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Counting Polynomials on Regular Iterative Structures

Lorentz JÄNTSCHI [1,*], Mugur C. BĂLAN [1] and Sorana D. BOLBOACĂ [2]

[1] Technical University, Cluj-Napoca, 103-105 Muncii Boulevard, 400641 Cluj-Napoca, Romania.
[2] "Iuliu Haţieganu" University of Medicine and Pharmacy, 6 Louis Pasteur, 400349 Cluj-Napoca, Romania.

E-mail(s): lori@academicdirect.org; Mugur.Balan@termo.utcluj.ro; sbolboaca@umfcluj.ro

* Author to whom correspondence should be addressed; Tel.: +4-0264-401775.

Abstract: Subgraphs can results through application of criteria based on matrix which characterize the entire graph. The most important categories of criteria are the ones able to produce connected subgraphs (fragments). Theoretical frame on graph theory, a series of three molecular fragmentation algorithms on pair of atoms, and construction of four square matrices (Szeged, Cluj, MaxF, and CMaxF) containing the fragment's size are presented. New theoretical results on fragment's size and the order based on sizes are presented. The obtained matrices were used to obtain the counting polynomials for two series of regular structures. The informational analysis on the obtained distinct counting polynomials was performed by using informational entropy and energy. Structure-property relationship analysis has been also conducted on the obtained counting polynomials. The obtained results are discussed and the main conclusions are highlighted.

Keywords: Graph theory; Subgraphs; Graph polynomials; Entropy; Energy.

Introduction

Molecular Topology creates one of the most important junction between Graph Theory and Organic Chemistry. Some books were published in this interdisciplinary field, just one of them being [1]. Two main operational tools on this field are square matrices (the cell of matrix contains a graph theoretical property associated to the pairs of vertices) and graph polynomials. Counting polynomials were recently introduced as a tool for substructures count and sizes for a given fragmentation criteria [2] applied on a graph-type structure. The formulas have important chemical application, dealing with cycles of four, five, and six atoms, most frequent rings in organic chemistry.

The paper presents the counting polynomial formulas obtained on some regular structures by applying of three pair-based fragmentation algorithms. The counting polynomials were further investigated from the informational perspective when another series of entropy and energy formulas of polynomials were obtained. Finally, a structure-activity relationships study was conducted using the entropy and the energy of a polynomial formula as structure descriptors.

Graph Theory

Connected Un-Oriented Graphs and Distance Matrix

Let V be a set and $E \subseteq V \times V$. Then $G = (V, E)$ is an *un-oriented* graph. More, a graph is *connected* if there is a path from one to any other vertex.

Let $G = (V, E)$ be an un-oriented connected graph. We will note with $V(G)$ the *set of vertices* from G, with $E(G)$ the *set of edges* from G, and with $d(G)$ the *distance matrix* of G. In terms of distance matrix $d(G)$ the *connectivity* of G is translated in: $d(G)_{i,j} < \infty$ for any $i,j \in V(G)$.

Pair-Based Fragmentation in Graphs

Gutman first introduced the Szeged criterion [3]. The *Szeged subgraphs* $Sz(G)_{i,j}$ are obtained for a pair of different vertices (*i* and *j*). They are connected graphs (the set resulting from a geodesic operator), and were recently defined [4]. For $i,j \in V(G)$:

$$
\begin{aligned}
&Sz(G)_{i,j} = (V(Sz(G)_{i,j}), E(Sz(G)_{i,j}))\\
&V(Sz(G)_{i,j}) = \{s \in V(G) \mid d(G)_{s,i} < d(G)_{s,j}\}\\
&E(Sz(G)_{i,j}) = \{(s,t) \in E(G) \mid s,t \in V(Sz(G)_{i,j})\}
\end{aligned}
\tag{1}
$$

Jäntschi et al. introduced the ClujF criterion [5]. The property obtained by the set $CjF(G)_{i,j,p}$ when the ClujF criterion is applied was proved in [1] (Theorem 2.1, p. 31). The *ClujF subgraphs* are defined based on a path *p* from vertex *i* to vertex *j*:

$$CjF(G)_{i,j,p} = Sz(Gp)_{i,j} \tag{2}$$

where *Gp* is obtained from *G* by withdrawing of the edges of the path *p*.

The largest subgraph obtained from *G* containing the *i* vertex and not containing the *j* vertex is considered to be a maximal connected subgraph (relative to i and j vertices). Let us call this subgraph $MaxF(G)_{i,j}$.

Maximal connected subgraphs can be defined through construction. Constructing a temporary graph, ($VTmp(G)_{i,j}$, $ETmp(G)_{i,j}$) defined below (which is a disconnected one), $V(MaxF(G)_{i,j})$ and $E(MaxF(G)_{i,j})$ sets result from it:

$$
\begin{aligned}
&VTmp(G)_{i,j} = \{s \in V(G) \mid s \neq j\}\\
&ETmp(G)_{i,j} = \{(u,v) \in E(G) \mid u,v \neq j\}\\
&V(MaxF(G)i,j) = \{s \in VTmp(G)i,j \mid d(VTmp(G)i,j)s,i < \infty\}\\
&E(MaxF(G)_{i,j}) = \{(s,t) \in E(G) \mid s,t \in V(MaxF(G)_{i,j})\}
\end{aligned}
\tag{3}
$$

The *complementary of the maximal connected* subgraph $MaxF(G)_{i,j}$ named $CMaxF(G)_{i,j}$ is a new graph structure that is relative to graph *G*:

$$
\begin{aligned}
&CMaxF(G)_{i,j} = (V(CMaxF(G)_{i,j})\\
&E(CMaxF(G)_{i,j}))\\
&V(CMaxF(G)_{i,j}) = \{s \in V(G) \mid s \notin V(MaxF(G)_{i,j})\}\\
&E(CMaxF(G)_{i,j}) = \{(s,t) \in E(G) \mid s,t \in V(CMaxF(G)_{i,j})\}
\end{aligned}
\tag{4}
$$

Pair-Based Matrices in Graphs

The counting matrices containing the number of subgraphs vertices are formally known as pair-based matrices in graphs. Note that, in general these are unsymmetrical matrices. We will note the associated matrices using brackets [$\cdot$] for every above-defined criterion.

The definition for [*MaxF*], [*CMaxF*], and [*Sz*] matrices are similar to each other. For *CjF* a consistent matrix definition was found (in [2]) if max function is used on all set of paths between vertices (and the name became [*CjFM*] consequently):

$$[C]_{i,j} = |C(G)_{i,j}| \tag{5}$$

where $C \in \{MaxF, CMaxF, Sz\}$

$$[CjFM]_{i,j} = \max\{|CjF(G)_{i,j,p}| \tag{6}$$

when $p \in P(G)_{i,j}\}$.

Subgraph Relationships

A graph $H=(W,F)$ is called subgraph of $G=(V,E)$ if $W \subseteq V$ and $F \subseteq E$ holds and note this relationship (of partial order) as $H \leq G$.

Following relations hold, and $CMaxF(G)_{i,j}$, $SzF(G)_{i,j}$, $CjF(G)_{i,j,p}$, $MaxF(G)_{i,j}$ are connected subgraphs of *G*:

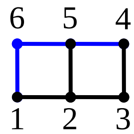
$$
\begin{aligned}
&\mathrm{CMaxF(G)}_{i,j} \leq \mathrm{G}\\
&\mathrm{SzF(G)}_{i,j} \leq \mathrm{MaxF(G)}_{i,j}\\
&\mathrm{CjF(G)}_{i,j,p} \leq \mathrm{MaxF(G)}_{i,j}\\
&\mathrm{MaxF(G)}_{i,j} \leq \mathrm{G}
\end{aligned}
\tag{7}
$$

Other results can be obtained as consequence of Eq(7):

$$
\begin{aligned}
&\mathrm{CMaxF(G)j,i} \leq \mathrm{SzF(G)i,j}\\
&\mathrm{CMaxF(G)j,i} \leq \mathrm{CjF(G)i,j,p}
\end{aligned}
\tag{8}
$$

Proving of the above result is reduced to checking of vertices inclusion, since all implied subgraphs were defined containing all possible edges borrowed from *G*. Let be $v \in CMaxF(G)_{j,i}$. Removing of *i* vertex from *G* makes the vertex *v* inaccessible from *j* through a path (according to *CMax* definition). It results that all paths from *j* to *v* visits *i* in *G*, including the shortest paths, and then the *v* vertex belongs also to the $SzF(G)_{i,j}$ set (having all paths from *j* to *v* longer than a path from *v* to *i*). Removing of a path from *i* to *j* in *G* does not affect the *v* vertices (because to arrive in these vertices from vertex *j* is necessary to visit vertex *i*), and thus the second partial order relationship is proved.

Even if, in general, $SzF(G)_{i,j}$ is a larger subgraph than $CjF(G)_{i,j,p}$ (because of removal of the path *p*) the partial ordering between $SzF(G)_{i,j}$ and $CjF(G)_{i,j,p}$ is not a general rule, and the following example gives the proof of this. Let us take the graph $G = (\{1..6\},\{(1,2),(1,6),(2,3),(2,5),(3,4),(4,5),(5,6)\})$ - see figure, and set *i* to 1 and *j* to 4. For this graph $CjF_{1,4,[1,6,5,4]}=\{1,2,5\}$ and $Sz_{1,4}=\{1,2,6\}$ and $CjF(G)_{i,j,p}$ is not in general a subgraph of $SzF(G)_{i,j}$.



Ordering of Sizes

According to the Theorem 5 in [4] (and the proof of the inequality may be found in [4]), using [{*j*}] and [*V(G)*\{*j*}] as notations for matrices having all entries equal with sizes of {*j*} and *V(G)*\{*j*} respectively, excepting first diagonal where are zeros, the followings are true:

$$
\begin{aligned}
&\sum_{i,j\in V(G)}[\{j\}]_{i,j} = |V(G)|\cdot(|V(G)|-1)\\
&\sum_{i,j\in V(G)}[V(G)\setminus\{j\}]_{i,j} = |V(G)|\cdot(|V(G)|-1)^2\\
&\sum_{i,j\in V(G)}[\{j\}]_{i,j} \leq \sum_{i,j\in V(G)}[\mathrm{CMaxF}]_{i,j} \leq \sum_{i,j\in V(G)}[\mathrm{CjF}]_{i,j} \leq \sum_{i,j\in V(G)}[\mathrm{Sz}]_{i,j} \leq \sum_{i,j\in V(G)}[\mathrm{MaxF}]_{i,j} \leq \sum_{i,j\in V(G)}[V(G)\setminus\{j\}]_{i,j}
\end{aligned}
\tag{9}
$$

Note that the inequality is slightly changed, including here $[CjF]_{i,j,p}$ in place of $[CjFM]_{i,j}$. The inequality still holds. Indeed, since for max was already proof (Theorem 5 in [4]), for remaining paths (which not provide the largest sets) only first part of the inequality must be prove ($\Sigma[CMaxF]_{i,j} \leq \Sigma[CjF]_{i,j}$). But, for this relationship we already have (from previous section) that $CMaxF(G)_{j,i} \leq CjF(G)_{i,j,p}$ which implies $[CMaxF]_{j,i} \leq [CjF]_{i,j,p}$ on every *(i,j)* pair and any path. Just applying the sum operator to this relationship, the proof is done.

Counting Polynomials

A counting polynomial for a graph structure (see Figure 1) is a polynomial formula depending on the structure, and on the applied criteria; it is frequently expressed using an undetermined variable X. The polynomial formula characterizes the entire graph though its monomes and every monome describes the results of an independent event on which counting operation is applied. Thus, a rank of a monome express the magnitude of the event - the size of the subgraphs obtained from the graph structure by applying the criteria, while a coefficient of a monome express the frequency of an event - number of subgraphs obtained from the graph structure having same size by applying the criteria.

Obtaining of polynomial formulas have important applications in chemical graph theory and structure-activity relationships [6,7]. Thus, theoretical approaches on counting polynomials may have important application in these fields.

Three Classical Regular Structures

The regular structures presented in Figure 1 were considered as classical regular structures in this study.

The obtained counting polynomials for the structures presented in Figure 1 based on MaxF, CMaxF, CJFM, and Sz criteria are presented in Table 1.

The sign [·] stands for "integer part of". The followings express the truncate function:

$$\left[\frac{Y}{2}\right]=\frac{Y+\frac{(-1)^{Y}-1}{2}}{2},\left[\frac{Y-1}{2}\right]=\frac{Y-\frac{(-1)^{Y}+3}{2}}{2},\left[\frac{Y+1}{2}\right]=\frac{Y-\frac{(-1)^{Y}-1}{2}}{2} \tag{10}$$

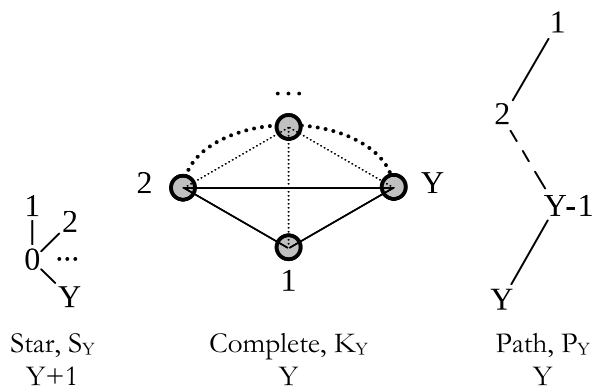


Figure 1. Regular structures and their number of vertices.

Table 1. Counting polynomials on regular structures from Figure 1.

