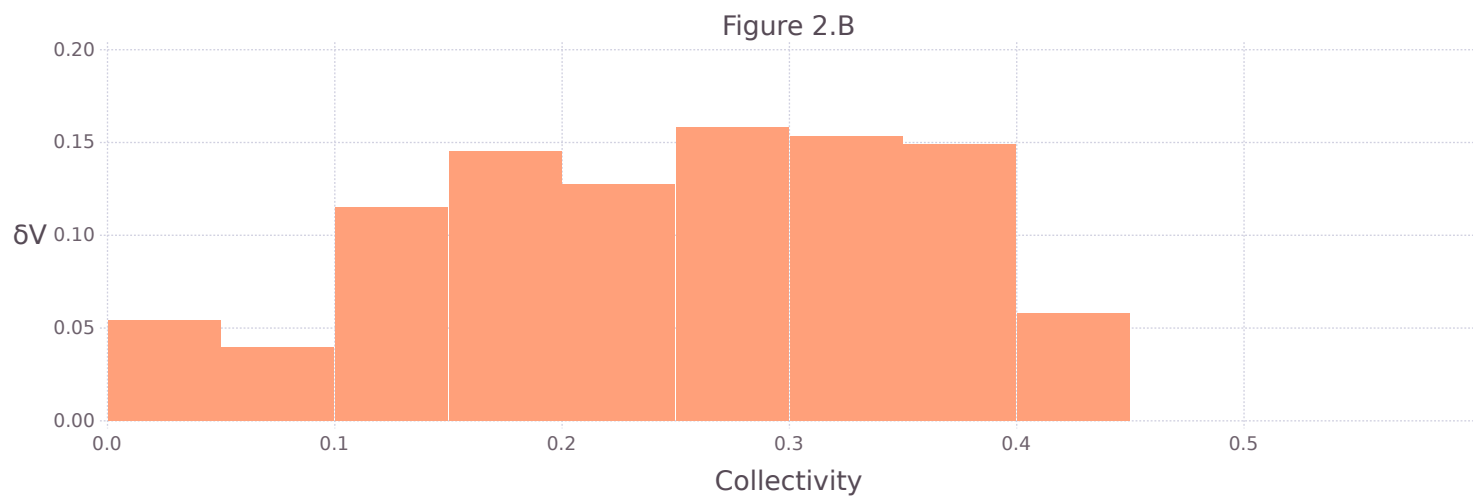


Figure 173. This is an inserted EPS graphic

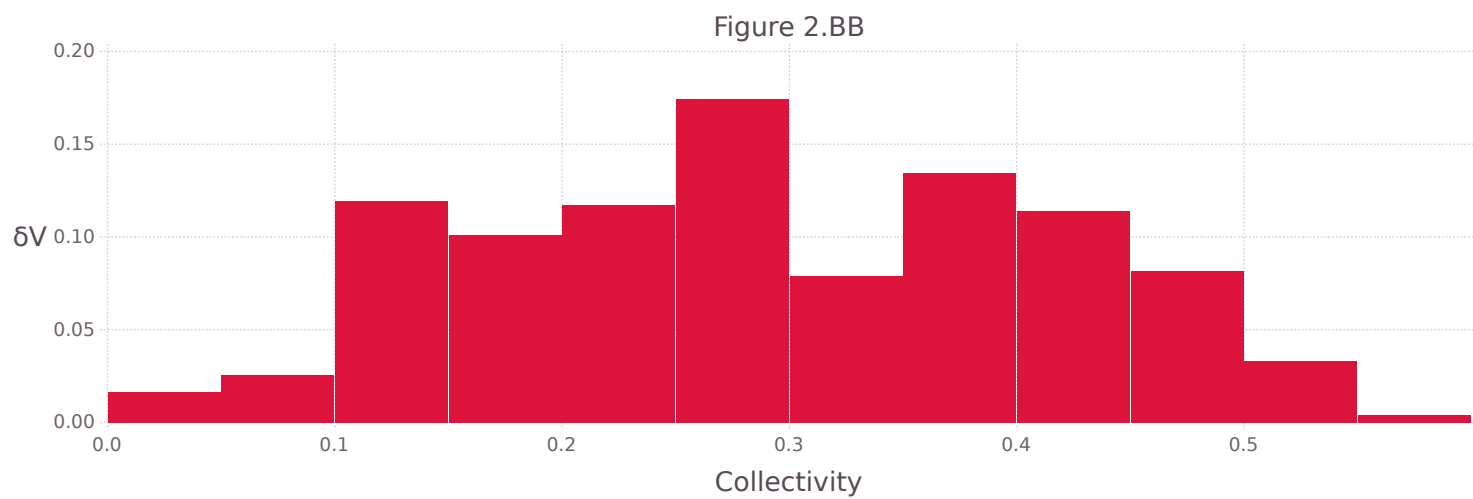


Figure 174. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with the **Participation Number**, as Fig.2 shows.