Criterion	Star (S_Y)	Complete (K_Y)	Path (P_Y)
MaxF	$P_1(Y,X)=YX^1+Y^2X^Y$	$P_3(Y,X)=Y(Y-1)X^{Y-1}$	$P_5(Y,X)$
CMaxF			
CJFM	$P_2(Y,X)=Y^2X^1+YX^Y$	$P_4(Y,X)=Y(Y-1)X$	$P_6(Y,X)$
Sz			$P_7(Y,X)$

The counting polynomials formulas on the structures presented in Figure 1 are:

$$P_5 = 2\sum_{p=1}^{Y-i} pX^p \tag{11}$$

$$P_6 = 2\sum_{p=1}^{Y-1} (Y-p)X^p \tag{12}$$

$$P_7 = \sum_{p=1}^{[(Y-1)/2]} 4pX^4 + \sum_{p=1}^{[Y/2]} (4p-2)X^{Y-p} \tag{13}$$

Other Repeated Structures

Four repeated cyclic structure (noted *$G_3(Y)$, $G_4(Y)$, $G_5(Y)$,* and *$G_6(Y)$*) were also considered (Figure 2). The abbreviations of counting polynomials of these structures are presented in Table 2.

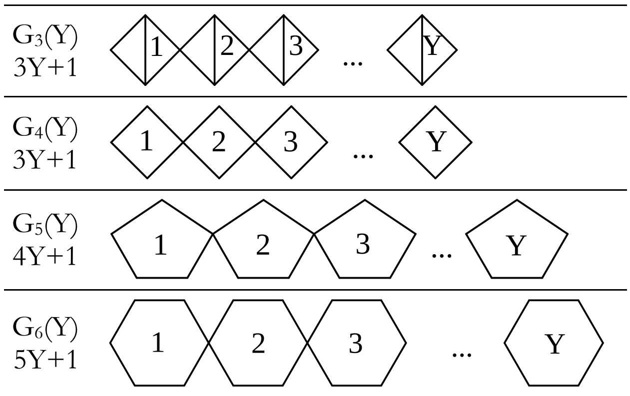


Figure 2. Four repeated cyclic structures and their sizes.

Table 2. Counting polynomials abbreviations of structures from Figure 2.

Criterion	$G_3(Y)$	$G_4(Y)$	$G_5(Y)$	$G_6(Y)$
MaxF	$P_8(Y,X)$	not computed	not computed	not computed
CMaxF	$P_9(Y,X)$	not computed	not computed	not computed
CJFM	$P_{10}(Y,X)$	not computed	not computed	not computed
Sz	$P_{11}(Y,X)$	$P_{12}(Y,X)$	$P_{13}(Y,X)$	$P_{14}(Y,X)$

Counting polynomials for the structures presented in Figure 2 are as follows:

$$P_8 = 6Y^2X^{3Y} + 6\sum_{P=1}^{Y} pX^{3p} = 6Y(Y+1)X^{3Y} + 6\sum_{p=1}^{Y-1} pX^{3p} \tag{14}$$

$$P_9 = 6Y^2X + 6\sum_{P=1}^{Y}(Y-P)X^{3p+1} = 6Y(Y+1)X + 6\sum_{p=1}^{Y-1}(Y-p)X^{3p+1} \tag{15}$$

$$P_{10} = 2(Y+3)X + 2(3Y-1)X^2 + \sum_{p=1}^{Y-1} 2X^{3p}(6(Y-p) + 3X + (3(Y-p)-1)X^2) \tag{16}$$

$$P_{11} = 2(Y+3)X + 4X^2 + \sum_{p=2}^{Y}\left(\frac{18p-7-(-1)^p}{2}X^{\frac{6p-1+(-1)^p}{4}} + \frac{18p-17+(-1)^p}{2}X^{3Y-\frac{6p-5+(-1)^p}{4}} + 4X^{3p-1}\right) \tag{17}$$

$$P_{12} = \sum_{p=2}^{Y}\left(\frac{18p-19-5(-1)^p}{2}X^{\frac{6p-1+(-1)^p}{4}} + \frac{18p-29+5(-1)^p}{2}X^{3Y-\frac{6p-5+(-1)_p}{4}} + 16X^{3p-4}\right) + 2(Y+1)X + 8X3Y - 1 \tag{18}$$

$$\begin{aligned} P_{13} = {} & 4(Y+4)X^2 + 8((-1)^Y + 1)X^{2Y-1}(X+1)(YX^2 - X + Y) + \\ & + 8\sum_{p=2}^{[(Y+1)/2]} X^{4p-5}(2p-2+(2p-3)X+(2p-2)X^2+2pX^3) + \\ & + \sum_{p=2}^{[(Y+1)/2]} X^{4Y-4p+3}(2p-1+(2p-3)X+(2p-3)X^2+(2p-2)X^3) \end{aligned} \tag{19}$$

$$\begin{aligned} P_{14} = {} & 4(Y+2)X^2 + 18X^{5Y-2} + 16\sum_{p=2}^{Y} X^{5p-6}(X^3+1) + \\ & + 2\sum_{p=2}^{(Y/2)+1}((17p-19)X^{5p-7} + (17p-31)X^{5p-5} + 4(4p-7)X^{5(Y-p)+6}) + \\ & + 2\sum_{p=2}^{[(Y+1)/2]}((17p-4)X^{5(Y-p)+3} + (17p-29)X^{5(Y-p)+5} + 4(4p-5)X^{5p-4}) \end{aligned} \tag{20}$$

Polynomials by Examples: Classical Regular and Repeated Structures

The definition formula of counting polynomials found some applications in investigation of structure-activity relationships [7], characterization of nanostructures [8], investigation of indeterminate over a finite field and with bounded degree polynomials [9], irreducible polynomials on a finite field [10], etc.

A series of calculations were performed on proposed regular structures (S_Y, K_Y, P_Y, G_3, G_4, G_5, and G6, see Figure 1 and 2) by using a series of graph patterns. The polynomials for different values of repeating parameter Y are presented in Table 3. Note that the obtained results of counting polynomials on investigated repeated structures are general and are parameterized by the type of repeated structure and by the number of iterations.

Table 3. Polynomials of some regular structures for different values of Y.

Y	Graph	Criteria	Polynomial	Hartley	Expression
2	S_2	MaxF	$P_1(2,X)$	log2	$2{\cdot}X+4{\cdot}X^2$
2	S_2	CMaxF	$P_2(2,X)$	log2	$4{\cdot}X+2{\cdot}X^2$
2	S_2	CJFM	$P_2(2,X)$	log2	$4{\cdot}X+2{\cdot}X^2$
2	S_2	Sz	$P_2(2,X)$	log2	$4{\cdot}X+2{\cdot}X^2$
2	K_2	MaxF	$P_3(2,X)$	log1	$2{\cdot}X$
2	K_2	CMaxF	$P_4(2,X)$	log1	$2{\cdot}X$
2	K_2	CJFM	$P_4(2,X)$	log1	$2{\cdot}X$
2	K_2	Sz	$P_4(2,X)$	log1	$2{\cdot}X$
2	P_2	MaxF	$P_5(2,X)$	log1	$2{\cdot}X$
2	P_2	CMaxF	$P_6(2,X)$	log1	$2{\cdot}X$
2	P_2	CJFM	$P_6(2,X)$	log1	$2{\cdot}X$
2	P_2	Sz	$P_7(2,X)$	log1	$2{\cdot}X$
2	$G_3(2)$	MaxF	$P_8(2,X)$	log2	$6{\cdot}X^3+36{\cdot}X^6$
2	$G_3(2)$	CMaxF	$P_9(2,X)$	log2	$36{\cdot}X^1+6{\cdot}X^4$
2	$G_3(2)$	CJFM	$P_{10}(2,X)$	log5	$10{\cdot}X+10{\cdot}X^2+12{\cdot}X^3+6{\cdot}X^4+4{\cdot}X^5$
2	$G_3(2)$	Sz	$P_{11}(2,X)$	log5	$10{\cdot}X+4{\cdot}X^2+14{\cdot}X^3+10{\cdot}X^4+4{\cdot}X^5$
2	$G_4(2)$	Sz	$P_{12}(2,X)$	log5	$6{\cdot}X+16{\cdot}X^2+6{\cdot}X^3+6{\cdot}X^4+8{\cdot}X^5$
2	$G_5(2)$	Sz	$P_{13}(2,X)$	log5	$24{\cdot}X^2+16{\cdot}X^3+8{\cdot}X^4+8{\cdot}X^5+16{\cdot}X^6$
2	$G_6(2)$	Sz	$P_{14}(2,X)$	log7	$16{\cdot}X^2+30{\cdot}X^3+16{\cdot}X^4+6{\cdot}X^5+8{\cdot}X^6+16{\cdot}X^7+18{\cdot}X^8$
3	S_3	MaxF	$P_1(3,X)$	log2	$3{\cdot}X+9{\cdot}X^3$
3	S_3	CMaxF	$P_2(3,X)$	log2	$9{\cdot}X+3{\cdot}X^3$
3	S_3	CJFM	$P_2(3,X)$	log2	$9{\cdot}X+3{\cdot}X^3$
3	S_3	Sz	$P_2(3,X)$	log2	$9{\cdot}X+3{\cdot}X^3$
3	K_3	MaxF	$P_3(3,X)$	log1	$6{\cdot}X^2$
3	K_3	CMaxF	$P_4(3,X)$	log1	$6{\cdot}X$
3	K_3	CJFM	$P_4(3,X)$	log1	$6{\cdot}X$
3	K_3	Sz	$P_4(3,X)$	log1	$6{\cdot}X$
3	P_3	MaxF	$P_5(3,X)$	log2	$2{\cdot}X+4{\cdot}X^2$
3	P_3	CMaxF	$P_6(3,X)$	log2	$4{\cdot}X+2{\cdot}X^2$
3	P_3	CJFM	$P_6(3,X)$	log2	$4{\cdot}X+2{\cdot}X^2$
3	P_3	Sz	$P_7(3,X)$	log2	$4{\cdot}X+2{\cdot}X^2$
3	$G_3(3)$	MaxF	$P_8(3,X)$	log3	$6{\cdot}X^3+12{\cdot}X^6+72{\cdot}X^9$
3	$G_3(3)$	CMaxF	$P_9(3,X)$	log3	$72{\cdot}X+12{\cdot}X^4+6{\cdot}X^7$
3	$G_3(3)$	CJFM	$P_{10}(3,X)$	log8	$12{\cdot}X+16{\cdot}X^2+24{\cdot}X^3+6{\cdot}X^4+10{\cdot}X^5+12{\cdot}X^6+6{\cdot}X^7+4{\cdot}X^8$
3	$G_3(3)$	Sz	$P_{11}(3,X)$	log8	$12{\cdot}X+4{\cdot}X^2+14{\cdot}X^3+24{\cdot}X^4+4{\cdot}X^5 + 18{\cdot}X^6+10{\cdot}X^7+4{\cdot}X^8$
3	$G_4(3)$	Sz	$P_{12}(3,X)$	log8	$8{\cdot}X+16{\cdot}X^2+6{\cdot}X^3+20{\cdot}X^4+16{\cdot}X^5+10{\cdot}X^6+6{\cdot}X^7+8{\cdot}X^8$
3	$G_5(3)$	Sz	$P_{13}(3,X)$	log9	$28{\cdot}X^2+16{\cdot}X^3+8{\cdot}X^4+16{\cdot}X^5+32{\cdot}X^6+24{\cdot}X^7+8{\cdot}X^8+8{\cdot}X^9+ 16{\cdot}X^{10}$
3	$G_6(3)$	Sz	$P_{14}(3,X)$	log12	$20{\cdot}X^2+30{\cdot}X^3+16{\cdot}X^4+6{\cdot}X^5+24{\cdot}X^6+16{\cdot}X^7+60{\cdot}X^8+16{\cdot}X^9+ 10{\cdot}X^{10}+8{\cdot}X^{11}+16{\cdot}X^{12}+18{\cdot}X^{13}$

S_Y = S_Y star; K_Y = K_Y complete; P_Y = P_Y path;
Harley = Harley's entropy; G_3, G_4, G_5, G_6 = repeated cyclic structures (see Figure 2)

Entropy and Energy of Counting Polynomials

Two parameters derived from the information obtained through graph theory on counting polynomials were analyzed: entropy and energy.

Let a counting polynomial be given by the general formula $P=\Sigma_{1\le i\le n}a_i x^{b_i}$. Let $A=(a_i)_{1\le i\le n}$ and $B=(b_i)_{1\le i\le n}$ being arrays of the counting polynomials coefficients (a_i) and powers (b_i), respectively. The coefficient a_i is the apparition frequency of a fragment of size b_i. The polynomial formula represents the probability space through A (the frequency space) and B (events space). This formula allows obtaining entropies (from a_i) and energies (from a_i and b_i) of counting polynomials.

The Rényi entropy formula [11] for a counting polynomial is given by the formula:

$$H_\alpha(P) = \frac{1}{1-\alpha}\log_2\sum_{i=1}^{n} p_i^\alpha \tag{21}$$

where α = non-negative number, and $p_i = a_i/\sum(a_i)$.

The following parameters were defined starting with Rényi entropy formula and were computed for the investigated patterns:

- $\alpha = 0$: $H_0(P)$ = logarithm of the cardinality of X, sometimes called the *Hartley's entropy* of X (max entropy) [12]. It is important for information reconciliation, which is an error correction:

$$H_0(P) = \log_2\sum_{i=1}^{n} 1 \tag{22}$$

- $\alpha = 1$: $H_1(P)$ = *Shannon's entropy* [13]:

$$H_1(P) = -\sum_{i=1}^{n} p_i \cdot \log_2 \cdot p_i \tag{23}$$

- $\alpha = 2$: $H_2(P)$ = negative logarithm of the *Simpson diversity index* [14]:

$$H_2(P) = -\log_2\sum_{i=1}^{n} p_i^2 \tag{24}$$

- $\alpha = \infty$: $H_\infty(X)$ = min entropy [15]:

$$H_\infty(P) = -\log_2\left(\max_{i=1}^{n} p_i\right) \tag{25}$$

The following property is applied on the above entropy equations: $H_\infty \le H_2 \le 2\cdot H_\infty$.

The energy, an attribute of systems, could also be computed for polynomials. Four formulas were used to compute the energy of investigated counting polynomials:

$$E_1(P) = \sum_{i=1}^{n} b_i \tag{26}$$

$$E_2(P) = \sum_{i=1}^{n} b_i^2 \tag{27}$$

$$HE_1(P) = \frac{\sum_{i=1}^{n} a_i b_i}{\sum_{i=1}^{n} a_i} \tag{28}$$

$$HE_2(P) = \frac{\sum_{i=1}^{n} a_i b_i^2}{\sum_{i=1}^{n} a_i} \qquad (29)$$

The entropy of a polynomial formula is defined by the frequency of apparition of molecular fragments of specified size and it is comprises in the coefficients of the formula. The energy of a polynomial formula take here four forms, two of them being obtained exclusively based on the size of molecular fragments comprises in the polynomial formula at the level of rank of polynomial variable. The other two energy formulas are obtained through weighting sizes fragments with frequencies of their occurrence.

Generic Equations: Entropies and Energies of Counting Polynomials on Investigated Structures

The generic equations of entropies and energies on investigated structures are presented in tables as follows:

- Hartley's entropy (H_0): Table 4. Some examples of equations describing Hartley's entropy [11] of the obtained connected structures through considered fragmentation criteria (MaxF, CMaxF, Sz, CJFM) on investigated graph patterns (S_Y, K_Y, P_Y, G_3, G_4, G_5, G_6) are presented in this table.
- Min entropy (H_∞): Table 5.
- Diversity (D_2) and Renyi's entropy (H_2) equations: Table 6.
- Shannon's entropy (H_1): Table 7.
- E_1 & E_2 energy: Table 8 & 9.
- HE_1 & HE_2 energy: Table 10.

Tables 4-11 contain whenever possible the exact formulas of entropies (see Table 4-7) and energies (see Table 8-11) on the investigated counting polynomials. Some exceptions are observed on the Shannon's entropy, where the exact formulas were obtained just for the first four counting polynomial formulas. The Shannon entropy for other than first four counting polynomials are just approximations of the exact formulas and are given with associated significance levels (see Table 7) obtained through comparison with the exact formula obtained based on counting polynomial formulas of first twenty representative. The limit values for entropy and energy associated to the iteration close to ∞ were also included in the tables (Table 4-11) when was appropriate.

Table 4. Hartley's entropy equations on investigated counting polynomials

P	H_0 Calculations	H_0 Formulas
P_1 P_2	$\log_2(1+1)$ $\log_2(1+1)$	$H_0(P_1,Y) = H_0(P_2,Y) = 1$
P_3 P_4	$\log_2(1)$ $\log_2(1)$	$H_0(P_3,Y) = H_0(P_4,Y) = 0$
P_5 P_6 P_7	$\log_2\Sigma_{1\le p\le Y-1}1$ $\log_2\Sigma_{1\le p\le Y-1}1$ $\log_2(\Sigma_{1\le p\le[(Y-1)/2]}1+\Sigma_{1\le p\le[Y/2]}1)$	$H_0(P_5,Y) = H_0(P_6,Y) = H_0(P_7,Y) = \log_2(Y-1)$ $H_0(P_5,Y) = H_0(P_6,Y) = H_0(P_7,Y) \rightarrow \log_2 Y$
P_8 P_9	$\log_2(1+\Sigma_{1\le p\le Y-1}1)$ $\log_2(1+\Sigma_{1\le p\le Y-1}1)$	$H_0(P_8,Y) = H_0(P_9,Y) = \log_2 Y$
P_{10} P_{11} P_{12}	$\log_2(2+3\Sigma_{1\le p\le Y-1}1)$ $\log_2(2+3\Sigma_{2\le p\le Y}1)$ $\log_2(2+3\Sigma_{2\le p\le Y}1)$	$H_0(P_{10},Y) = H_0(P_{11},Y) = H_0(P_{12},Y) = \log_2(3Y-1)$ $H_0(P_{10},Y) = H_0(P_{11},Y) = H_0(P_{12},Y) \rightarrow \log_2 Y$
P_{13}	$\log_2(3+2(-1)^Y)+8\Sigma_{2\le p\le[(Y+1)/2]}1)$	$H_0(P_{13},Y) = \log_2(4Y-3)$ $H_0(P_{13},Y) \rightarrow \log_2 Y$
P_{14}	$\log_2(2+2\Sigma_{2\le p\le Y}1+3\Sigma_{2\le p\le Y}1)$	$H_0(P_{14},Y) = \log_2(5Y-3)$ $H_0(P_{14},Y) \rightarrow \log_2 Y$

Table 5. Min-entropy equations on counting polynomials

P	H_∞ Formula*
P_1	$H_\infty N(P_1,Y) = H_\infty N(P_2,Y) = Y^2$
P_2	$H_\infty D(P_1,Y) = H_\infty D(P_2,Y) = Y^2+Y$
	$H_\infty(P_1,Y) = H_\infty(P_2,Y) = \log_2(1+Y^{-1})$
	$H_\infty(P_1,Y) = H_\infty(P_2,Y) \to 0$
P_3	$H_\infty N(P_3,Y) = H_\infty N(P_4,Y) = Y(Y-1)$
P_4	$H_\infty D(P_3,Y) = H_\infty D(P_4,Y) = Y(Y-1)$
	$H_\infty(P_3,Y) = H_\infty(P_4,Y) = 0$
P_5	$H_\infty N(P_5,Y) = H_\infty N(P_6,Y) = H_\infty N(P_7,Y) = 2(Y-1)$
P_6	$H_\infty D(P_5,Y) = H_\infty D(P_6,Y) = H_\infty D(P_7,Y) = Y(Y-1)$
P_7	$H_\infty(P_5,Y) = H_\infty(P_6,Y) = H_\infty(P_7,Y) = \max(0,\log_2 Y)$
	$H_\infty(P_5,Y) = H_\infty(P_6,Y) = H_\infty(P_7,Y) \to \log_2 Y$
P_8	$H_\infty N(P_8,Y) = H_\infty N(P_9,Y) = 6Y(Y+1)$
P_9	$H_\infty D(P_8,Y) = H_\infty D(P_9,Y) = 3Y(3Y+1)$
	$H_\infty(P_8,Y) = H_\infty(P_9,Y) = \log_2[(3Y+1)/(Y+1)]-1$
	$H_\infty(P_8,Y) = H_\infty(P_9,Y) \to \log_2 3 - 1$
P_{10}	$H_\infty N(P_{10},1) = 8$; $H_\infty N(P_{10},Y) = 12(Y-1)$, $Y>1$
	$H_\infty D(P_{10},Y) = 3Y(3Y+1)$
	$H_\infty(P_{10},1) = 2-\log_2 3$; $H_\infty(P_{10},Y) = \log_2[Y(3Y+1)/(Y-1)]-2$, $Y>1$
	$H_\infty(P_{10},Y) \to \log_2 Y$
P_{11}	$H_\infty N(P_{11},1) = 8$; $H_\infty N(P_{11},Y) = [18Y-7-(-1)^Y]/2$, $Y>1$
	$H_\infty D(P_{11},Y) = 3Y(3Y+1)$
	$H_\infty(P_{11},1) = 2-\log_2 3$; $H_\infty(P_{11},Y) = \log_2[Y(18Y+6)/[18Y-7-(-1)^Y]]$, $Y>1$
	$H_\infty(P_{11},Y) \to \log_2 Y$
P_{12}	$H_\infty N(P_{12},1) = 8$; $H_\infty N(P_{12},2) = 16$; $H_\infty N(P_{12},Y) = [18Y-19+5(-1)^Y]/2$, $Y>2$
	$H_\infty D(P_{12},Y) = 3Y(3Y+1)$
	$H_\infty(P_{12},1) = 2-\log_2 3$; $H_\infty(P_{12},2) = \log_2 21-3$; $H_\infty(P_{12},Y) = \log_2[6Y(3Y+1)/[18Y-19+5(-1)^Y]]$, $Y>2$
	$H_\infty(P_{12},Y) \to \log_2 Y$
P_{13}	$H_\infty N(P_{13},1) = 20$; $H_\infty N(P_{13},Y) = 8Y + 4 + 4(-1)^Y$, $Y>1$
	$H_\infty D(P_{13},Y) = 4Y(4Y+1)$
	$H_\infty(P_{13},1) = 0$; $H_\infty(P_{13},Y) = \log_2[Y(4Y+1)/[2Y+1+(-1)^Y]]$, $Y>1$
	$H_\infty(P_{13},Y) \to \log_2 Y$
P_{14}	$H_\infty N(P_{14},1) = 18$; $H_\infty N(P_{14},Y) = [34Y+5-13(-1)^Y]/2$, $Y>1$
	$H_\infty D(P_{14},Y) = 5Y(5Y+1)$
	$H_\infty(P_{14},1) = \log_2 5-\log_2 3$; $H_\infty(P_{13},Y) = \log_2[10Y(5Y+1)/[34Y+5-13(-1)^Y]]$, $Y>1$
	$H_\infty(P_{14},Y) \to \log_2 Y$

* $H_\infty N(\cdot)$ - $H_\infty(\cdot)$ Numerator; $H_\infty N(\cdot)$ - $H_\infty D(\cdot)$ Denominator; limit formula = for large Y

Table 6. Diversity (D_2) and Renyi entropy (H_2) equations on counting polynomials

P	H_2 Formula *
P_1	$H_2N(P_1,Y) = H_2N(P_2,Y) = Y^2(Y^2+1)$
P_2	$H_2D(P_1,Y) = H_2D(P_2,Y) = H_\infty D^2(P_1,Y) = H_\infty D^2(P_2,Y)$
	$D_2(P_1,Y) = D_2(P_2,Y) = (Y^2+1)/(Y+1)^2$
	$H_2(P_1,Y) = H_2(P_2,Y) = \log_2(Y+1)^2/(Y^2+1)$
	$D_2(P_1,Y) = D_2(P_2,Y) \to 1$
	$H_2(P_1,Y) = H_2(P_2,Y) \to 0$
P_3	$H_2N(P_3,Y) = H_2N(P_4,Y) = Y^2(Y-1)^2$
P_4	$H_2D(P_3,Y) = H_2D(P_4,Y) = H_\infty D^2(P_3,Y) = H_\infty D^2(P_4,Y)$
	$D_2(P_3,Y) = D_2(P_4,Y) = 1$
	$H_2(P_3,Y) = H_2(P_4,Y) = 0$
P_5	$H_2N(P_5,Y) = H_2N(P_6,Y) = H_2N(P_7,Y) = (2Y/3)(2Y^2-Y+1)$
P_6	$H_2D(P_5,Y) = H_2D(P_6,Y) = H_2D(P_7,Y) = H_\infty D^2(P_5,Y) = H_\infty D^2(P_6,Y) = H_\infty D^2(P_7,Y)$
P_7	$D_2(P_4,Y) = D_2(P_5,Y) = D_2(P_6,Y) = (4Y^2-2Y+2)/(6Y(Y-1)^2)$
	$H_2(P_5,Y) = H_2(P_6,Y) = H_2(P_7,Y) = \log_2[6Y(Y-1)^2]/(4Y^2-2Y+2)$
	$D_2(P_5,Y) = D_2(P_6,Y) = D_2(P_7,Y) \to 2Y^{-1}/3$
	$H_2(P_5,Y) = H_2(P_6,Y) = H_2(P_7,Y) \to \log_2 Y$