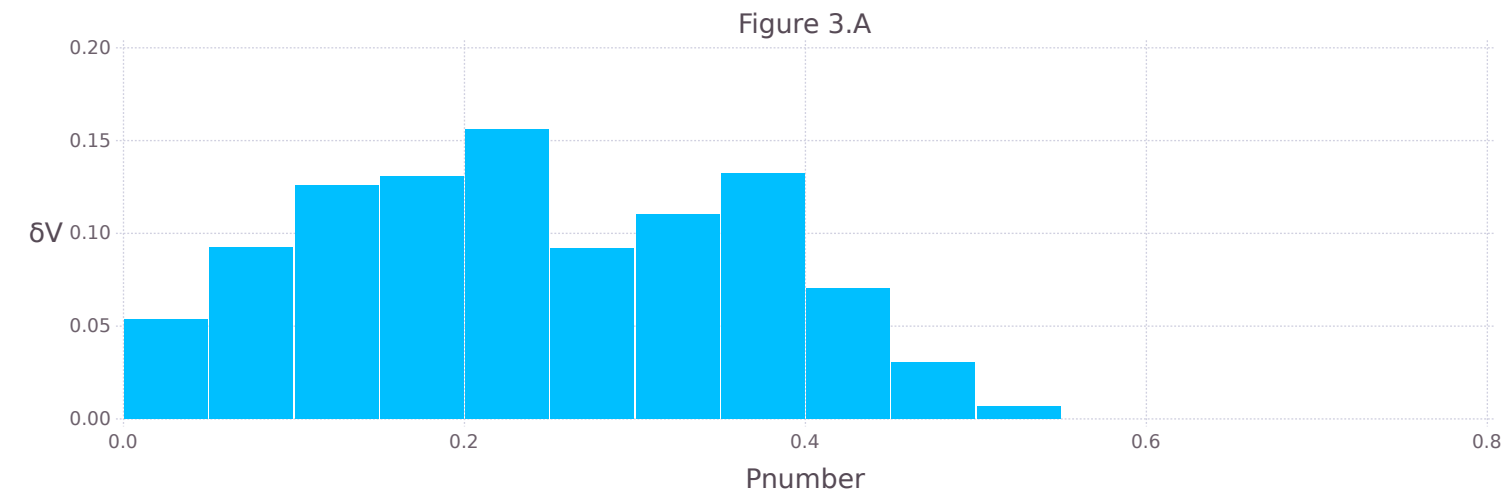


Figure 175. This is an inserted EPS graphic

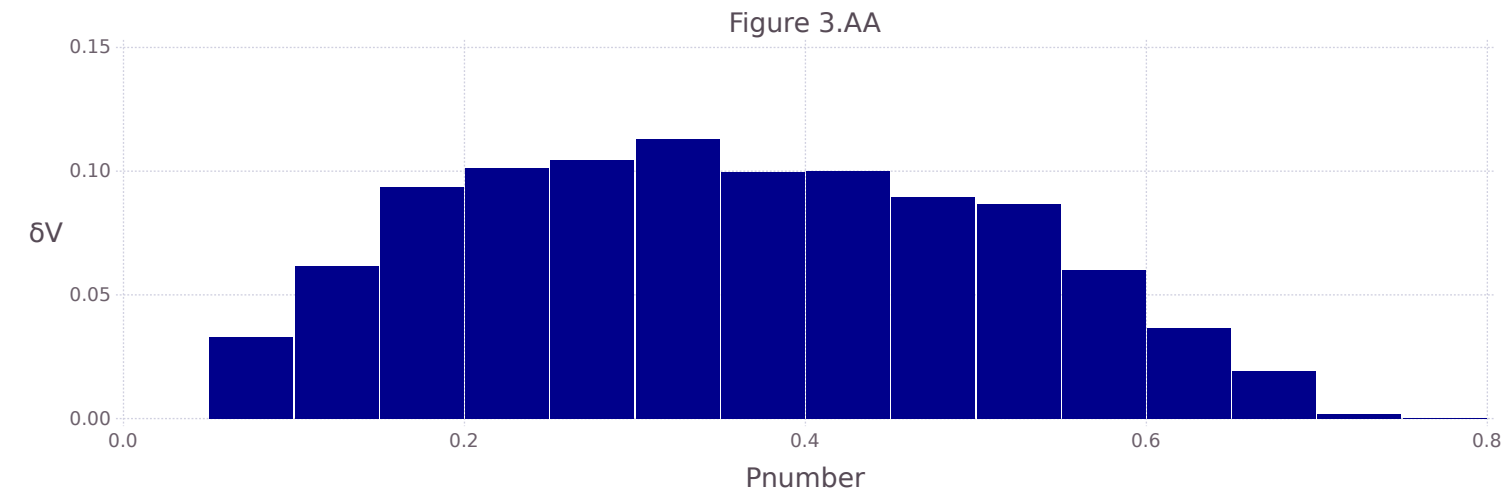


Figure 176. This is an inserted EPS graphic

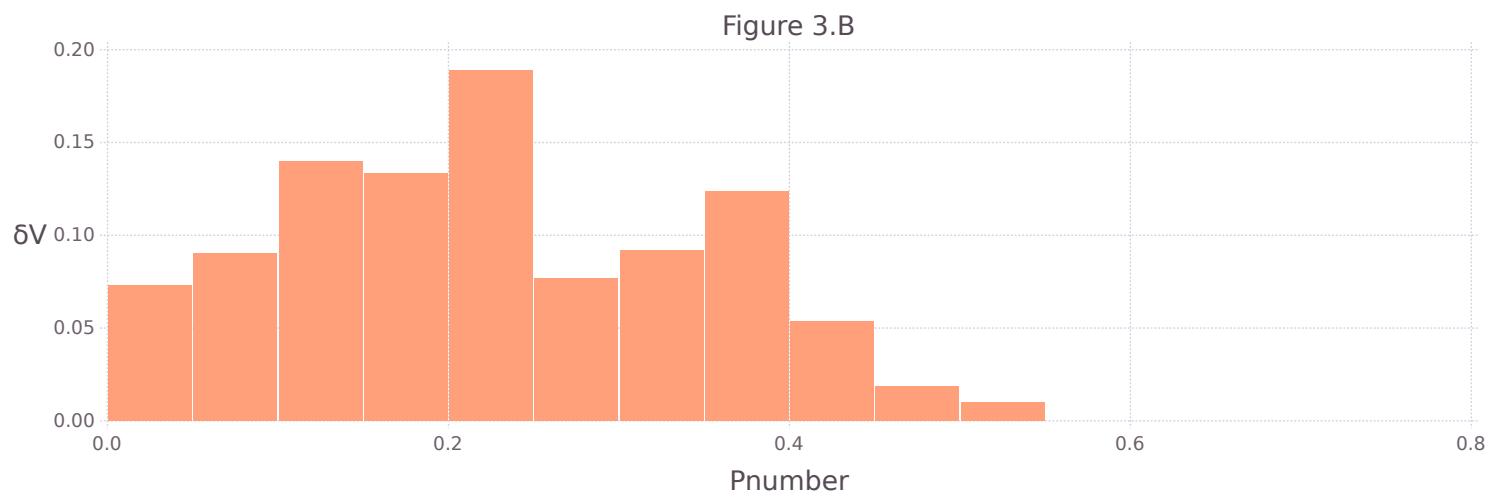


Figure 177. This is an inserted EPS graphic

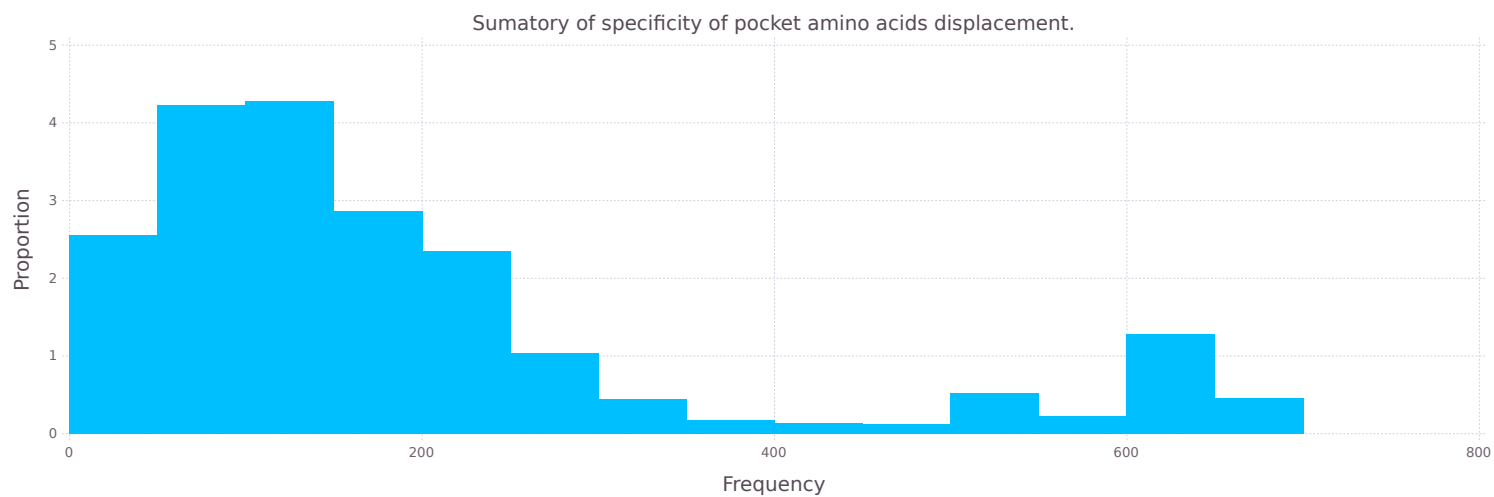


Figure 178. This is an inserted EPS graphic

VG_V can be translated into cartesian coordinates and the module of the X, Y, Z coordinates obtained.