Table 6. Continuation

P	H_2 Formula *
P_8	$H_2N(P_8,Y) = H_2N(P_9,Y) = 6Y(6Y^3+14Y^2+3Y+1)$
P_9	$H_2D(P_8,Y) = H_2D(P_9,Y) = H_\infty D^2(P_8,Y) = H_\infty D^2(P_9,Y)$
	$D_2(P_8,Y) = D_2(P_9,Y) = (12Y^3+28Y^2+6Y+2)/[3Y(3Y+1)^2]$
	$H_2(P_8,Y) = H_2(P_9,Y) = \log_2[3Y(3Y+1)^2]/(12Y^3+28Y^2+6Y+2)$
	$D_2(P_8,Y) = D_2(P_9,Y) \to 4/9$
	$H_2(P_8,Y) = H_2(P_9,Y) \to 2\log_2 3-2$
P_{10}	$H_2N(P_{10},Y) = 2Y(30Y^2-31Y+41)$
	$H_2D(P_{10},Y) = H_\infty D^2(P_{10},Y)$
	$D_2(P_{10},Y) =(60Y^2-62Y+82)/[9Y(3Y+1)^2]$
	$H_2(P_{10},Y) = \log_2[9Y(3Y+1)^2]/(60Y^2-62Y+82)$
	$D_2(P_{10},Y) \to 20Y^{-1}/27$
	$H_2(P_{10},Y) \to \log_2 Y$
P_{11}	$H_2N(P_{11},1) = 80$; $H_2N(P_{11},Y) = Y(54Y^2-23Y+44)+5/2[1-(-1)^Y]$, $Y>1$
	$H_2D(P_{11},Y) = H_\infty D^2(P_{11},Y)$
	$D_2(P_{11},1) = 5/9$; $D_2(P11,Y) = [Y(54Y^2-23Y+44)+5/2[1-(-1)]^2]/[9Y^2(3Y+1)^2]$
	$H_2(P_{11},1) = 2\log_2 3-\log_2 5$; $H_2(P11,Y) = \log_2[9Y^2(3Y+1)^2/(Y(54Y^2-23Y+44)+5/2(1-(-1))^Y)]$, $Y>1$
	$D_2(P_{11},Y) \to 2Y^{-1}/3$
	$H_2(P_{11},Y) \to \log_2 Y$
P_{12}	$H_2N(P_{12},1) = 80$; $H_2N(P_{12},2) = 428$;
	$H_2N(P_{12},Y) =54Y^3-131Y^2+388Y-256+25/2(1-(-1)^Y)$, $Y>2$
	$H_2D(P_{12},Y) = H_\infty D^2(P_{12},Y)$
	$D_2(P_{12},1) = 5/9$; $D_2(P_{12},Y) = 107/441$;
	$D_2(P_{12},Y) =[Y(54Y^2-23Y+44)+5/2(1-(-1)^Y)]/(9Y^2(3Y+1)^2)$, $Y>2$
	$H_2(P_{12},1) = 2\log_2 3-\log_2 5$; $H_2(P_{12},2) = \log_2 441-\log_2 107$;
	$H_2(P_{12},Y) =[9Y^3(3Y+1)^2]/[Y(54Y^2-23Y+44)+5/2(1-(-1)^Y)]$, $Y>2$
	$D_2(P_{12},Y) \to 2Y^{-1}/3$
	$H_2(P_{12},Y) \to \log_2 Y$
P_{13}	$H_2N(P_{13},1) = 20$; $H_2N(P_{13},2) = 1216$;
	$H_2N(P_{13},Y) = (85+1/3)Y^3+16Y^2+(298+2/3)Y-64-64(-1)^Y$, $Y>2$
	$H_2D(P_{13},Y) = H_\infty D^2(P_{13},Y)$
	$D_2(P_{13},1) = 1$; $D_2(P_{13},2) = 19/81$;
	$D_2(P_{13},Y) =[(85+1/3)Y^3+16Y^2+(298+2/3)Y-64-64(-1)^Y]/(16Y^2(4Y+1)^2)$, $Y>2$
	$H_2(P_{13},Y) = 0$; $H_2(P13,Y) = 4\log_2 3-\log_2 19$;
	$H_2(P_{13},Y) =(16Y^2(4Y+1)^2)/[(85+1/3)Y^3+16Y^2+(298+2/3)Y-64-64(-1)^Y]$
	$D_2(P_{13},Y) \to Y^{-1}/3$
	$H_2(P_{13},Y) \to \log_2 Y$
P_{14}	$H_2N(P_{14},1) = 468$; $H_2N(P_{14},Y) =278Y^3-495Y^2+1664Y-959-481/2(1+(-1)^Y)$, $Y>1$
	$H_2D(P_{14},Y) = H_\infty D^2(P_{14},Y)$
	$D_2(P_{14},1) = 13/25$; $D_2(P_{14},Y) =[278Y^3-495Y^2+1664Y-959-481/2(1+(-1)^Y)]/(25Y^2(5Y+1)^2)$, $Y>1$
	$H_2(P_{14},Y) = 2\log_2 5-\log_2 13$; $H_2(P_{14},Y) =(25Y^2(5Y+1)^2)/[278Y^3-495Y^2+1664Y-959-481/2(1+(-1)^Y)]$, $Y>1$
	$D_2(P_{14},Y) \to 278Y^{-1}/625$
	$H_2(P_{14},Y) \to \log_2 Y$
P_{12}	$H_2N(P_{12},1) = 80$; $H_2N(P_{12},2) = 428$; $H_2N(P_{12},Y) =54Y^3-131Y^2+388Y-256+25/2(1-(-1)^Y)$, $Y>2$
	$H_2D(P_{12},Y) = H_\infty D^2(P_{12},Y)$
	$D_2(P_{12},1) = 5/9$; $D_2(P_{12},Y) = 107/441$;
	$D_2(P_{12},Y) =[Y(54Y^2-23Y+44)+5/2(1-(-1)^Y)]/(9Y^2(3Y+1)^2)$, $Y>2$
	$H_2(P_{12},1) = 2\log_2 3-\log_2 5$; $H_2(P_{15},2) = \log_2 441-\log_2 107$;
	$H_2(P_{12},Y) =()/[9Y^2(3Y+1)^2]/[Y(54Y^2-23Y+44)+5/2(1-(-1)^Y)]$, $Y>2$
	$D_2(P_{12},Y) \to 2Y^{-1}/3$
	$H_2(P_{12},Y) \to \log_2 Y$

Table 6. Continuation

P	H_2 Formula *
P_{13}	$H_2N(P_{13},1) = 20$; $H_2N(P_{13},2) = 1216$; $H_2N(P_{13},Y) = (85+1/3)Y^3+16Y^2+(298+2/3)Y-64-64(-1)^Y$, $Y>2$ $H_2D(P_{13},Y) = H_\infty D^2(P_{13},Y)$ $D_2(P_{13},1) = 1$; $D_2(P_{13},2) = 19/81$; $D_2(P_{13},Y) =[(85+1/3)Y^3+16Y^2+(298+2/3)Y-64-64(-1)^Y]/(16Y^2(4Y+1)^2)$, $Y>2$ $H_2(P_{13},Y) = 0$; $H_2(P_{13},Y) = 4\log_2 3-\log_2 19$; $H_2(P_{13},Y) = (16Y^2(4Y+1)^2)/[(85+1/3)Y^3+16Y^2+(298+2/3)Y-64-64(-1)^Y]$ $D_2(P_{13},Y) \to Y^{-1}/3$ $H_2(P_{13},Y) \to \log_2 Y$
P_{14}	$H_2N(P_{14},1) = 468$; $H_2N(P_{14},Y) =278Y^3-495Y^2+1664Y-959-481/2(1+(-1)^Y)$, $Y>1$ $H_2D(P_{14},Y) = H_\infty D^2(P_{14},Y)$ $D_2(P_{14},1) = 13/25$; $D_2(P_{14},Y) = [279Y^3-495Y^2+1664-959-481/2(1+(-1)^Y)]/(25Y^2(5Y+1)^2)$, $Y>1$ $H_2(P_{14},Y) = 2\log_2 5-\log_2 13$; $H_2(P_{14},Y) = (25Y^2(5Y+1)^2)/[278Y^3-495Y^2+1664Y-959-481/2(1+(-1)^Y)]$, $Y>1$ $D_2(P_{14},Y) \to 278Y^{-1}/625$ $H_2(P_{14},Y) \to \log_2 Y$

Table 7. Shannon's entropy equations on counting polynomials

P	H_1 Formulas*
P_1 P_2	$H_1(P_1,Y) = H_1(P_2,Y) =\log_2(Y+1)-[Y/(Y+1)]\log_2(Y)$; $H_1(P_1,Y) = H_1(P_2,Y) \to 0$
P_3 P_4	$H_1(P_3,Y) = H_1(P_4,Y) = 0$
P_5 P_6 P_7	$H_1(P_5,Y) = H_1(P_6,Y) = H_1(P_7,Y) \approx -(3.18(\pm0.02))/10+[1.0054(\pm0.0004)\log_2(Y-(7.88(\pm0.02))/10)]/[1+[1.55(\pm0.03)/10]/[Y-9.0(\pm0.3)/10]]$ $\approx$ $r^2 > 0.9999$; $F \approx 3\cdot10^9$ $H_1(P_5,Y) = H_1(P_6,Y) = H_1(P_7,Y) \to \log_2 Y$
P8 P9	$H_1(P8,Y) = H_1(P9,Y) \approx 6.60(\pm0.01)/10+5/14+\log_2[Y^2/(Y+2.60(\pm0.02))]$; $r^2 > 0.9999$; $F \approx 10^7$ $H_1(P8,Y) = H_1(P9,Y) \to (5/14)\log_2 Y$
P_{10}	$H_1(P_{10},Y) \approx 6.67(\pm0.01)/10+\log_2[Y+2.96(\pm0.02)-7.34(\pm0.14)/(Y+1.65(\pm0.03))]$; $r^2 > 0.9999$; $F \approx 3\cdot10^7$ $H_1(P10,Y) \to \log_2 Y$
P_{11}	$H_1(P_{11},Y) \approx 7.44(\pm0.02)/10+\log_2[Y+2.02(\pm0.03)-4.83(\pm0.17)/(Y+1.54(\pm0.06))]$; $r^2 > 0.9999$; $F \approx 10^7$ $H_1(P11,Y) \to \log_2 Y$
P_{12}	$H_1(P_{12},Y) \approx 1.71(\pm0.01)+6/7\log_2[Y-4.7(\pm0.2)/10]$; $r^2 > 0.999$; $F \approx 10^5$ $H_1(P_{12},Y) \to (6/7)\log_2 Y$
P_{13}	$H_1(P_{13},Y) \approx 1.878(\pm0.003)+125/128\log_2[Y-7.37(\pm0.03)/10]$; $r^2 > 0.9999$; $F \approx 10^6$ $H_1(P_{13},Y) \to (125/128)\log_2 Y$
P_{14}	$H_1(P_{14},Y) \approx 2.326(\pm0.004)+21/25\log_2[Y-6.74(\pm0.06)/10]$; $r^2 > 0.9999$; $F \approx 4\cdot10^5$ $H_1(P14,Y) \to (21/25)\log_2 Y$

* P_1-P_4: exact formula;

* P_5 - P_{14}: approximate formulas

Table 8. E_1 energy equations on counting polynomials

P	E_1 Formula
P_1 P_2	$E_1(P_1,1) = E_1(P_2,1) = 1$; $E_1(P_1,Y) = E_1(P_2,Y) = Y+1$, $Y>1$ $E_1(P_1,Y) = E_1(P_2,Y) \to Y$
P_3	$E_1(P_3,Y) = Y-1$ $E_1(P_3,Y) \to Y$
P_4	$E_1(P_4,Y) = 1$
P_5 P_6 P_7	$E_1(P_5,Y) = E_1(P_6,Y) = E_1(P_7,Y) =(Y^2-Y)/2$ $E_1(P_5,Y) = E_1(P_6,Y) = E_1(P_7,Y) \to Y^2/2$
P_8	$E_1(P_8,Y) =[3Y(Y+1)]/2$ $E_1(P_8,Y) \to 3Y^2/2$
P_9	$E_1(P_9,1) = 0$; $E_1(P_9,Y) =[Y(3Y-1)/2]$, $Y>1$ $E_1(P_9,Y) \to 3Y^2/2$
P_{10} P_{11} P_{12}	$E_1(P_{10},Y) = E_1(P_{11},Y) = E_1(P_{12},Y) =[3Y(3Y-1)/2]$ $E_1(P_{10},Y) = E_1(P_{11},Y) = E_1(P_{12},Y) \to 9Y^2/2$
P_{13}	$E_1(P_{13},Y) = 2Y(4Y-3)$ $E_1(P_{13},Y) \to 8Y^2$
P_{14}	$E_1(P_{14},Y) =[5Y(5Y-3)/2]$ $E_1(P_{14},Y) \to 25Y^2/2$

Table 9. E_2 energy equations on counting polynomials

P	E_2 Formula
P_1 P_2	$E_2(P_1,1) = E_2(P_2,1) = 1$; $E_2(P_1,Y) = E_2(P_2,Y) = Y^2+1$, $Y>1$ $E_2(P_1,Y) = E_2(P_2,Y) \to Y^2$
P_3	$E_2(P_3,Y) = (Y-1)^2$ $E_2(P_3,Y) \to Y^2$
P_4	$E_2(P_4,Y) = 1$
P_5 P_6 P_7	$E_2(P_5,Y) = E_2(P_6,Y) = E_2(P_7,Y) =Y^3/3-Y^2/2+Y/6$ $E_2(P_5,Y) = E_2(P_6,Y) = E_2(P_7,Y) \to Y^3/3$
P_8	$E_2(P_8,Y) =3Y^3+9/2Y^2+3Y/2$ $E_2(P_8,Y) \to 3Y^3$
P_9	$E_2(P_9,Y) =3Y^3-3/2Y^2-Y/2$ $E_2(P_8,Y) \to 3Y^3$
P_{10} P_{11} P_{12}	$E_2(P_{10},Y) = E_2(P_{11},Y) = E_2(P_{12},Y) =9Y^3-9/2Y^2+Y/2$ $E_2(P_{10},Y) = E_2(P_{11},Y) = E_2(P_{12},Y) \to 9Y^3$
P_{13}	$E_2(P_{13},Y) =64/3Y^3-24Y^2+26/3Y-2$ $E_2(P_{13},Y) \to 64Y^3/3$
P_{14}	$E_2(P_{14},Y) = 125/3Y^3-75/2Y^2+65/6Y-2$ $E_2(P_{14},Y) \to 125Y^3/3$

Table 10. HE_1 equations on counting polynomials

P	HE_1 Formula
P_1	$HE_1N(P_1,Y) = Y(Y^2+1)$ $HE_1D(P_1,Y) = H_\infty D(P_1,Y)$ $HE_1(P_1,Y) =(Y^2+1)/(Y+1)$ $HE_1(P_1,Y) \to Y$
P_2	$HE_1N(P_2,Y) = 2Y^2$ $HE_1D(P_2,Y) = H_\infty D(P_2,Y)$ $HE_1(P_2,Y) =2Y/(Y+1)$ $HE_1(P_2,Y) \to 2$

Table 10. Continuation

P	HE_1 Formula
P_3	$HE_1N(P_3,Y) = Y(Y-1)^2$ $HE_1D(P_3,Y) = H_\infty D(P_3,Y)$ $HE_1(P_3,Y) = Y-1$ $HE_1(P_3,Y) \to Y$
P_4	$HE_1N(P_4,Y) = Y(Y-1)$ $HE_1D(P_4,Y) = H_\infty D(P_4,Y)$ $HE_1(P_4,Y) = 1$
P_5	$HE_1N(P_5,Y) =[Y(2Y^2-Y+1)]/3$ $HE_1D(P_5,Y) = H_\infty D(P_5,Y)$ $HE_1(P_5,Y) = (2Y^2-Y+1)/(Y-1)$ $HE_1(P_5,Y) \to 2Y$
P_6	$HE_1N(P_6,Y) = Y(Y^2-1)/3$ $HE_1D(P_6,Y) = H_\infty D(P_6,Y)$ $HE_1(P_6,Y) = (Y+1)/3$ $HE_1(P_6,Y) \to Y/3$
P_7	$HE_1N(P_7,Y) = (4Y^3-6Y^2+4Y-1+(-1)^Y)/8$ $HE_1D(P_7,Y) = H_\infty D(P_7,Y)$ $HE_1(P_7,Y) = (4Y^3-6Y^2+4Y-1+(-1)^Y)/[8Y(Y-1)]$ $HE_1(P_7,Y) \to Y/2$
P_8	$HE_1N(P_8,Y) = 3Y(8Y^2+3Y+1)$ $HE_1D(P_8,Y) = H_\infty D(P_8,Y)$ $HE_1(P_8,Y) = (8Y^2+3Y+1)/(3Y+1)$ $HE_1(P_8,Y) \to 8Y/3$
P_9	$HE_1N(P_9,Y) = 3Y^2(Y+3)$ $HE_1D(P_9,Y) = H_\infty D(P_9,Y)$ $HE_1(P_9,Y) = [Y(Y+3)/(3Y+1)]$ $HE_1(P_9,Y) \to Y/3$
P_{10}	$HE_1N(P_{10},Y) = Y(9Y^2+12Y+5)$ $HE_1D(P_{10},Y) = H_\infty D(P_{10},Y)$ $HE_1(P_{10},Y) =(9Y^2+12Y+5)/(9Y+3)$ $HE_1(P_{10},Y) \to Y$
P_{11}	$HE_1N(P_{11},Y) = [108Y^3+18Y^2+12Y-5+5(-1)^Y]/8$ $HE_1D(P_{11},Y) = H_\infty D(P_{11},Y)$ $HE_1(P_{11},Y) =[108Y^3+18Y^2+12Y-5+5(-1)^Y]/[24Y(3Y+1)]$ $HE_1(P_{11},Y) \to 3Y/2$
P_{12}	$HE_1N(P_{12},Y) = [108Y^3+18Y^2-20Y+27+5(-1)^Y]/8$ $HE_1D(P_{12},Y) = H_\infty D(P_{12},Y)$ $HE_1(P_{12},Y) = [108Y^3+18Y^2-20Y+27+5(-1)^Y]/[24Y(3Y+1)]$ $HE_1(P_{12},Y) \to 3Y/2$
P_{13}	$HE_1N(P_{13},Y) = 8(4Y^3+1)$ $HE_1D(P_{13},Y) = H_\infty D(P_{13},Y)$ $HE_1(P_{13},Y) = 2(4Y^3+1)/Y(4Y+1)$ $HE_1(P_{13},Y) \to 2Y$
P_{14}	$HE_1N(P_{14},Y) = [500Y^3+38Y^2-92Y+185+7(-1)^Y]/8$ $HE_1D(P_{14},Y) = H_\infty D(P_{14},Y)$ $HE_1(P_{14},Y) = [500Y^3+38Y^2-92Y+185+7(-1)^Y]/40Y(5Y+1)$ $HE_1(P_{14},Y) \to 5Y/2$

Table 11. HE_2 equations on counting polynomials

P	HE_2 Formula
P_1	$HE_2N(P_1,Y) = Y(Y^3+1)$ $HE_2D(P_1,Y) = H_\infty D(P_1,Y)$ $HE_2(P_1,Y) = (Y^3+1)/(Y+1$ $HE_2(P_1,Y) \to Y^2$
P_2	$HE_2N(P_2,Y) = Y^2(Y+1)$ $HE_2D(P_2,Y) = H_\infty D(P_2,Y)$ $HE_2(P_2,Y) = Y$
P_3	$HE_2N(P_3,Y) = Y(Y-1)^3$ $HE_2D(P_3,Y) = H_\infty D(P_3,Y)$ $HE_2(P_3,Y) = (Y-1)^2$ $HE_2(P_3,Y) \to Y^2$
P_4	$HE_2N(P_4,Y) = Y(Y-1)$ $HE_2D(P_4,Y) = H_\infty D(P_4,Y)$ $HE_2(P_4,Y) = 1$
P_5	$HE_2N(P_5,Y) = (Y^2(Y-1)^2)/2$ $HE_2D(P_5,Y) = H_\infty D(P_5,Y)$ $HE_2(P_5,Y) = Y(Y-1)/2$ $HE_2(P_5,Y) \to Y^2/2$
P_6	$HE_2N(P_6,Y) = (Y^2(Y^2+1))/6$ $HE_2D(P_6,Y) = H_\infty D(P_6,Y)$ $HE_2(P_6,Y) = Y(Y+1)/6$ $HE_2(P_6,Y) \to Y^2/6$
P_7	$HE_2N(P_7,Y) =7/24[Y(Y-1)(Y^2+1)]+1/16[2Y(-1)^Y+1-(-1)^Y]$ $HE_2D(P_7,Y) = H_\infty D(P_7,Y)$ $HE_2(P_7,Y) =7/24(Y^2+1)+[2Y(-1)^Y+1-(-1)^Y]/16Y(Y-1)$ $HE_2(P_7,Y) \to 7Y^2/24$
P_8	$HE_2N(P_8,Y) = 27Y^2(5Y^2+2Y+1)/2$ $HE_2D(P_8,Y) = H_\infty D(P_8,Y)$ $HE_2(P_8,Y) = 9Y(5Y^2+2Y+1)/2(3Y+1)$ $HE_2(P8,Y) \to 15Y^2/2$
P_9	$HE_2N(P_9,Y) =3Y(3Y^3+2Y^2+3Y-1)/2$ $HE_2D(P_9,Y) = H_\infty D(P9,Y)$ $HE_2(P_9,Y) = (3Y^3+2Y^2+3Y-1)/2(3Y+1)$ $HE_2(P_9,Y) \to Y^2/2$
P_{10}	$HE_2N(P_{10},Y) = 3Y^2(9Y^2+16Y-9)/2$ $HE_2D(P_{10},Y) = H_\infty D(P_{10},Y)$ $HE_2(P10,Y) = Y(9Y^2+16Y-9)/2(3Y+1)$ $HE_2(P10,Y) \to 3Y^2/2$
P_{11}	$HE_2N(P_{11},Y) = (189Y^4+42Y^3-6Y^2-20Y)/8-(30Y-17)(1+(-1)^Y)/16$ $HE_2D(P_{11},Y) = H_\infty D(P_{11},Y)$ $HE_2(P_{11},Y) = (189Y^4+42Y^3-6Y^2-20Y)/24Y(3Y+1)-(30Y-17)(1+(-1)^Y)/48Y(3Y+1)$ $HE_2(P_{11},Y) \to 21Y^2/8$
P_{12}	$HE_2N(P_{12},Y) = (189Y^4+42Y^3-102Y^2+206Y-47)/8+(30Y-17)(1+(-1)^Y)/16$ $HE_2D(P_{12},Y) = H_\infty D(P_{12},Y)$ $HE_2(P_{12},Y) = (189Y^4+42Y^3-102Y^2+206Y-47)/24Y(3Y+1)+(30Y-17)(1+(-1)^Y)/48Y(3Y+1)$ $HE_2(P12,Y) \to 21Y^2/8$
P_{13}	$HE_2N(P_{13},Y) = 8Y(28Y^3-13Y^2+18Y-3)/2$ $HE_2D(P_{13},Y) = H_\infty D(P_{13},Y)$ $HE_2(P_{13},Y) =2(28Y^3-13Y^2+18Y-3)/3(4Y+1)$ $HE_2(P13,Y) \to 14Y^2/3$
P_{14}	$HE_2N(P_{14},Y) = (4375Y^4+470Y^3-2362Y^2+4066Y-1509)/24+(70Y+215)/8\times(1+(-1)^Y)/2$ $HE_2D(P_{14},Y) = H_\infty D(P_{14},Y)$ $HE_2(P_{14},Y) = (4375Y^4+470Y^3-2362Y^2+4066Y-1509)/120Y(5Y+1)+(70Y+215)(1+(-1)^Y)/80Y(5Y+1)$ $HE_2(P_{14},Y) \to 175Y^2/24$

The results obtained in this section revealed a series of important aspects from the perspective of entropy and energy of investigated counting polynomials (see Table 12).

Table 12. Summary of entropy and energy analysis

Observation	Informational parameter	Counting polynomial formula(s)
Constant value		
0	H_α, $\alpha > 0$	P_3, P_4
1	H_0	P_1, P_2
	E_1, E_2, HE_1, HE_2	P_4
Finite limit value		
0	H_∞	P_1, P_2
$\log_2 3$ - 1		P_8, P_9
$2\log_2 3$-2	H_2	P_8, P_9
2	HE_1	P_2
Limit value of $\log_2 Y$	H_0	P_5-P14
	H_∞, H_2	P_5-P_7, P_{10}-P_{14}
	H_1	P_5-P_7, P_{10}, P_{11}

The analysis of the entropies and energies generic equations on investigated counting polynomials revealed the followings:

- The following counting polynomials on regular structures have systematically the same formulas:
  - P_1 & P_2 (see Hartley's entropy - Table 4, min-entropy - Table 5, diversity and Renyi's entropy - Table 6, Shannon's entropy - Table 7, E_1 energy - Table 8, E_2 energy - Table 9);
  - P_3 & P_4 (see Hartley's entropy - Table 4, min-entropy - Table 5, diversity and Renyi's entropy - Table 6, Shannon's entropy - Table 7);
  - P_5 & P_6 & P_7 (see Hartley's entropy - Table 4, min-entropy - Table 5, diversity and Renyi's entropy - Table 6, Shannon's entropy - Table 7, E_1 energy - Table 8, E_2 energy - Table 9);
  - P_8 & P_9 (see Hartley's entropy - Table 4, min-entropy - Table 5, diversity and Renyi's entropy - Table 6, Shannon's entropy - Table 7);
  - P_{10} & P_{11} & P_{12} (see Hartley's entropy - Table 4, E_1 energy - Table 8, E_2 energy - Table 9).

  The counting polynomials, which proved to have the same generic formulas for different measures of entropies and energy, were grouped in most of the cases according to the type of repeated structure. The exception was observed on the following cyclic repeated structure: P_{10} ($G_3(Y)$ on CJFM criterion) & P_{11} ($G_3(Y)$ on Sz criterion) & P_{12} ($G_4(Y)$ on Sz criterion).
- Identical generic formulas were obtained for $HE_2(P_5)$ and $E_1(P_5)$, $E_1(P_6)$ and $E_1(P_7)$ (see Table 11 and 8).
- The generic formulas of energy on counting polynomials that comprise both (Eq(28) and Eq(29)) the counting polynomials (as entropy component) and the powers (the energy component) are individual for each type of investigated regular structure.
- The values are equal to or tend to be 0 for the following parameters: Hartley entropy for P_3, P_4 (see Table 4), min-entropy for P_1, P_2, P_3, and P4 (see Table 5), Renyi entropy for P_1, P_2, P_3, and P4 (see Table 6), Shannon entropy for P_1, P_2, P_3, and P4 (see Table 7).
- The values are equal to or tend to be 1 for the following parameters: Hartley entropy for P_1 and P_2 (see Table 4), diversity for P_1, P_2, P_3, and P4 (see Table 6), E_1 energy for P_4 (see Table 8), E_2 energy for P_4 (see Table 9), HE_1 energy for P_5 (see Table 10), HE_2 energy for P_5 (see Table 11).

The values is equal to or tends to be $\log_2 Y$ for the following parameters: Hartley entropy for P_5, P_6, P_7, P_8, P_9, P_{10}, P_{11}, P_{12}, P_{13}, P_{14} (see Table 4), min-entropy for P_5, P_6, P_7, P_{10}, P_{11}, P_{12}, P_{13}, P_{14} (see Table 5), Renyi entropy for P_5, P_6, P_7, P_{10}, P_{11}, P_{12}, P_{13}, P_{14} (see Table 6), Shannon entropy for P_5, P_6, P_7, P_{10}, P_{11} (see Table 7).

The energies (Eq(26)-Eq(29)) and entropies (Eq(22)-Eq(25)) for proposed structures were calculated and the results are presented in Supplementary materials online (Table 13 – Table 21).