124
125

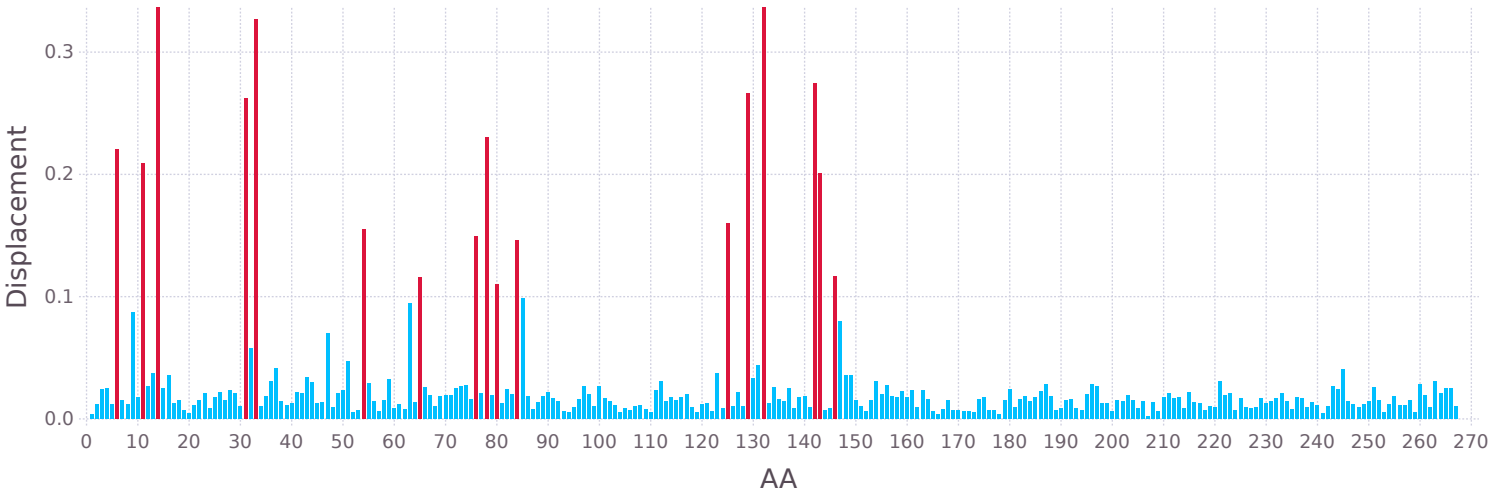


Figure 179. This is an inserted EPS graphic

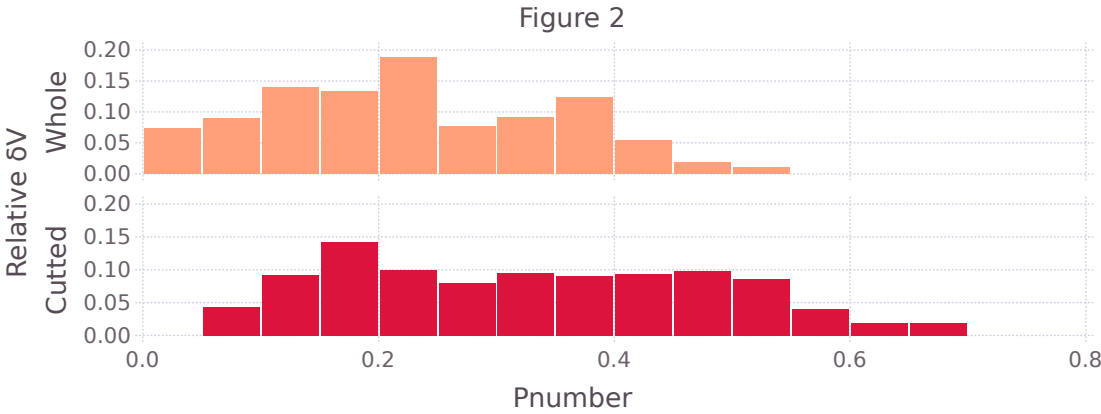


Figure 180. This is an inserted EPS graphic

6.4 1M14

126

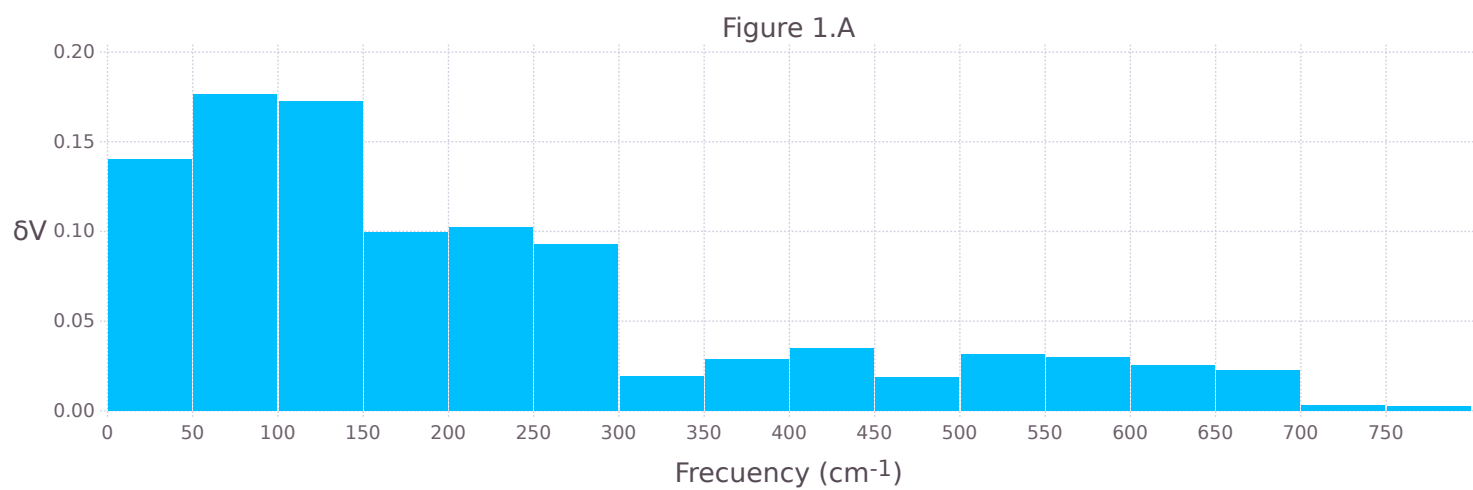


Figure 181. This is an inserted EPS graphic

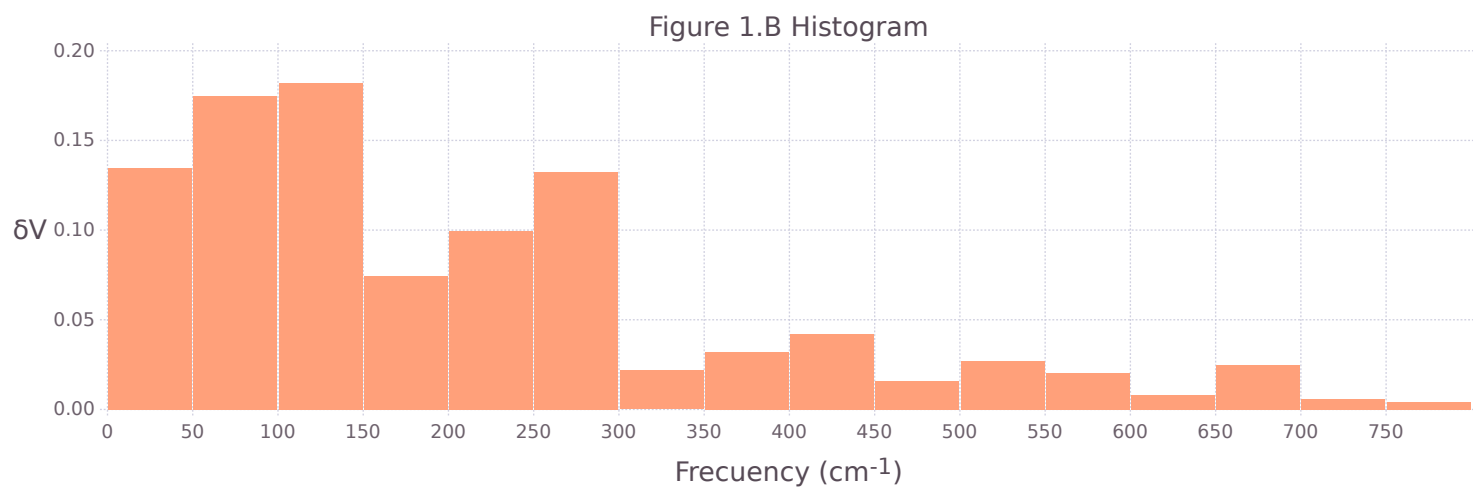


Figure 182. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

127

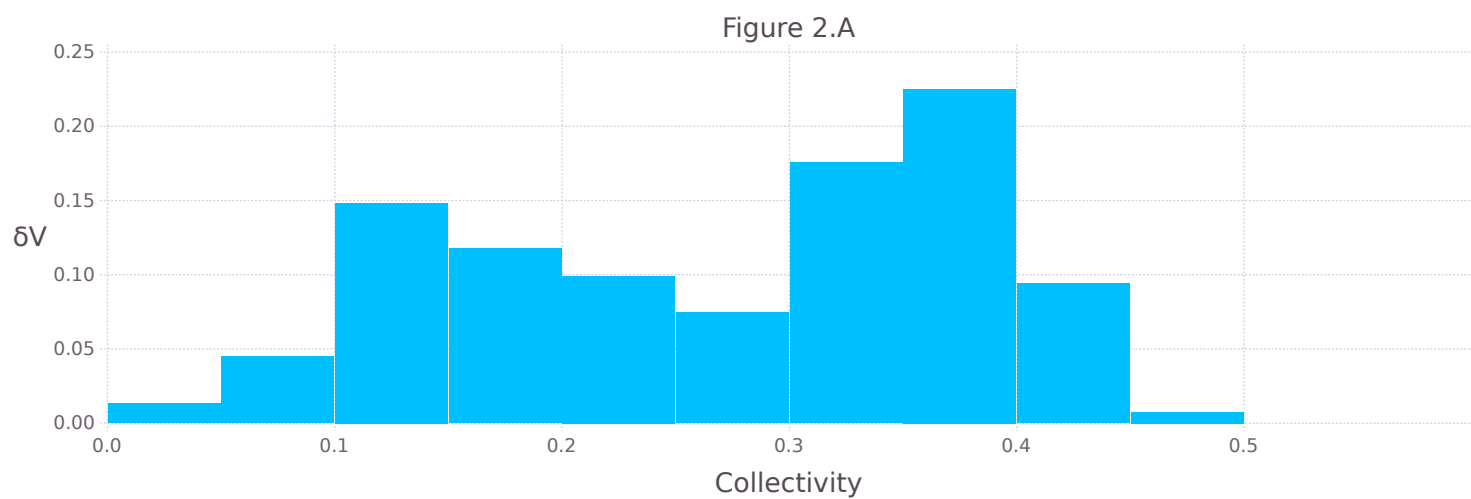


Figure 183. This is an inserted EPS graphic

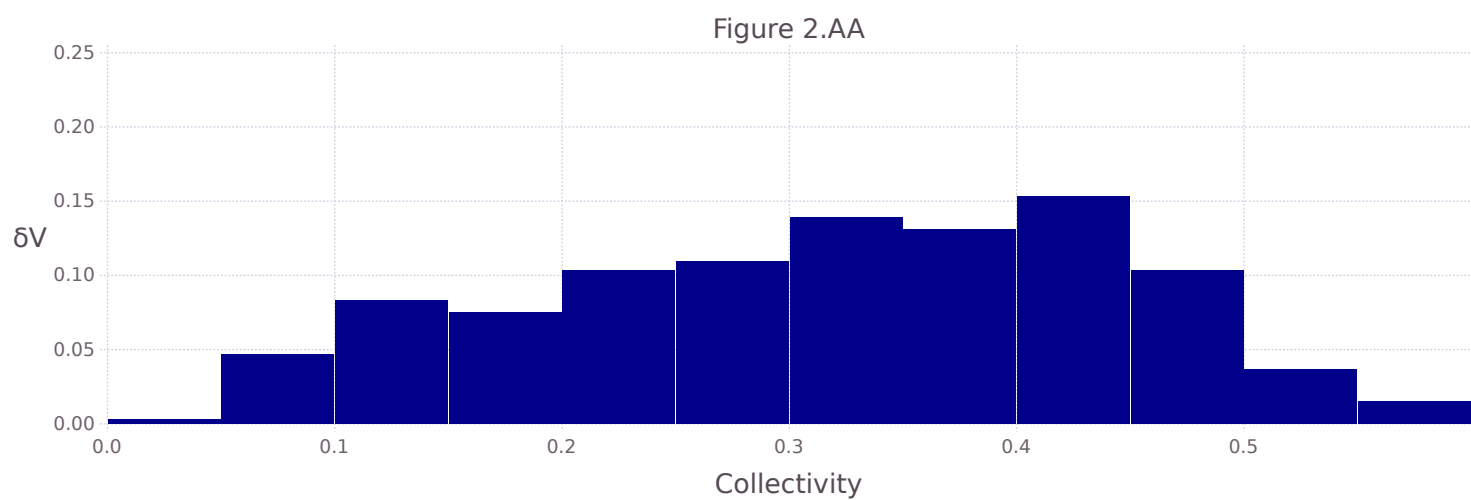


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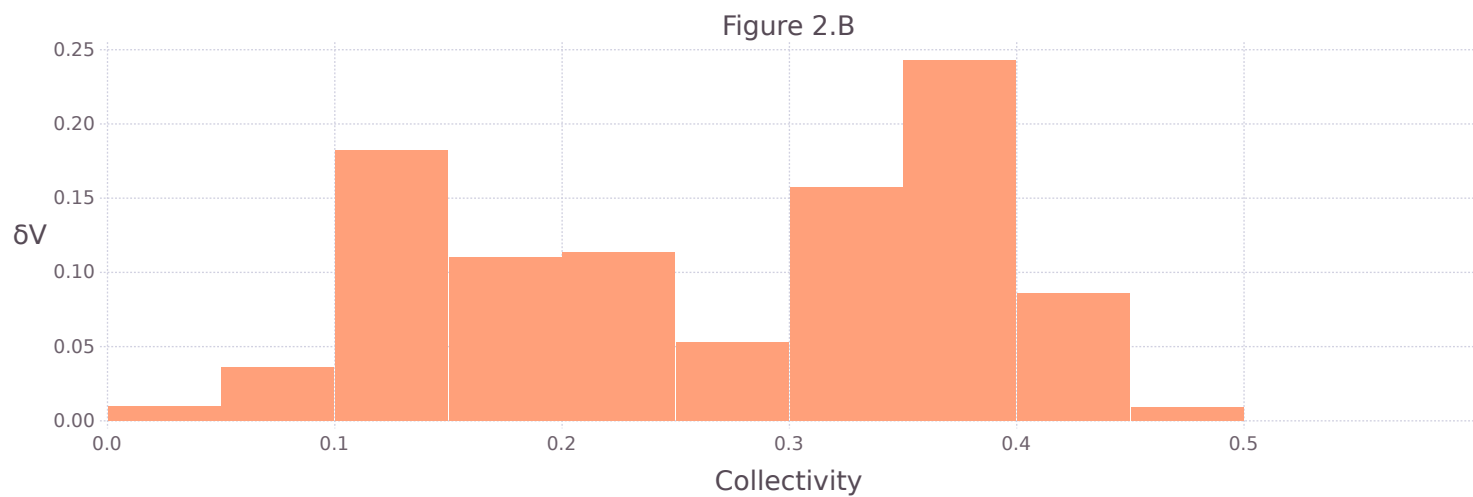


Figure 185. This is an inserted EPS graphic

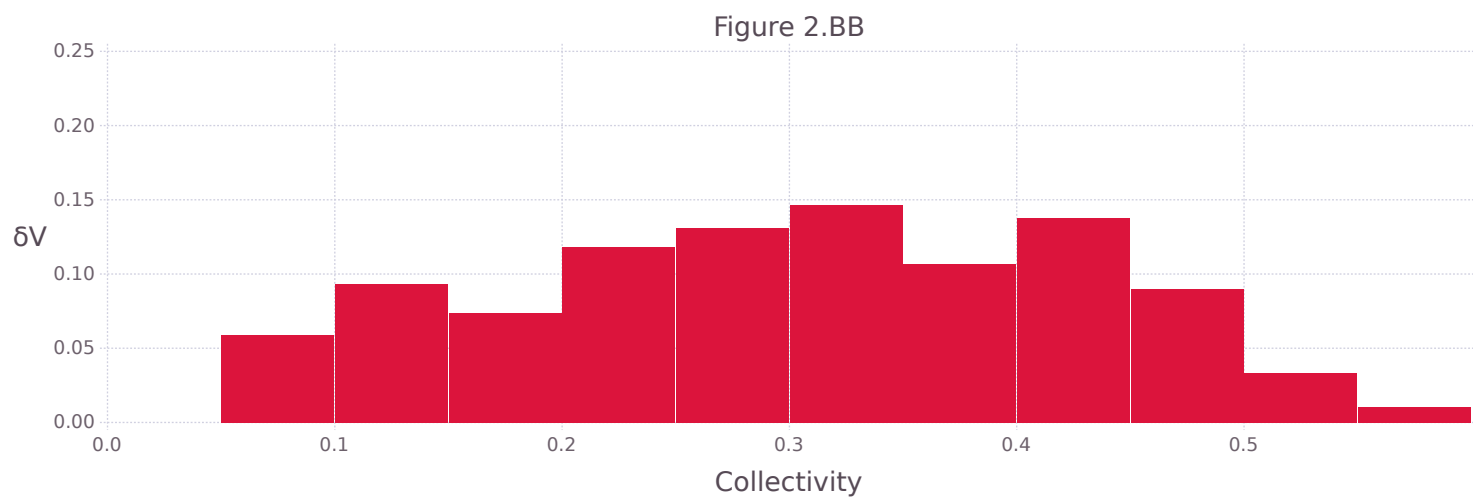


Figure 186. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with the **Participation Number**, as Fig.2 shows.

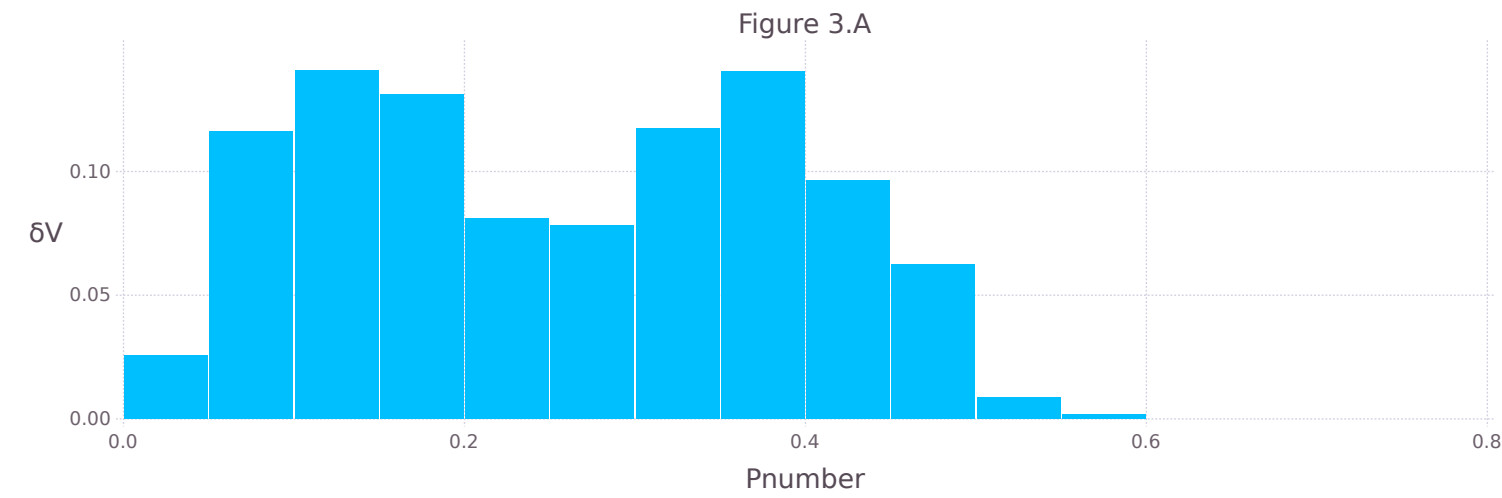


Figure 187. This is an inserted EPS graphic

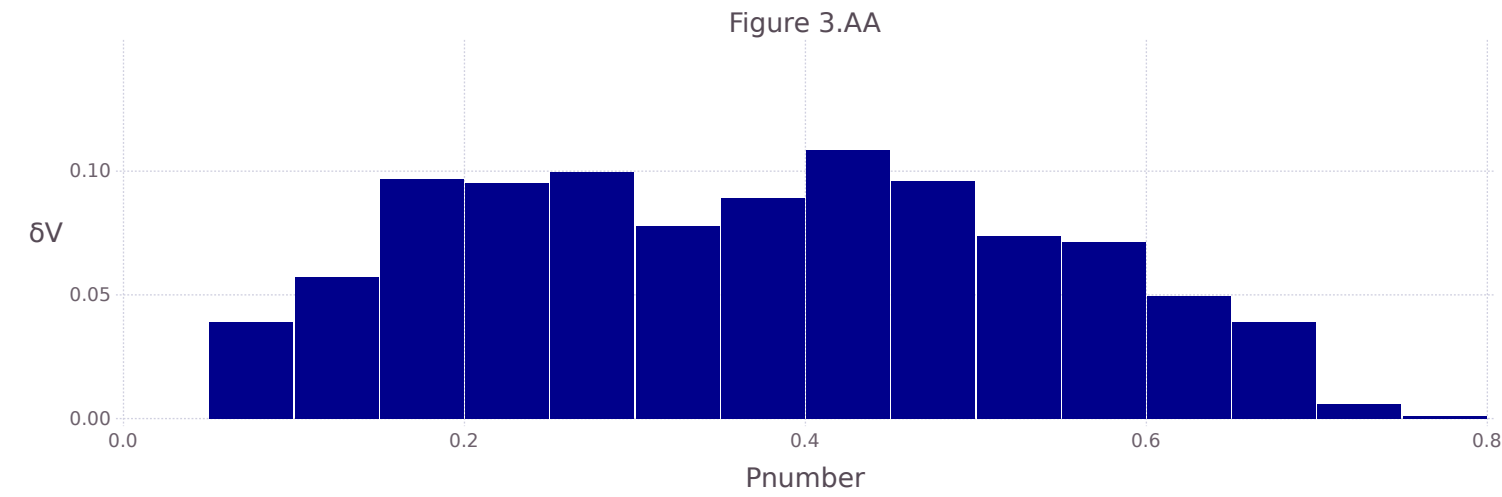


Figure 188. This is an inserted EPS graphic

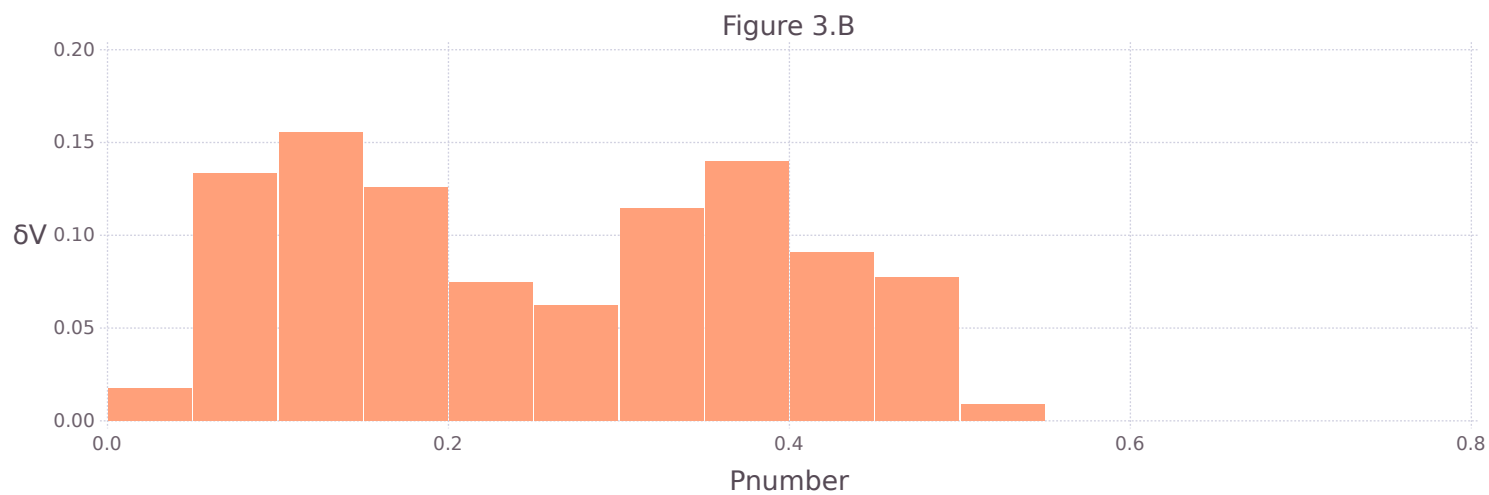


Figure 189. This is an inserted EPS graphic

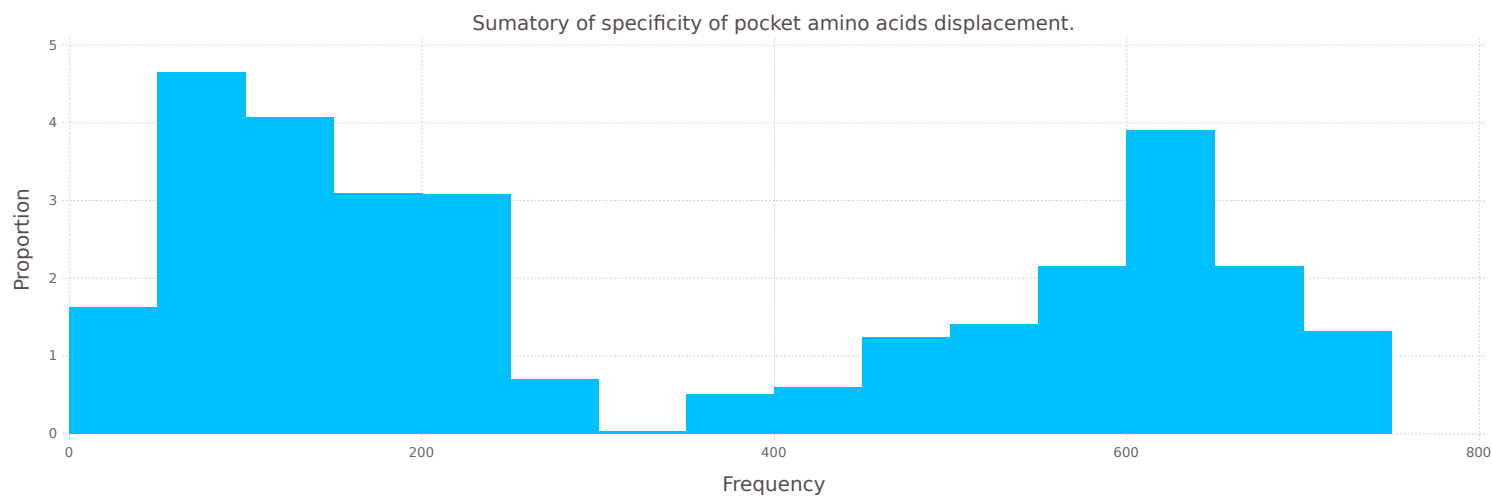


Figure 190. This is an inserted EPS graphic

VGV can be translated into cartesian coordinates and the module of the X, Y, Z coordinates obtained.