Table 13. Entropies (H) and energies (E, HE) of P_1 (S_Y graph, MaxF criterion) and P_2 (S_Y graph, CMaxF, CJFM, Sz criteria) polynomials

Y	H_0	H_1	H_∞	H_2	$HE_1(P_1)$	$E_1(P_1)$	$HE_2(P_1)$	$E_2(P_1)$	$HE_1(P_2)$	$HE_2(P_2)$
1	0	0.0000	0.0000	0.0000	1.0000	1	1	1	1	1
2	1	0.9183	0.5850	0.8480	1.6667	3	3	5	1.3333	2
3	1	0.8113	0.4150	0.6781	2.5000	4	7	10	1.5000	3
4	1	0.7219	0.3219	0.5564	3.4000	5	13	17	1.6000	4
5	1	0.6500	0.2630	0.4695	4.3333	6	21	26	1.6667	5
6	1	0.5917	0.2224	0.4053	5.2857	7	31	37	1.7143	6
7	1	0.5436	0.1926	0.3561	6.2500	8	43	50	1.7500	7
8	1	0.5033	0.1699	0.3175	7.2222	9	57	65	1.7778	8
9	1	0.4690	0.1520	0.2863	8.2000	10	73	82	1.8000	9
10	1	0.4395	0.1375	0.2607	9.1818	11	91	101	1.8182	10
11	1	0.4138	0.1255	0.2392	10.1667	12	111	122	1.8333	11
12	1	0.3912	0.1155	0.2210	11.1538	13	133	145	1.8462	12
13	1	0.3712	0.1069	0.2053	12.1429	14	157	170	1.8571	13
14	1	0.3534	0.0995	0.1917	13.1333	15	183	197	1.8667	14
15	1	0.3373	0.0931	0.1798	14.1250	16	211	226	1.8750	15
16	1	0.3228	0.0875	0.1693	15.1176	17	241	257	1.8824	16
17	1	0.3095	0.0825	0.1599	16.1111	18	273	290	1.8889	17
18	1	0.2975	0.0780	0.1516	17.1053	19	307	325	1.8947	18
19	1	0.2864	0.0740	0.1440	18.1000	20	343	362	1.9000	19
20	1	0.2762	0.0704	0.1372	19.0952	21	381	401	1.9048	20

Table 14. Entropies (H) and energies (E, HE) of P_5 (P_Y graph, MaxF criterion), P_6 (P_Y graph, CMaxF, CJFM criteria) and P_7(P_Y graph, Sz criterion) polynomials

Y	H_0	H_1	H_∞	H_2	$HE_1(P_5)$	$HE_2(P_5)$	E_1	E_2	$HE_1(P_6)$	$HE_2(P_6)$	$HE_1(P_7)$	$HE_2(P_7)$
1	0.000	0.000	0.000	0.000	0.000	0	0	0	0.000	0.000	0.000	0.000
2	0.000	0.000	0.000	0.000	1.000	1	1	1	1.000	1.000	1.000	1.000
3	1.000	0.918	0.585	0.848	1.667	3	3	5	1.333	2.000	1.333	2.000
4	1.585	1.459	1.000	1.363	2.333	6	6	14	1.667	3.333	1.833	3.833
5	2.000	1.846	1.322	1.737	3.000	10	10	30	2.000	5.000	2.300	6.100
6	2.322	2.149	1.585	2.032	3.667	15	15	55	2.333	7.000	2.800	9.067
7	2.585	2.398	1.807	2.277	4.333	21	21	91	2.667	9.333	3.286	12.524
8	2.807	2.610	2.000	2.485	5.000	28	28	140	3.000	12.000	3.786	16.643
9	3.000	2.794	2.170	2.667	5.667	36	36	204	3.333	15.000	4.278	21.278
10	3.170	2.957	2.322	2.829	6.333	45	45	285	3.667	18.333	4.778	26.556
11	3.322	3.104	2.459	2.974	7.000	55	55	385	4.000	22.000	5.273	32.364
12	3.459	3.236	2.585	3.106	7.667	66	66	506	4.333	26.000	5.773	38.803
13	3.585	3.358	2.700	3.227	8.333	78	78	650	4.667	30.333	6.269	45.782
14	3.700	3.470	2.807	3.338	9.000	91	91	819	5.000	35.000	6.769	53.385
15	3.807	3.574	2.907	3.441	9.667	105	105	1015	5.333	40.000	7.267	61.533
16	3.907	3.671	3.000	3.538	10.333	120	120	1240	5.667	45.333	7.767	70.300
17	4.000	3.761	3.088	3.628	11.000	136	136	1496	6.000	51.000	8.265	79.618
18	4.087	3.847	3.170	3.713	11.667	153	153	1785	6.333	57.000	8.765	89.549
19	4.170	3.927	3.248	3.793	12.333	171	171	2109	6.667	63.333	9.263	100.035
20	4.248	4.004	3.322	3.869	13.000	190	190	2470	7.000	70.000	9.763	111.132

Table 15. Entropies (H) and energies (E, HE) of P_8 (G_3 graph, MaxF criterion) polynomials

Y	H_0	H_1	H_∞	H_2	HE_1	E_1	HE_2	E_2
1	0.0000	0.0000	0.0000	0.0000	3.0000	3	$9.00 \cdot 10^0$	$9.00 \cdot 10^0$
2	1.0000	0.5917	0.2224	0.4053	5.5714	9	$3.21 \cdot 10^1$	$4.50 \cdot 10^1$
3	1.5850	0.9056	0.3219	0.5946	8.2000	18	$7.02 \cdot 10^1$	$1.26 \cdot 10^2$
4	2.0000	1.1161	0.3785	0.7074	10.8462	30	$1.23 \cdot 10^2$	$2.70 \cdot 10^2$
5	2.3219	1.2729	0.4150	0.7828	13.5000	45	$1.91 \cdot 10^2$	$4.95 \cdot 10^2$
6	2.5850	1.3971	0.4406	0.8369	16.1579	63	$2.74 \cdot 10^2$	$8.19 \cdot 10^2$
7	2.8074	1.4994	0.4594	0.8776	18.8182	84	$3.72 \cdot 10^2$	$1.26 \cdot 10^3$
8	3.0000	1.5863	0.4739	0.9094	21.4800	108	$4.85 \cdot 10^2$	$1.84 \cdot 10^3$
9	3.1699	1.6615	0.4854	0.9350	24.1429	135	$6.13 \cdot 10^2$	$2.57 \cdot 10^3$
10	3.3219	1.7277	0.4948	0.9559	26.8065	165	$7.56 \cdot 10^2$	$3.47 \cdot 10^3$
11	3.4594	1.7868	0.5025	0.9735	29.4706	198	$9.14 \cdot 10^2$	$4.55 \cdot 10^3$
12	3.5850	1.8401	0.5090	0.9883	32.1351	234	$1.09 \cdot 10^3$	$5.85 \cdot 10^3$
13	3.7004	1.8887	0.5146	1.0011	34.8000	273	$1.28 \cdot 10^3$	$7.37 \cdot 10^3$
14	3.8074	1.9331	0.5194	1.0122	37.4651	315	$1.48 \cdot 10^3$	$9.14 \cdot 10^3$
15	3.9069	1.9742	0.5236	1.0219	40.1304	360	$1.70 \cdot 10^3$	$1.12 \cdot 10^4$
16	4.0000	2.0123	0.5272	1.0305	42.7959	408	$1.93 \cdot 10^3$	$1.35 \cdot 10^4$
17	4.0875	2.0478	0.5305	1.0382	45.4615	459	$2.18 \cdot 10^3$	$1.61 \cdot 10^4$
18	4.1699	2.0811	0.5334	1.0450	48.1273	513	$2.44 \cdot 10^3$	$1.90 \cdot 10^4$
19	4.2479	2.1124	0.5361	1.0512	50.7931	570	$2.72 \cdot 10^3$	$2.22 \cdot 10^4$
20	4.3219	2.1418	0.5384	1.0568	53.4590	630	$3.01 \cdot 10^3$	$2.58 \cdot 10^4$

Table 16. Entropies (H) and energies (E, HE) of P_9 (G_3 graph, CMaxF criterion) polynomials

Y	H_0	H_1	H_∞	H_2	HE_1	E_1	HE_2	E_2
1	0.0000	0.0000	0.0000	0.0000	0.0000	0	$0.00 \cdot 10^0$	$0.00 \cdot 10^0$
2	1.0000	0.5917	0.2224	0.4053	1.4286	5	$3.14 \cdot 10^0$	$1.70 \cdot 10^1$
3	1.5850	0.9056	0.3219	0.5946	1.8000	12	$6.20 \cdot 10^0$	$6.60 \cdot 10^1$
4	2.0000	1.1161	0.3785	0.7074	2.1538	22	$1.02 \cdot 10^1$	$1.66 \cdot 10^2$
5	2.3219	1.2729	0.4150	0.7828	2.5000	35	$1.53 \cdot 10^1$	$3.35 \cdot 10^2$
6	2.5850	1.3971	0.4406	0.8369	2.8421	51	$2.13 \cdot 10^1$	$5.91 \cdot 10^2$
7	2.8074	1.4994	0.4594	0.8776	3.1818	70	$2.83 \cdot 10^1$	$9.52 \cdot 10^2$
8	3.0000	1.5863	0.4739	0.9094	3.5200	92	$3.63 \cdot 10^1$	$1.44 \cdot 10^3$
9	3.1699	1.6615	0.4854	0.9350	3.8571	117	$4.53 \cdot 10^1$	$2.06 \cdot 10^3$
10	3.3219	1.7277	0.4948	0.9559	4.1935	145	$5.53 \cdot 10^1$	$2.85 \cdot 10^3$
11	3.4594	1.7868	0.5025	0.9735	4.5294	176	$6.63 \cdot 10^1$	$3.81 \cdot 10^3$
12	3.5850	1.8401	0.5090	0.9883	4.8649	210	$7.83 \cdot 10^1$	$4.96 \cdot 10^3$
13	3.7004	1.8887	0.5146	1.0011	5.2000	247	$9.13 \cdot 10^1$	$6.33 \cdot 10^3$
14	3.8074	1.9331	0.5194	1.0122	5.5349	287	$1.05 \cdot 10^2$	$7.93 \cdot 10^3$
15	3.9069	1.9742	0.5236	1.0219	5.8696	330	$1.20 \cdot 10^2$	$9.78 \cdot 10^3$
16	4.0000	2.0123	0.5272	1.0305	6.2041	376	$1.36 \cdot 10^2$	$1.19 \cdot 10^4$
17	4.0875	2.0478	0.5305	1.0382	6.5385	425	$1.53 \cdot 10^2$	$1.43 \cdot 10^4$
18	4.1699	2.0811	0.5334	1.0450	6.8727	477	$1.71 \cdot 10^2$	$1.70 \cdot 10^4$
19	4.2479	2.1124	0.5361	1.0512	7.2069	532	$1.90 \cdot 10^2$	$2.00 \cdot 10^4$
20	4.3219	2.1418	0.5384	1.0568	7.5410	590	$2.10 \cdot 10^2$	$2.34 \cdot 10^4$

Table 17. Entropies (H) and energies (E, HE) of P_{10} (G_3 graph, CJFM criterion) polynomials

Y	H_0	H_1	H_∞	H_2	HE_1	E_1	HE_2	E_2
1	1.0000	0.9183	0.5850	0.8480	1.3333	3	$2.00\cdot10^{0}$	$5.00\cdot10^{0}$
2	2.3219	2.2264	1.8074	2.1553	2.6190	15	$8.43\cdot10^{0}$	$5.50\cdot10^{1}$
3	3.0000	2.7994	1.9069	2.6306	3.7333	36	$1.80\cdot10^{1}$	$2.04\cdot10^{2}$
4	3.4594	3.1679	2.1155	2.9378	4.7949	66	$3.06\cdot10^{1}$	$5.06\cdot10^{2}$
5	3.8074	3.4434	2.3219	3.1790	5.8333	105	$4.63\cdot10^{1}$	$1.02\cdot10^{3}$
6	4.0875	3.6659	2.5110	3.3819	6.8596	153	$6.49\cdot10^{1}$	$1.79\cdot10^{3}$
7	4.3219	3.8535	2.6818	3.5585	7.8788	210	$8.65\cdot10^{1}$	$2.87\cdot10^{3}$
8	4.5236	4.0165	2.8365	3.7153	8.8933	276	$1.11\cdot10^{2}$	$4.32\cdot10^{3}$
9	4.7004	4.1609	2.9773	3.8565	9.9048	351	$1.39\cdot10^{2}$	$6.20\cdot10^{3}$
10	4.8580	4.2908	3.1062	3.9850	10.9140	435	$1.70\cdot10^{2}$	$8.56\cdot10^{3}$
11	5.0000	4.4089	3.2250	4.1030	11.9216	528	$2.03\cdot10^{2}$	$1.14\cdot10^{4}$
12	5.1293	4.5174	3.3350	4.2120	12.9279	630	$2.40\cdot10^{2}$	$1.49\cdot10^{4}$
13	5.2479	4.6177	3.4374	4.3133	13.9333	741	$2.80\cdot10^{2}$	$1.90\cdot10^{4}$
14	5.3576	4.7111	3.5332	4.4080	14.9380	861	$3.22\cdot10^{2}$	$2.38\cdot10^{4}$
15	5.4594	4.7985	3.6231	4.4969	15.9420	990	$3.68\cdot10^{2}$	$2.94\cdot10^{4}$
16	5.5546	4.8806	3.7078	4.5806	16.9456	1128	$4.16\cdot10^{2}$	$3.57\cdot10^{4}$
17	5.6439	4.9580	3.7879	4.6597	17.9487	1275	$4.68\cdot10^{2}$	$4.29\cdot10^{4}$
18	5.7279	5.0313	3.8638	4.7347	18.9515	1431	$5.23\cdot10^{2}$	$5.10\cdot10^{4}$
19	5.8074	5.1009	3.9360	4.8060	19.9540	1596	$5.80\cdot10^{2}$	$6.01\cdot10^{4}$
20	5.8826	5.1672	4.0047	4.8739	20.9563	1770	$6.41\cdot10^{2}$	$7.02\cdot10^{4}$

Table 18. Entropies (H) and energies (E, HE) of P_{11} (G_3 graph, Sz criterion) polynomials

Y	H_0	H_1	H_∞	H_2	HE_1	E_1	HE_2	E_2
1	1.0000	0.9183	0.5850	0.8480	1.3333	$3.00\cdot10^{0}$	$2.00\cdot10^{0}$	$5.00\cdot10^{0}$
2	2.3219	2.1604	1.5850	2.0432	2.8571	$1.50\cdot10^{1}$	$9.81\cdot10^{0}$	$5.50\cdot10^{1}$
3	3.0000	2.7292	1.9069	2.5449	4.3111	$3.60\cdot10^{1}$	$2.26\cdot10^{1}$	$2.04\cdot10^{2}$
4	3.4594	3.1089	2.2854	2.8984	5.8077	$6.60\cdot10^{1}$	$4.08\cdot10^{1}$	$5.06\cdot10^{2}$
5	3.8074	3.3951	2.5146	3.1699	7.2917	$1.05\cdot10^{2}$	$6.41\cdot10^{1}$	$1.02\cdot10^{3}$
6	4.0875	3.6279	2.7740	3.3974	8.7895	$1.53\cdot10^{2}$	$9.27\cdot10^{1}$	$1.79\cdot10^{3}$
7	4.3219	3.8242	2.9449	3.5914	10.2814	$2.10\cdot10^{2}$	$1.27\cdot10^{2}$	$2.87\cdot10^{3}$
8	4.5236	3.9949	3.1414	3.7624	11.7800	$2.76\cdot10^{2}$	$1.66\cdot10^{2}$	$4.32\cdot10^{3}$
9	4.7004	4.1459	3.2768	3.9144	13.2751	$3.51\cdot10^{2}$	$2.10\cdot10^{2}$	$6.20\cdot10^{3}$
10	4.8580	4.2816	3.4348	4.0521	14.7742	$4.35\cdot10^{2}$	$2.60\cdot10^{2}$	$8.56\cdot10^{3}$
11	5.0000	4.4048	3.5469	4.1773	16.2709	$5.28\cdot10^{2}$	$3.14\cdot10^{2}$	$1.14\cdot10^{4}$
12	5.1293	4.5178	3.6789	4.2927	17.7703	$6.30\cdot10^{2}$	$3.74\cdot10^{2}$	$1.49\cdot10^{4}$
13	5.2479	4.6222	3.7744	4.3993	19.2679	$7.41\cdot10^{2}$	$4.40\cdot10^{2}$	$1.90\cdot10^{4}$
14	5.3576	4.7192	3.8878	4.4986	20.7674	$8.61\cdot10^{2}$	$5.10\cdot10^{2}$	$2.38\cdot10^{4}$
15	5.4594	4.8098	3.9710	4.5914	22.2657	$9.90\cdot10^{2}$	$5.86\cdot10^{2}$	$2.94\cdot10^{4}$
16	5.5546	4.8948	4.0704	4.6787	23.7653	$1.13\cdot10^{3}$	$6.67\cdot10^{2}$	$3.57\cdot10^{4}$
17	5.6439	4.9750	4.1440	4.7609	25.2640	$1.28\cdot10^{3}$	$7.54\cdot10^{2}$	$4.29\cdot10^{4}$
18	5.7279	5.0508	4.2325	4.8387	26.7636	$1.43\cdot10^{3}$	$8.45\cdot10^{2}$	$5.10\cdot10^{4}$
19	5.8074	5.1226	4.2986	4.9124	28.2626	$1.60\cdot10^{3}$	$9.42\cdot10^{2}$	$6.01\cdot10^{4}$
20	5.8826	5.1910	4.3782	4.9826	29.7623	$1.77\cdot10^{3}$	$1.04\cdot10^{3}$	$7.02\cdot10^{4}$

Table 19. Entropies (H) and energies (E, HE) of P_{12} (G_4 graph, Sz criterion) polynomials

Y	H_0	H_1	H_∞	H_2	HE_1	E_1	HE_2	E_2
1	1.0000	0.9183	0.5850	0.8480	1.6667	$3.00\cdot10^{0}$	$3.00\cdot10^{0}$	$5.00\cdot10^{0}$
2	2.3219	2.1892	1.3923	2.0432	2.8571	$1.50\cdot10^{1}$	$1.00\cdot10^{1}$	$5.50\cdot10^{1}$
3	3.0000	2.8621	2.1699	2.7405	4.2667	$3.60\cdot10^{1}$	$2.24\cdot10^{1}$	$2.04\cdot10^{2}$
4	3.4594	3.3112	2.7004	3.1958	5.7564	$6.60\cdot10^{1}$	$4.03\cdot10^{1}$	$5.06\cdot10^{2}$
5	3.8074	3.6244	2.6590	3.4739	7.2417	$1.05\cdot10^{2}$	$6.34\cdot10^{1}$	$1.02\cdot10^{3}$
6	4.0875	3.8710	3.0255	3.6968	8.7427	$1.53\cdot10^{2}$	$9.20\cdot10^{1}$	$1.79\cdot10^{3}$
7	4.3219	4.0703	3.0444	3.8710	10.2381	$2.10\cdot10^{2}$	$1.26\cdot10^{2}$	$2.87\cdot10^{3}$
8	4.5236	4.2406	3.3219	4.0251	11.7400	$2.76\cdot10^{2}$	$1.65\cdot10^{2}$	$4.32\cdot10^{3}$
9	4.7004	4.3879	3.3528	4.1580	13.2381	$3.51\cdot10^{2}$	$2.09\cdot10^{2}$	$6.20\cdot10^{3}$
10	4.8580	4.5192	3.5757	4.2799	14.7398	$4.35\cdot10^{2}$	$2.59\cdot10^{2}$	$8.56\cdot10^{3}$
11	5.0000	4.6368	3.6083	4.3896	16.2389	$5.28\cdot10^{2}$	$3.13\cdot10^{2}$	$1.14\cdot10^{4}$
12	5.1293	4.7443	3.7944	4.4920	17.7402	$6.30\cdot10^{2}$	$3.73\cdot10^{2}$	$1.49\cdot10^{4}$
13	5.2479	4.8428	3.8260	4.5862	19.2397	$7.41\cdot10^{2}$	$4.39\cdot10^{2}$	$1.90\cdot10^{4}$
14	5.3576	4.9342	3.9857	4.6750	20.7409	$8.61\cdot10^{2}$	$5.09\cdot10^{2}$	$2.38\cdot10^{4}$
15	5.4594	5.0192	4.0154	4.7579	22.2406	$9.90\cdot10^{2}$	$5.85\cdot10^{2}$	$2.94\cdot10^{4}$
16	5.5546	5.0990	4.1553	4.8366	23.7415	$1.13\cdot10^{3}$	$6.66\cdot10^{2}$	$3.57\cdot10^{4}$
17	5.6439	5.1740	4.1830	4.9108	25.2413	$1.28\cdot10^{3}$	$7.53\cdot10^{2}$	$4.29\cdot10^{4}$
18	5.7279	5.2448	4.3074	4.9815	26.7421	$1.43\cdot10^{3}$	$8.44\cdot10^{2}$	$5.10\cdot10^{4}$
19	5.8074	5.3120	4.3333	5.0486	28.2420	$1.60\cdot10^{3}$	$9.41\cdot10^{2}$	$6.01\cdot10^{4}$
20	5.8826	5.3759	4.4453	5.1129	29.7426	$1.77\cdot10^{3}$	$1.04\cdot10^{3}$	$7.02\cdot10^{4}$

Table 20. Entropies (H) and energies (E, HE) of P_{13} (G_5 graph, Sz criterion) polynomials

Y	H_0	H_1	H_∞	H_2	HE_1	E_1	HE_2	E_2
1	0.0000	0.0000	0.0000	0.0000	2.0000	$2.00\cdot10^{0}$	$4.00\cdot10^{0}$	$4.00\cdot10^{0}$
2	2.3219	2.1972	1.5850	2.0919	3.6667	$2.00\cdot10^{1}$	$1.59\cdot10^{1}$	$9.00\cdot10^{1}$
3	3.1699	2.9992	2.2854	2.8634	5.5897	$5.40\cdot10^{1}$	$3.76\cdot10^{1}$	$3.84\cdot10^{2}$
4	3.7004	3.5503	3.0875	3.4470	7.5588	$1.04\cdot10^{2}$	$6.89\cdot10^{1}$	$1.01\cdot10^{3}$
5	4.0875	3.9256	3.1293	3.8119	9.5429	$1.70\cdot10^{2}$	$1.10\cdot10^{2}$	$2.11\cdot10^{3}$
6	4.3923	4.2290	3.6439	4.1222	11.5333	$2.52\cdot10^{2}$	$1.60\cdot10^{2}$	$3.79\cdot10^{3}$
7	4.6439	4.4715	3.6653	4.3584	13.5271	$3.50\cdot10^{2}$	$2.19\cdot10^{2}$	$6.20\cdot10^{3}$
8	4.8580	4.6810	4.0444	4.5692	15.5227	$4.64\cdot10^{2}$	$2.88\cdot10^{2}$	$9.45\cdot10^{3}$
9	5.0444	4.8604	4.0575	4.7444	17.5195	$5.94\cdot10^{2}$	$3.66\cdot10^{2}$	$1.37\cdot10^{4}$
10	5.2095	5.0209	4.3576	4.9047	19.5171	$7.40\cdot10^{2}$	$4.53\cdot10^{2}$	$1.90\cdot10^{4}$
11	5.3576	5.1635	4.3663	5.0444	21.5152	$9.02\cdot10^{2}$	$5.50\cdot10^{2}$	$2.56\cdot10^{4}$
12	5.4919	5.2938	4.6147	5.1741	23.5136	$1.08\cdot10^{3}$	$6.56\cdot10^{2}$	$3.35\cdot10^{4}$
13	5.6147	5.4123	4.6210	5.2905	25.5123	$1.27\cdot10^{3}$	$7.72\cdot10^{2}$	$4.29\cdot10^{4}$
14	5.7279	5.5221	4.8329	5.3998	27.5113	$1.48\cdot10^{3}$	$8.97\cdot10^{2}$	$5.40\cdot10^{4}$
15	5.8329	5.6235	4.8376	5.4996	29.5104	$1.71\cdot10^{3}$	$1.03\cdot10^{3}$	$6.67\cdot10^{4}$
16	5.9307	5.7184	5.0224	5.5940	31.5096	$1.95\cdot10^{3}$	$1.17\cdot10^{3}$	$8.14\cdot10^{4}$
17	6.0224	5.8071	5.0261	5.6815	33.5090	$2.21\cdot10^{3}$	$1.33\cdot10^{3}$	$9.80\cdot10^{4}$
18	6.1085	5.8908	5.1898	5.7648	35.5084	$2.48\cdot10^{3}$	$1.49\cdot10^{3}$	$1.17\cdot10^{5}$
19	6.1898	5.9695	5.1928	5.8427	37.5079	$2.77\cdot10^{3}$	$1.66\cdot10^{3}$	$1.38\cdot10^{5}$
20	6.2668	6.0444	5.3399	5.9171	39.5074	$3.08\cdot10^{3}$	$1.84\cdot10^{3}$	$1.61\cdot10^{5}$

Table 21. Entropies (H) and energies (E, HE) of P_{14} (G_6 graph, Sz criterion) polynomials

Y	H_0	H_1	H_∞	H_2	HE_1	E_1	HE_2	E_2
1	1.0000	0.9710	0.7370	0.9434	2.6000	$5.00\cdot10^{0}$	$7.00\cdot10^{0}$	$1.30\cdot10^{1}$
2	2.8074	2.6561	1.8745	2.5321	4.7273	$3.50\cdot10^{1}$	$2.69\cdot10^{1}$	$2.03\cdot10^{2}$
3	3.5850	3.3157	2.0000	3.0357	7.1583	$9.00\cdot10^{1}$	$6.19\cdot10^{1}$	$8.18\cdot10^{2}$
4	4.0875	3.8018	2.7142	3.5550	9.6524	$1.70\cdot10^{2}$	$1.12\cdot10^{2}$	$2.11\cdot10^{3}$
5	4.4594	4.1176	2.7897	3.8335	12.1477	$2.75\cdot10^{2}$	$1.76\cdot10^{2}$	$4.32\cdot10^{3}$
6	4.7549	4.3743	3.2464	4.0938	14.6516	$4.05\cdot10^{2}$	$2.56\cdot10^{2}$	$7.71\cdot10^{3}$
7	5.0000	4.5758	3.2992	4.2813	17.1524	$5.60\cdot10^{2}$	$3.50\cdot10^{2}$	$1.25\cdot10^{4}$
8	5.2095	4.7511	3.6351	4.4581	19.6561	$7.40\cdot10^{2}$	$4.58\cdot10^{2}$	$1.90\cdot10^{4}$
9	5.3923	4.9004	3.6756	4.6023	22.1575	$9.45\cdot10^{2}$	$5.82\cdot10^{2}$	$2.74\cdot10^{4}$
10	5.5546	5.0349	3.9412	4.7390	24.6604	$1.18\cdot10^{3}$	$7.19\cdot10^{2}$	$3.80\cdot10^{4}$
11	5.7004	5.1544	3.9740	4.8574	27.1617	$1.43\cdot10^{3}$	$8.72\cdot10^{2}$	$5.10\cdot10^{4}$
12	5.8329	5.2644	4.1938	4.9701	29.6639	$1.71\cdot10^{3}$	$1.04\cdot10^{3}$	$6.67\cdot10^{4}$
13	5.9542	5.3645	4.2213	5.0710	32.1650	$2.02\cdot10^{3}$	$1.22\cdot10^{3}$	$8.53\cdot10^{4}$
14	6.0661	5.4580	4.4087	5.1673	34.6668	$2.35\cdot10^{3}$	$1.42\cdot10^{3}$	$1.07\cdot10^{5}$
15	6.1699	5.5445	4.4324	5.2554	37.1677	$2.70\cdot10^{3}$	$1.63\cdot10^{3}$	$1.32\cdot10^{5}$
16	6.2668	5.6260	4.5957	5.3398	39.6691	$3.08\cdot10^{3}$	$1.85\cdot10^{3}$	$1.61\cdot10^{5}$
17	6.3576	5.7022	4.6165	5.4181	42.1699	$3.49\cdot10^{3}$	$2.09\cdot10^{3}$	$1.94\cdot10^{5}$
18	6.4429	5.7746	4.7612	5.4933	44.6711	$3.92\cdot10^{3}$	$2.35\cdot10^{3}$	$2.31\cdot10^{5}$
19	6.5236	5.8429	4.7798	5.5638	47.1717	$4.37\cdot10^{3}$	$2.62\cdot10^{3}$	$2.72\cdot10^{5}$
20	6.5999	5.9081	4.9098	5.6317	49.6727	$4.85\cdot10^{3}$	$2.90\cdot10^{3}$	$3.19\cdot10^{5}$