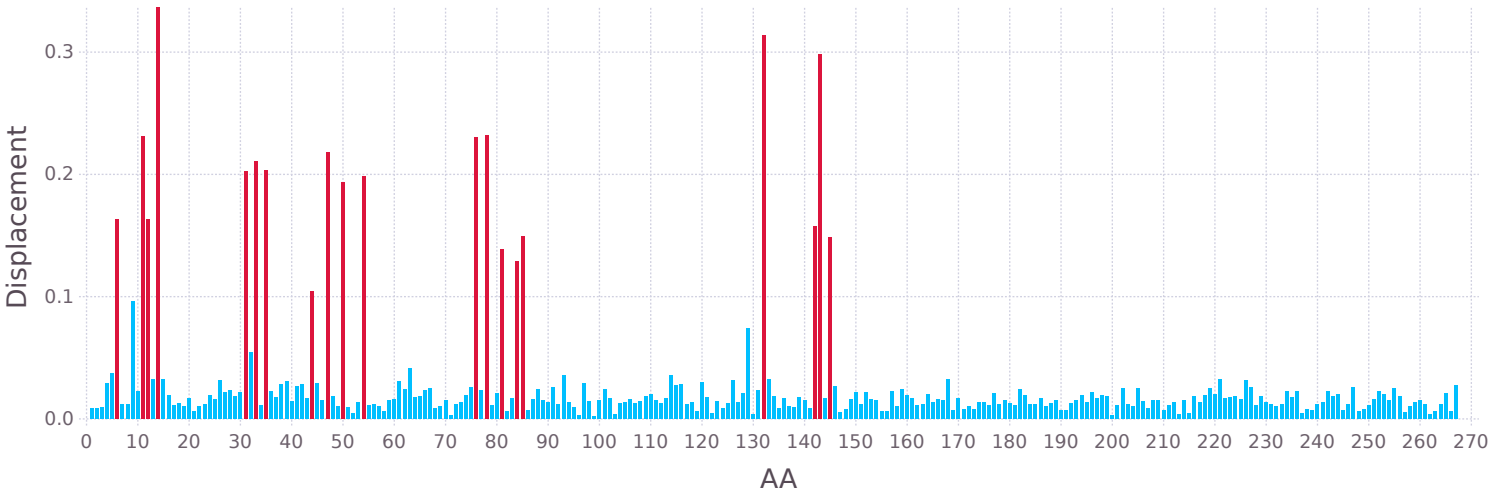


Figure 191. This is an inserted EPS graphic

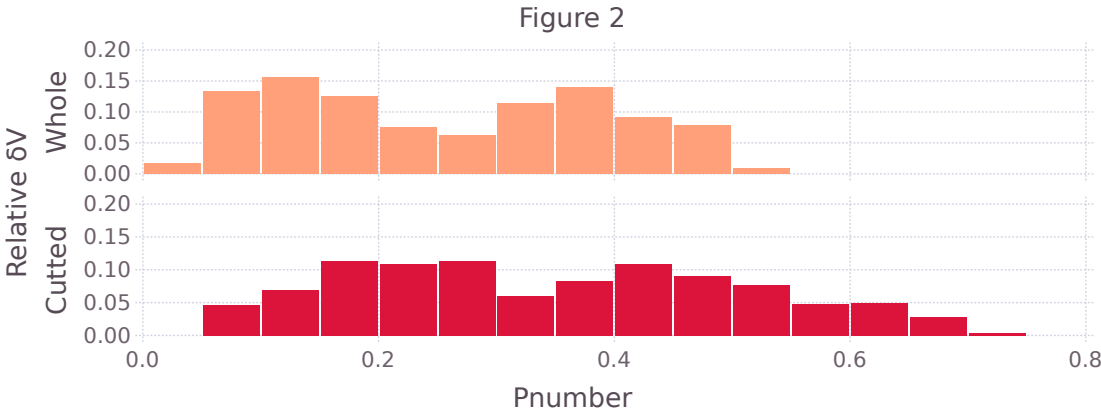


Figure 192. This is an inserted EPS graphic

6.5 1PRN

132

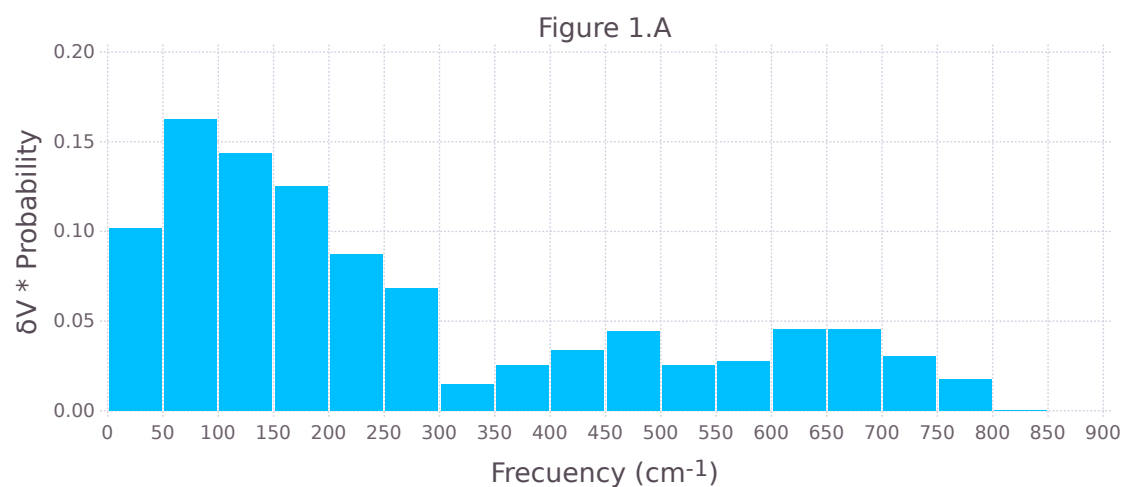


Figure 193. This is an inserted EPS graphic

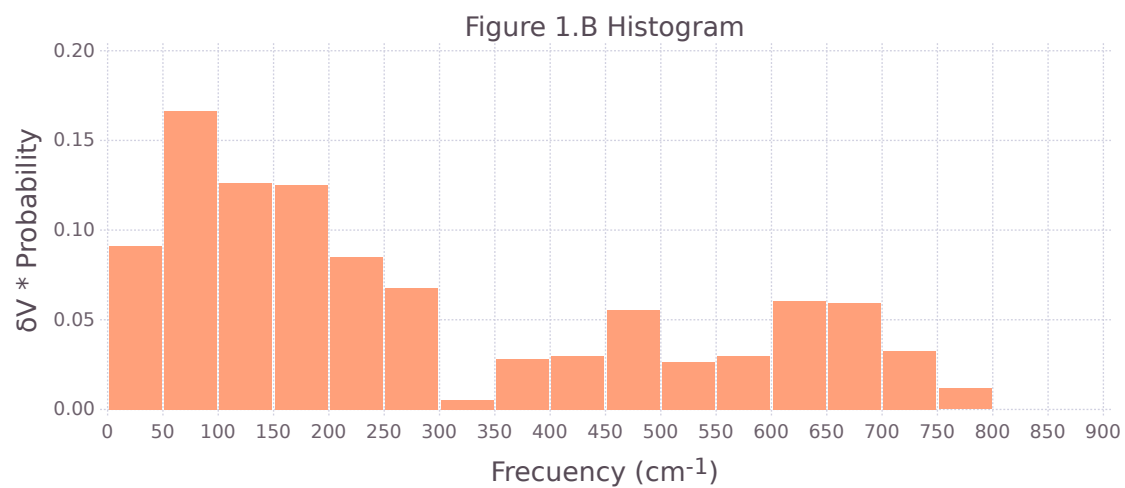


Figure 194. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

133

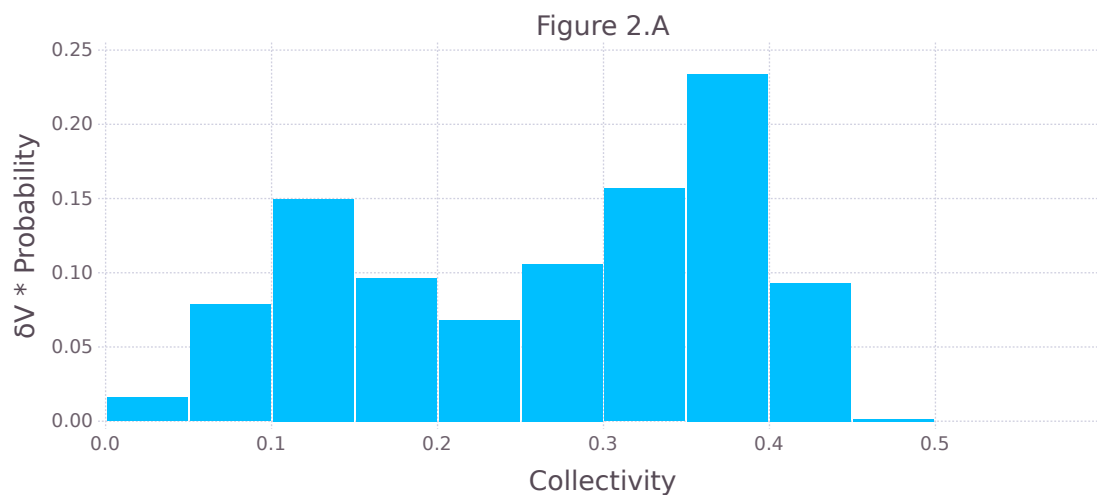


Figure 195. This is an inserted EPS graphic

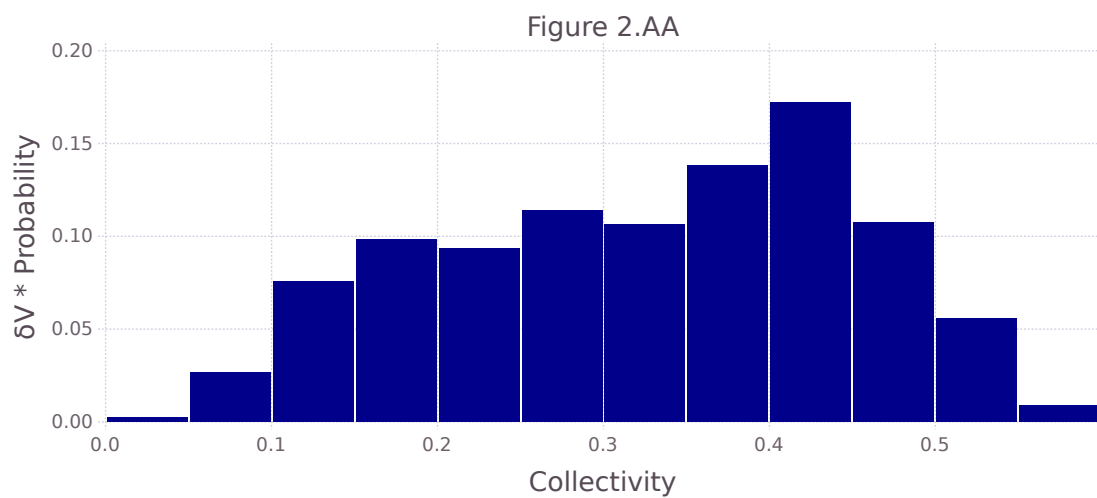


Figure 196. This is an inserted EPS graphic

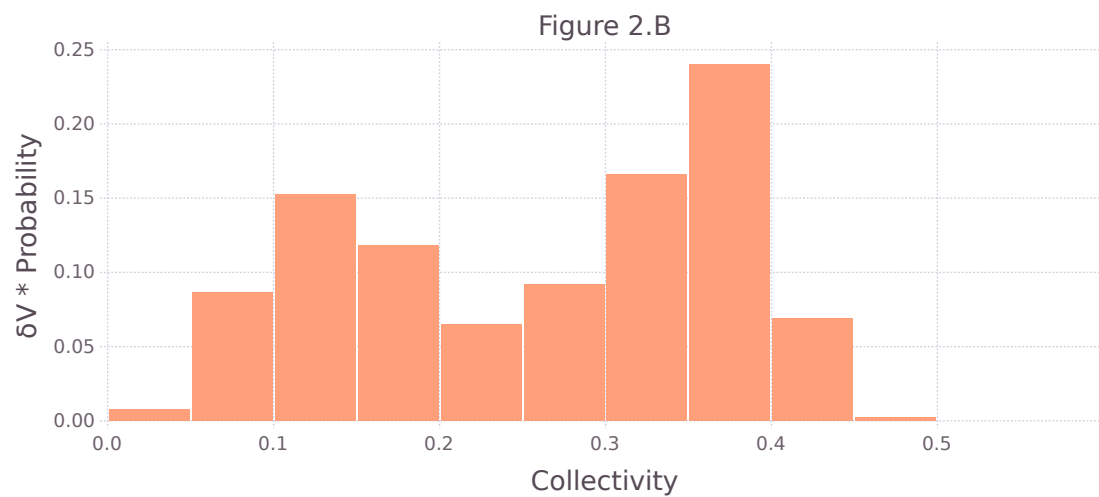


Figure 197. This is an inserted EPS graphic

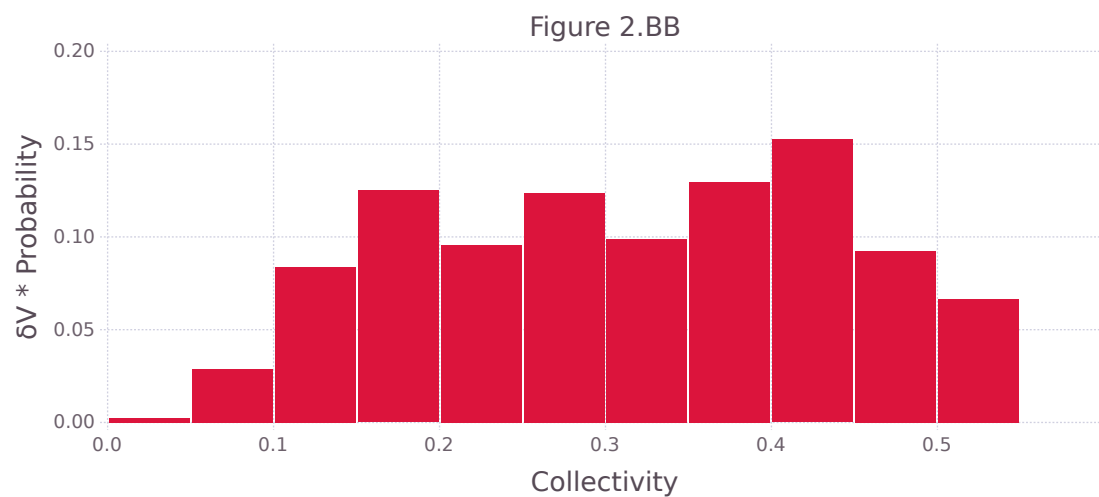


Figure 198. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with the **Participation Number**, as Fig.2 shows.

134
135

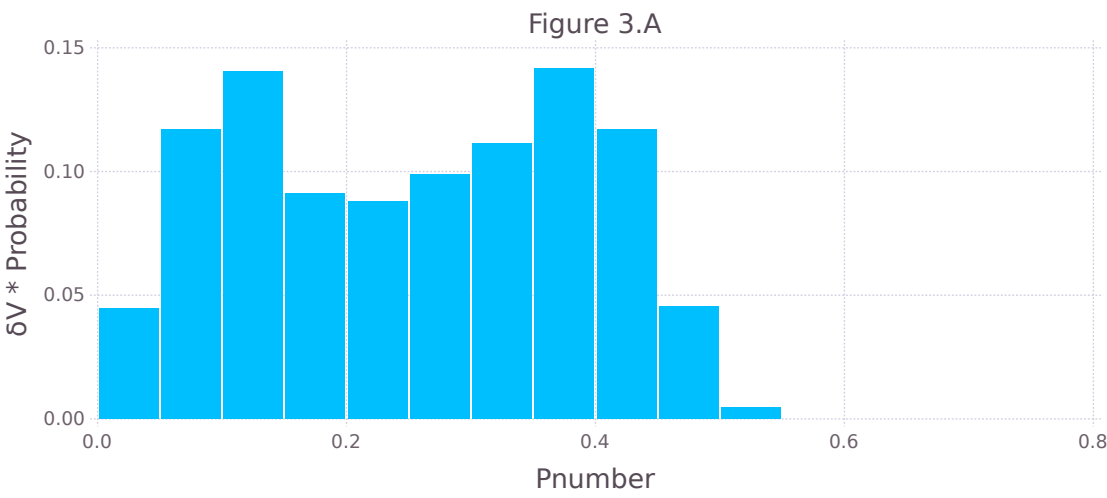


Figure 199. This is an inserted EPS graphic

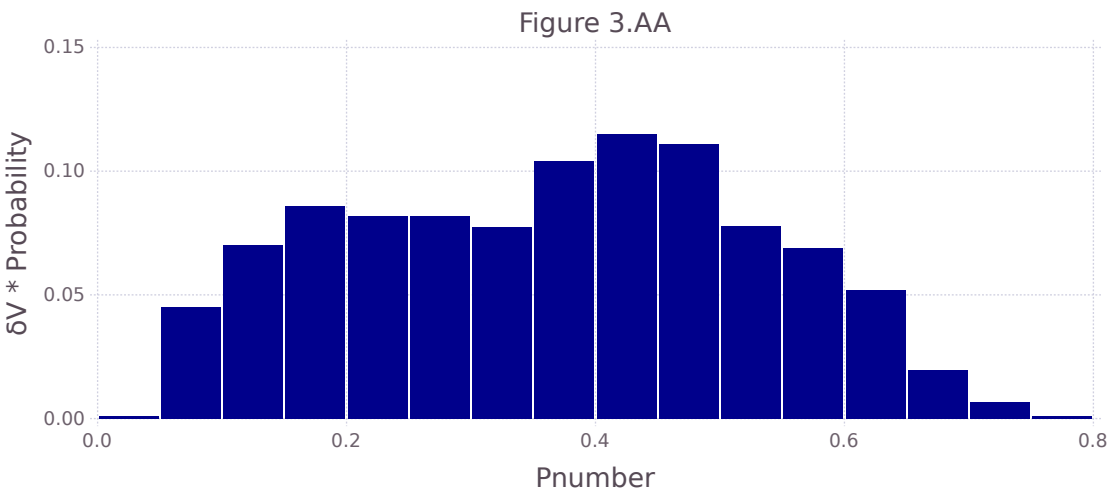


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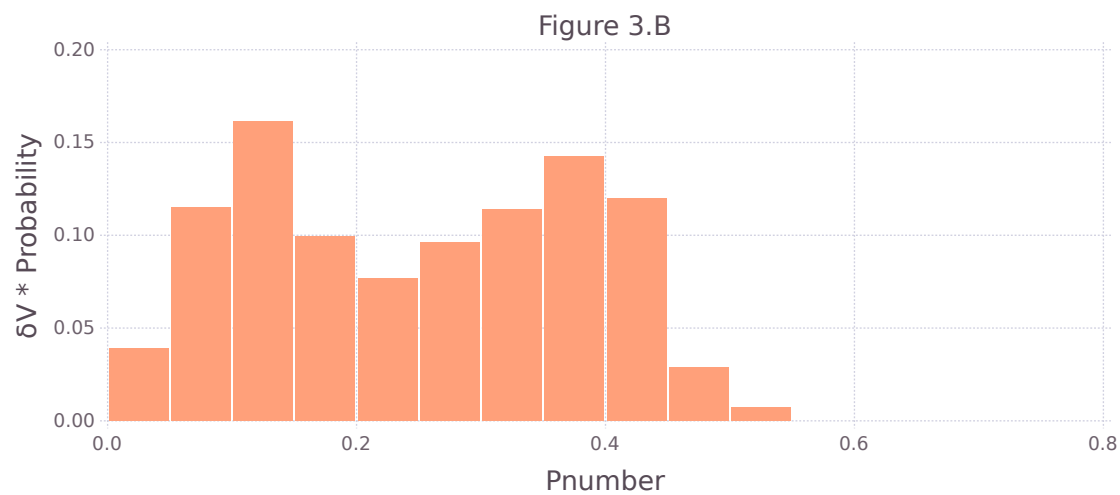


Figure 201. This is an inserted EPS graphic

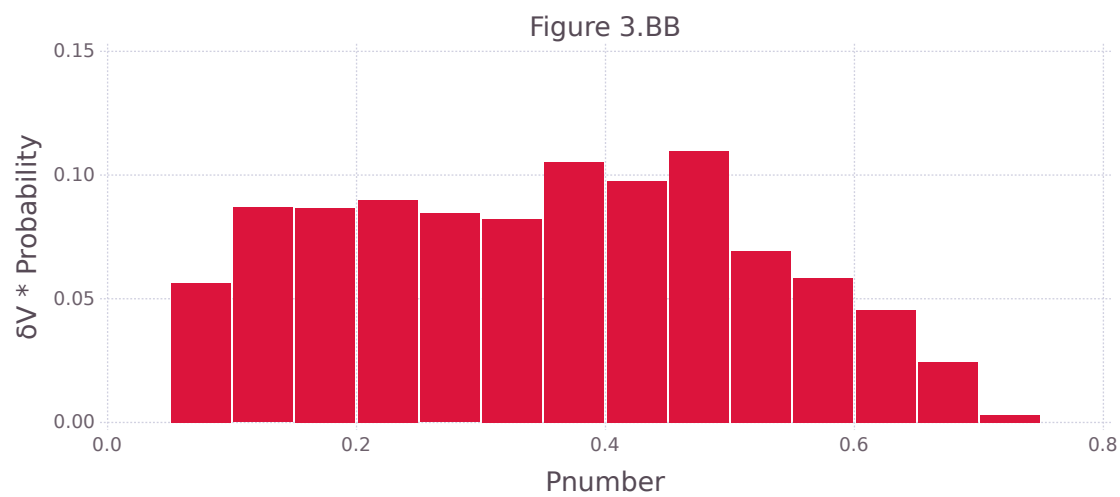


Figure 202. This is an inserted EPS graphic

VGV can be translated into cartesian coordinates and the module of the X, Y, Z coordinates obtained.

136
137

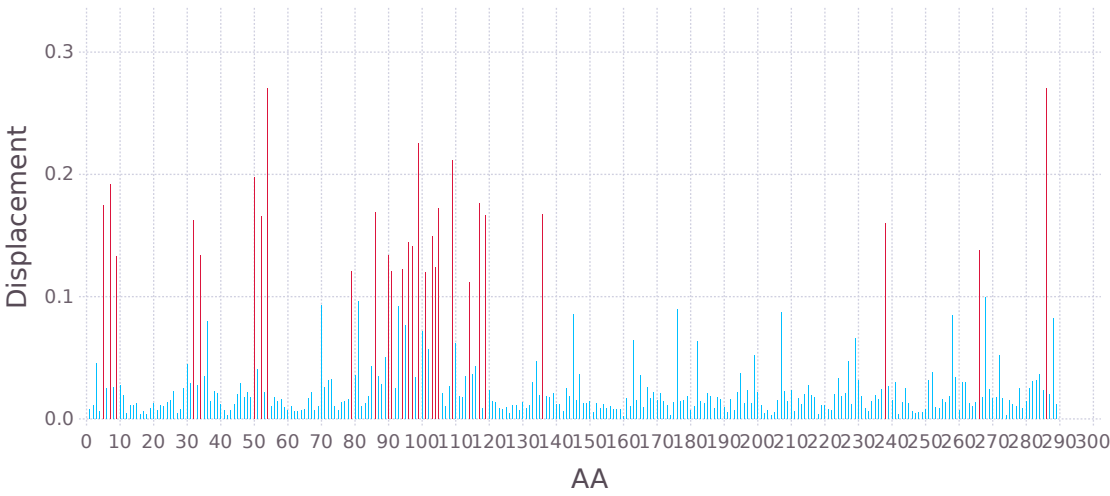


Figure 203. This is an inserted EPS graphic

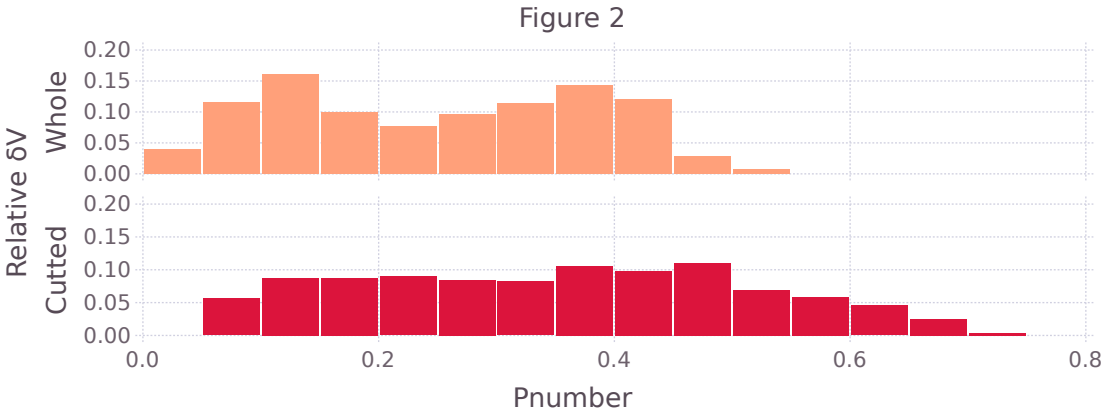


Figure 204. This is an inserted EPS graphic

6.6 256L

138

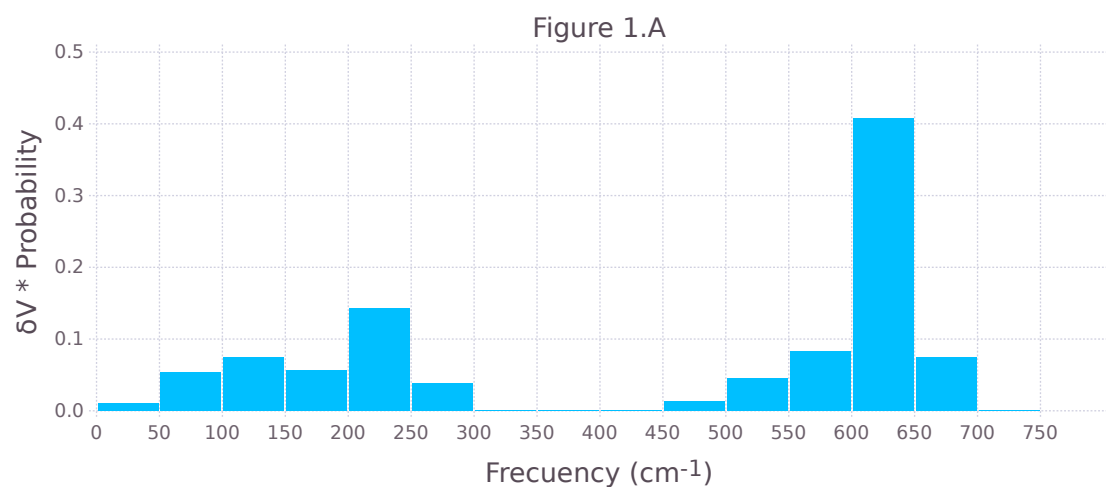


Figure 205. This is an inserted EPS graphic

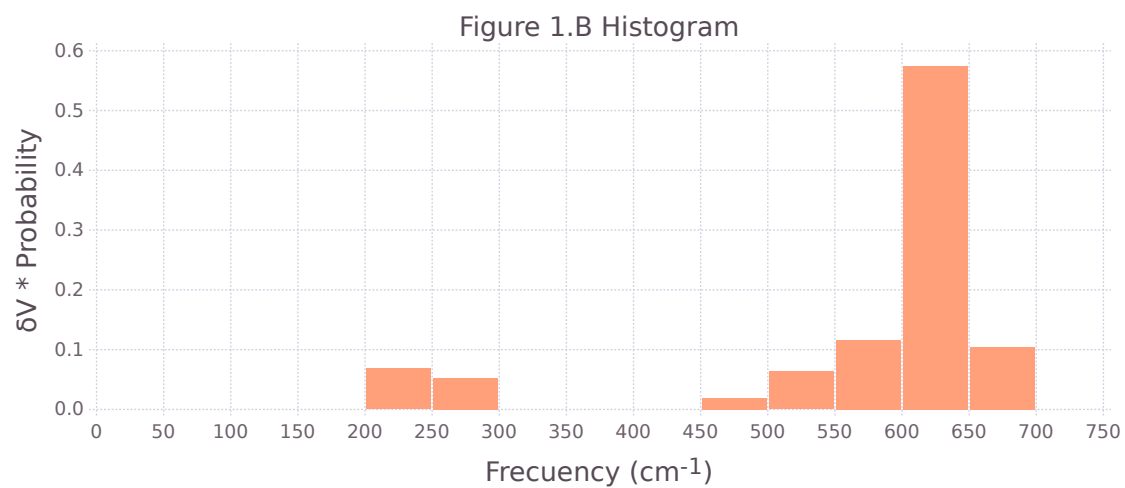


Figure 206. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with collectivity, as Fig.2 shows.

139

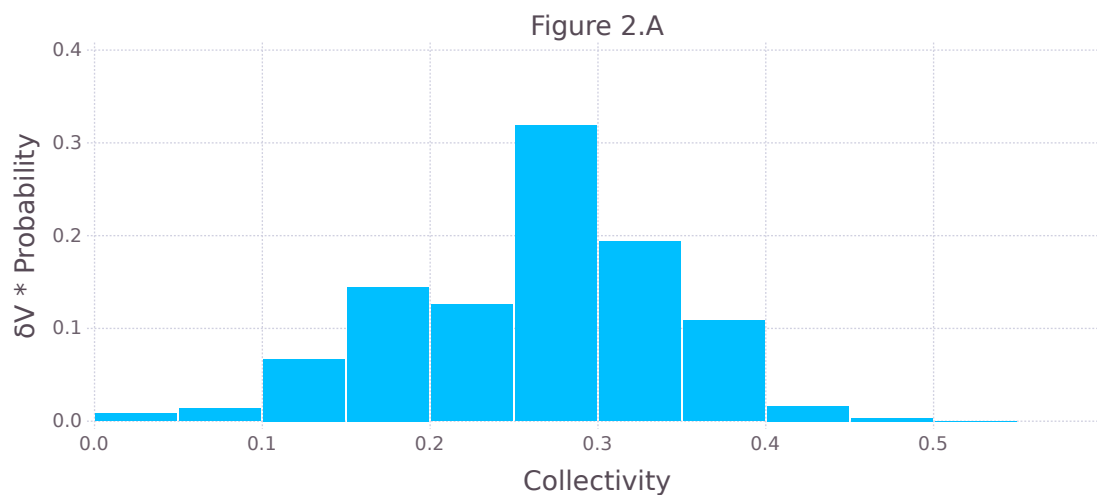


Figure 207. This is an inserted EPS graphic

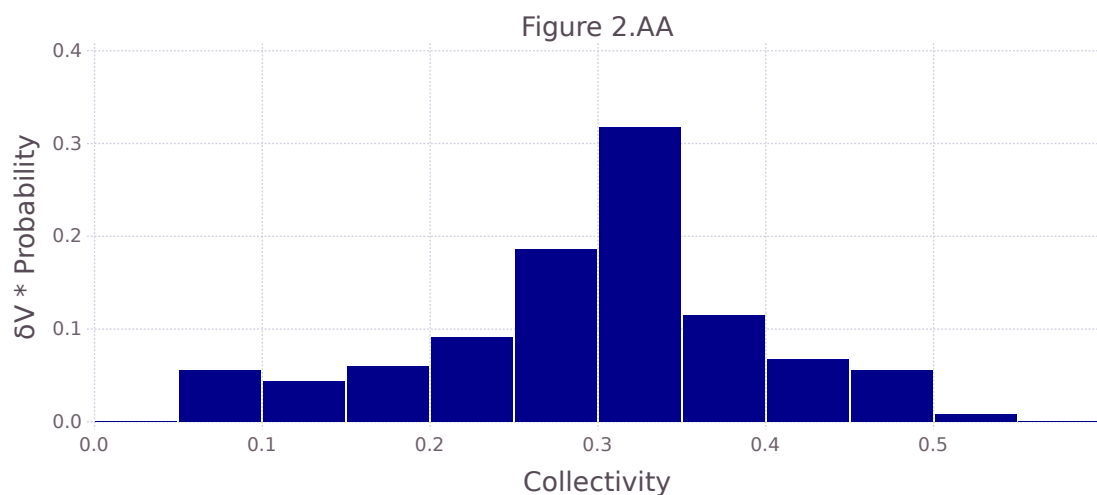


Figure 208. This is an inserted EPS graphic

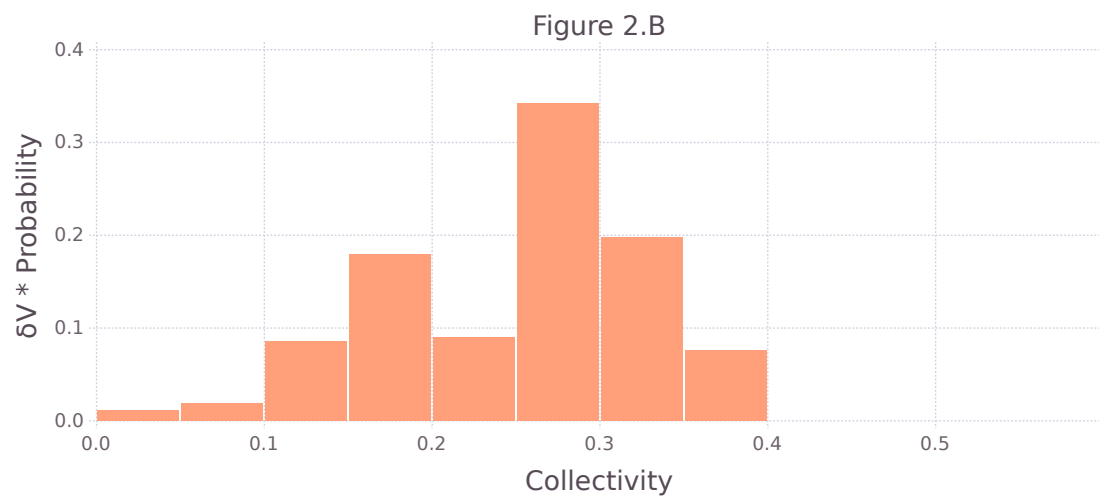


Figure 209. This is an inserted EPS graphic

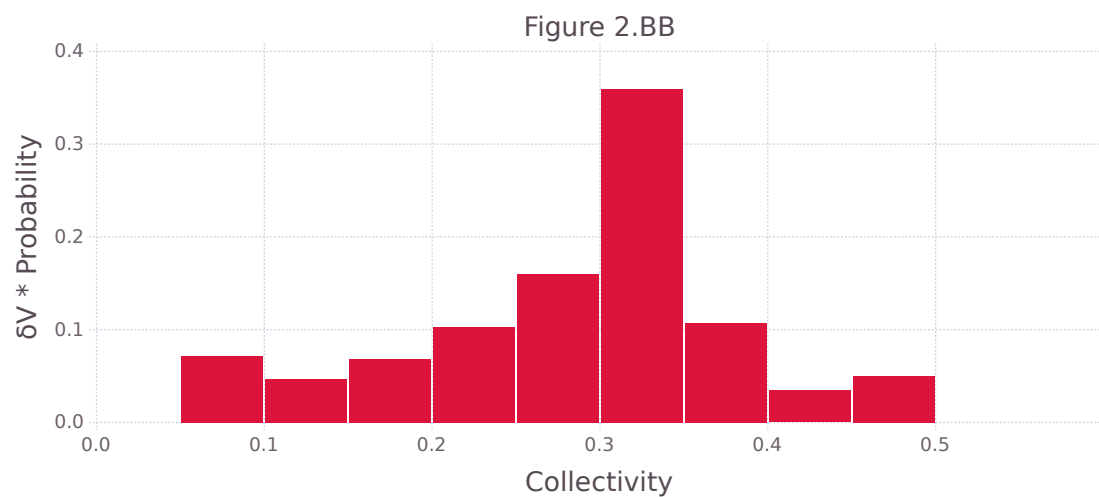


Figure 210. This is an inserted EPS graphic

As in Fig.1, the analogous can be done with the **Participation Number**, as Fig.2 shows.

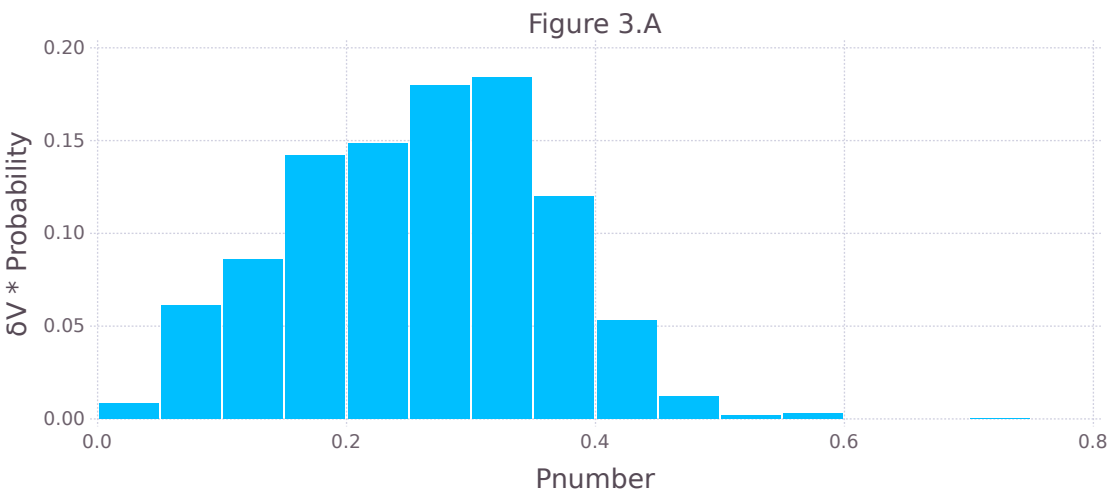


Figure 211. This is an inserted EPS graphic

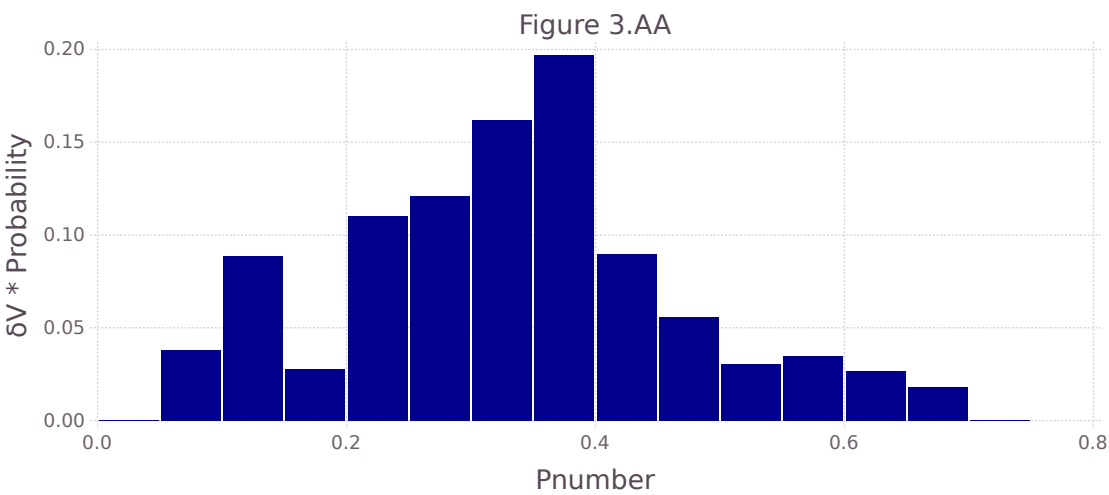


Figure 212. This is an inserted EPS graphic

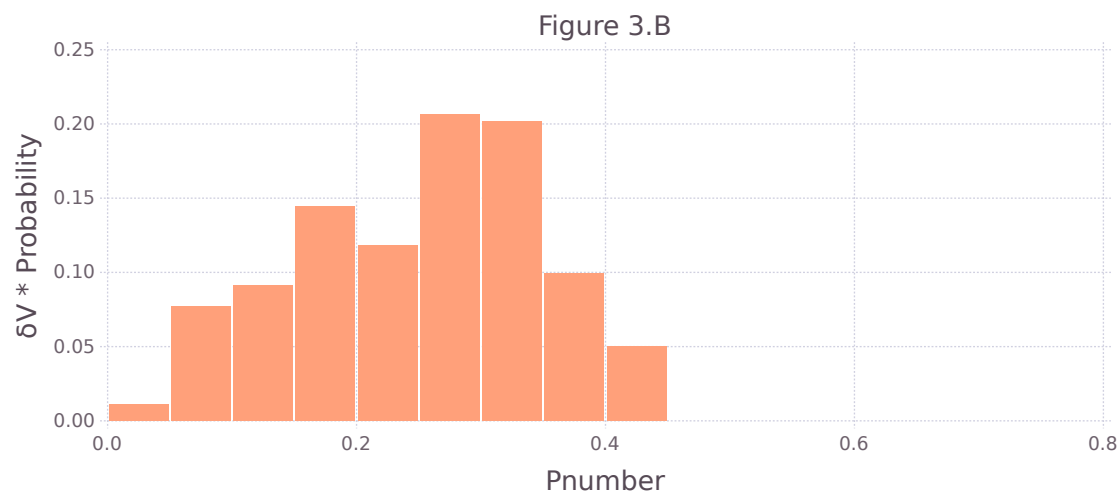


Figure 213. This is an inserted EPS graphic

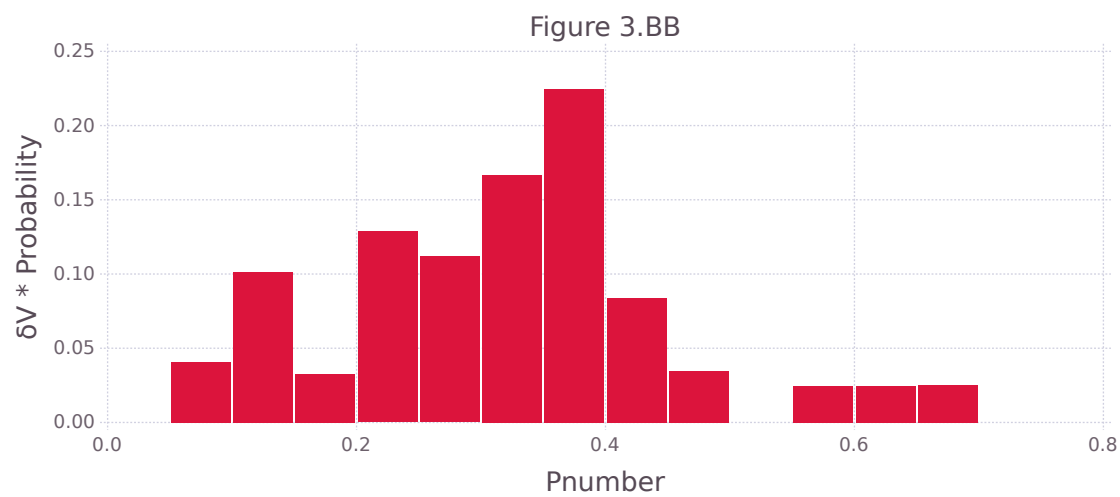


Figure 214. This is an inserted EPS graphic

VGV can be translated into cartesian coordinates and the module of the X, Y, Z coordinates obtained.

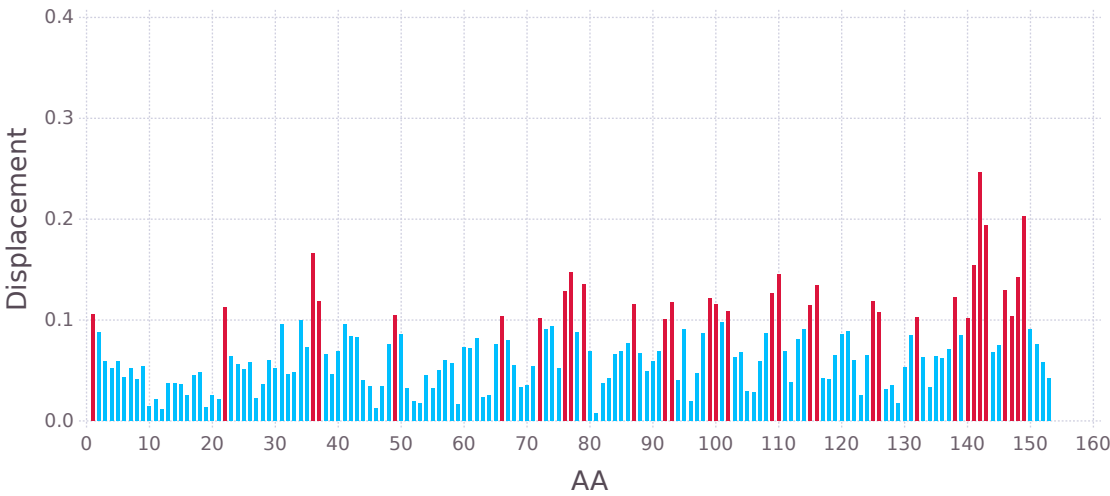


Figure 215. This is an inserted EPS graphic

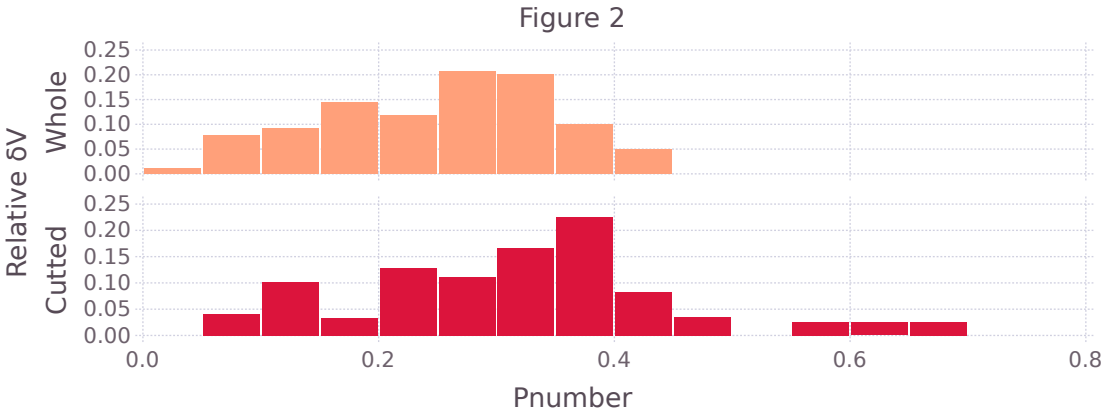


Figure 216. This is an inserted EPS graphic

7 Discussion

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8 Supporting Information

8.1 Molecular Dynamics

The 2 S-Hydroxycysteine amino acids in 1HVR were parametrized using the GAFF force field following AMBER developers recommendations. All molecules were simulated with leaprc.protein.ff14SB force field and solvated with TIP3P waters, forming a truncated octahedric box. Ions were added to neutralize each system.

All simulations were performed in the constant temperature and pressure (NTP) ensemble with $T = 300\text{K}$, $P = 1\text{bar}$, using the berendsen barostat and the Langevin thermostat with a γ collision frequency of 2 ps^{-1} .

The simulation step was 2fs, water molecules and all bond lengths to hydrogen atoms were constrained using the SHAKE algorithm. Nonbonded interactions were cutoff at 10 \AA . Long-range electrostatic interactions were calculated using the Particle Mesh Ewald method.

Essential modes were extracted from the mass-weighted correlation matrix of the alpha carbon atoms. All $3 * N - 6$ — where N is the number of amino acids—, vectors were used for the calculations.

References

1. Devaraju P, Gulati R, Antony PT, Mithun CB, Negi VS. Susceptibility to SLE in South Indian Tamils may be influenced by genetic selection pressure on TLR2 and TLR9 genes. *Mol Immunol.* 2014 Nov 22. pii: S0161-5890(14)00313-7. doi: 10.1016/j.molimm.2014.11.005