The analysis of the values of entropies and energies obtained on investigated counting polynomials revealed the followings:

- Identical values of entropies and energies calculated with a certain formula were obtained as was remarked in the analysis of the genetic formulas.
- In all cases, the values obtained by applying the Eq(28) and Eq(29) are individual for each investigated counting polynomial as resulted in the analysis of the generic formulas.
- The Hartley's entropy was equal to 1 for P_1 and P_2 when Y > 1.
- The values of entropies were equal to 1 for Y = 1 for the following counting polynomials P_1 = P_2 (see Table 13), P_5 = P_6 = P_7 (see Table 14), P_8 (see Table 15), and P_9 (see Table 16).
- The values of entropies increase with increases of Y with two exceptions. One exception is seen for P_1 = P_2 (see Table 13) when the values decreases with increasing of Y.
- Without any exception, the values of energies increases with the increase of Y (see Table 13 - Table 21).

Molecular Properties

Ten properties were calculated by using the HyperChem or Molecular Modelling Pro software for the investigated counting polynomials on stars, completes, paths, and on the four proposed cyclic structures: energy (abbreviated as Energy), surface area approximation (abbreviated as SAreaA), surface area grid (abbreviated as SAreaG), volume (abbreviated as Volume), hydration energy (abbreviated as HydE), octanol-water partition coefficient in logarithmic scale (abbreviated as LogP), refractivity (abbreviated as Refr), Polarizability (abbreviated as Polar), melting point (abbreviated as MeltP), and boiling point (abbreviated as BoilP). A series of parameters on different investigated structure were not calculated due to the limitations of software used; instead of these values the "n.a." (not available) abbreviation appears in the tables. The values of the properties of interest are presented in Supplementary materials online Tables 22 – 27. The linear relationships between the investigated properties on different counting polynomials and entropy, energy respectively were analyzed by using SPSS 16, stepwise method.

The simple- and multivariate linear regression models are presented in Supplementary materials online Tables 28 - 33. The following abbreviations were used in these tables: n = sample size, v = number of variable into the model, r^2 = coefficient of determination, SError = standard error of estimate; F = Fisher parameter, p = significance of Fisher parameter. The equations presented in tables contain the values of the intercept and the coefficients with associated constant used for obtaining 95% confidence intervals (presented in round brackets). The models with intercept and/or coefficients not significantly differed by zero were not considered as being significant models.

Table 22. Chemical-based properties of $P_Y(C)$ structures (Y>1)

Y	Energy	SAreaA	SAreaG	Volume	HydE	LogP	Refr	Polar	MeltP	BoilP
2	0.507	202.8	174	216.1	2.06	1.30	11.00	4.44	112.3	245.4
3	1.539	241.6	206.7	270.1	2.47	1.69	15.61	6.28	123.6	268.2
4	2.492	277.5	238.7	326.2	2.85	2.09	20.21	8.11	134.8	291.2
5	3.408	310.9	268.5	379.4	3.20	2.49	24.81	9.95	146.1	314.0
6	4.312	345.8	300.3	434.6	3.56	2.88	29.41	11.78	157.4	336.9
7	5.211	382.0	331.1	488.1	3.94	3.28	34.01	13.62	168.7	359.8
8	6.108	418.2	362.1	542.3	4.31	3.67	38.61	15.45	179.9	382.6
9	7.004	454.5	391.7	596.9	4.69	4.07	43.21	17.29	191.2	405.5
10	7.900	490.8	413.5	651.9	5.06	4.47	47.81	19.12	202.5	428.4
11	8.795	527.1	447.1	703.7	5.44	4.86	52.41	20.96	213.7	451.3
12	9.690	563.3	490.5	759.8	5.82	5.26	57.01	22.79	225.0	474.2
13	10.586	599.6	506.8	812.4	6.19	5.66	61.62	24.63	236.3	497.0
14	11.480	635.9	554.9	869.0	6.57	6.05	66.22	26.46	247.5	519.9
15	12.376	672.2	567.2	921.0	6.95	6.45	70.82	28.30	258.8	542.8
16	13.270	708.4	596.2	975.8	7.32	6.84	75.42	30.13	270.1	565.7
17	14.165	744.7	627.4	1029	7.70	7.24	80.02	31.97	281.4	588.6
18	15.060	781.0	656.9	1084	8.08	7.64	84.62	33.80	292.6	611.4
19	15.955	817.2	688.2	1137	8.45	8.03	89.22	35.64	303.9	634.3
20	16.850	853.5	717.3	1192	8.83	8.43	93.82	37.47	315.2	657.2

Energy = energy; SAreaA = surface area approximation; SAreaG = surface area grid; Volume = volume; HydE = hydration energy; LogP = octanol-water partition coefficient in logarithmic scale; Refr = refractivity; Polar = Polarizability; MeltP = melting point; BoilP = boiling point.

Table 23. Chemical-based properties of $G_{3,Y}(O,N,C)$ structures (Y≥1)

Y	Energy	SAreaA	SAreaG	Volume	HydE	LogP	Refr	Polar
1	252	121	156	183	-22.3	0.34	3.24	3.20
2	558	124	201	265	-18.8	0.96	15.5	6.19
3	900	124	249	347	-17.4	1.68	22.9	9.18
4	1191	151	300	435	-21.0	2.41	30.2	12.2
5	1438	182	360	532	-24.2	3.13	37.5	15.2
6	1734	199	410	619	-25.7	3.85	44.8	18.2
7	2030	216	460	705	-27.1	4.57	52.1	21.1
8	2326	233	510	793	-28.6	5.30	59.4	24.1
9	2622	250	560	880	-30.1	6.02	66.7	27.1
10	2917	267	610	967	-31.5	6.74	74.0	30.1
11	3213	284	661	1054	-33.0	7.46	81.3	33.1
12	3509	302	712	1140	-34.5	8.19	88.6	36.1
13	3805	319	762	1227	-35.9	8.91	95.9	39.1
14	4101	335	810	1313	-37.3	9.63	103	42.1
15	4396	318	819	1377	-33.1	10.4	110	45.1
16	4692	325	847	1454	-33.3	11.1	118	48.0
17	4987	303	850	1504	-31.7	11.8	125	51.0
18	5282	303	874	1569	-31.7	12.5	132	54.0
19	5578	294	880	1622	-31.1	13.3	140	57.0
20	5873	318	943	1719	-32.7	14.0	147	60.0

Energy = energy; SAreaA = surface area approximation; SAreaG = surface area grid; Volume = volume; HydE = hydration energy; LogP = octanol-water partition coefficient in logarithmic scale; Refr = refractivity; Polar = Polarizability; MeltP = melting point; BoilP = boiling point.

Table 24. Chemical-based properties of $G_{3,Y}(C)$ structures ($Y \geq 1$)

Y	Energy	SAreaA	SAreaG	Volume	HydE	LogP	Refr	Polar
1	36.63	149	207	269	1.56	0.95	16.5	6.57
2	74	165	264	317	1.66	0.97	26.4	10.5
3	111	183	318	473	1.79	0.99	36.3	14.5
4	148	204	372	576	1.97	1.01	46.2	18.4
5	185	225	428	679	2.15	1.03	56.2	22.4
6	222	246	484	780	2.33	1.05	66.1	26.4
7	259	267	538	883	2.52	1.07	76.0	30.3
8	296	288	596	986	2.70	1.09	85.9	34.3
9	333	309	649	1087	2.88	1.11	95.8	38.2
10	370	330	701	1190	3.07	1.13	106	42.2
11	407	351	759	1292	3.25	1.15	116	46.2
12	444	372	810	1396	3.43	1.17	126	50.1
13	481	393	872	1497	3.62	1.19	135	54.1
14	518	414	920	1599	3.80	1.21	145	58.0
15	555	435	985	1702	3.98	1.24	155	62.0
16	592	456	1031	1803	4.17	1.26	165	65.9
17	629	477	1087	1907	4.35	1.28	175	69.9
18	666	498	1148	2009	4.53	1.30	185	73.8
19	703	519	1196	2113	4.72	1.32	195	77.8
20	740	540	1247	2211	4.90	1.34	205	81.8

Energy = energy; SAreaA = surface area approximation; SAreaG = surface area grid; Volume = volume;
HydE = hydration energy; LogP = octanol-water partition coefficient in logarithmic scale;
Refr = refractivity; Polar = Polarizability.

Table 25. Chemical-based properties of $G_{4,Y}(C)$ structures ($Y \geq 1$)

Y	Energy	SAreaA	SAreaG	Volume	HydE	LogP	Refr	Polar
1	53.56	197	212	285	2.10	1.59	18.4	7.34
2	78.57	248	276	412	2.47	2.24	30.2	12.1
3	117.8	289	344	529	2.77	2.90	42.1	16.8
4	158.3	339	404	647	3.17	3.55	53.9	21.5
5	233.6	384	448	756	3.52	4.21	65.7	26.3
6	239.4	440	525	885	4.00	4.87	77.5	31.0
7	281.5	492	589	1010	4.44	5.52	89.3	35.7
8	322.1	543	638	1129	4.86	6.18	101	40.4
9	361.0	591	705	1241	5.26	6.83	113	45.2
10	401.5	642	767	1357	5.67	7.49	125	49.9
11	443.9	695	830	1487	6.12	8.15	137	54.7
12	482.5	743	887	1603	6.51	8.80	148	59.4
13	522.8	794	944	1722	6.93	9.46	160	64.1
14	563.1	844	1005	1842	7.35	10.1	172	68.8
15	603.2	895	1065	1963	7.77	10.8	184	73.6
16	643.2	945	1122	2083	8.19	11.4	196	78.3
17	683.3	996	1180	2203	8.60	12.1	208	83.0
18	723.4	1046	1243	2322	9.02	12.7	219	87.8
19	763.4	1097	1304	2441	9.44	13.4	231	92.5
20	803.5	1148	1361	2559	9.86	14.1	243	97.2

Energy = energy; SAreaA = surface area approximation; SAreaG = surface area grid; Volume = volume;
HydE = hydration energy; LogP = octanol-water partition coefficient in logarithmic scale;
Refr = refractivity; Polar = Polarizability.

Table 26. Chemical-based properties of $G_{5,Y}(C)$ structures ($Y \geq 1$)

Y	Energy	SAreaA	SAreaG	Volume	HydE	LogP	Refr	Polar
1	9.91	223	241	334	2.37	1.98	23.0	9.18
2	21.6	269	316	488	2.69	3.03	39.4	15.7
3	33.6	319	386	638	3.09	4.09	55.9	22.3
4	45.4	373	461	790	3.52	5.14	72.3	28.9
5	57.0	423	524	934	3.92	6.19	88.7	35.4
6	68.0	457	568	1059	4.15	7.24	105	42.0
7	79.6	497	619	1192	4.47	8.30	122	48.6
8	90.1	541	669	1322	4.82	9.35	138	55.1
9	100.1	602	734	1471	5.35	10.4	154	61.7
10	111.0	636	764	1593	5.58	11.5	171	68.3
11	119.9	641	780	1683	5.54	12.5	187	74.8
12	131.2	705	846	1831	6.13	13.6	204	81.4
13	142.0	737	880	1944	6.33	14.6	220	88.0
14	152.6	784	940	2078	6.73	15.7	237	94.5
15	161.6	801	963	2182	6.81	16.7	253	101
16	170.7	841	993	2299	7.13	17.8	269	108
17	180.9	857	1008	2396	7.20	18.8	286	114
18	190.7	909	1063	2530	7.64	19.9	302	121
19	200.9	957	1108	2659	8.05	20.9	319	127
20	211.7	1006	1156	2792	8.47	22.0	335	134
21	223.9	1061	1212	2931	8.94	23.0	351	140

Energy = energy; SAreaA = surface area approximation; SAreaG = surface area grid; Volume = volume;
HydE = hydration energy; LogP = octanol-water partition coefficient in logarithmic scale;
Refr = refractivity; Polar = Polarizability.

Table 27. Chemical-based properties of $G_{6,Y}(C)$ structures ($Y \geq 1$)

Y	Energy	SAreaA	SAreaG	Volume	HydE	LogP	Refr	Polar
1	12	236	261	378	2.50	2.38	28	11
2	21	291	349	568	2.92	3.83	49	19
3	37	360	437	757	3.51	5.28	70	28
4	51	436	529	949	4.19	6.72	91	36
5	61	510	618	1139	4.85	8.17	112	45
6	76	581	706	1328	5.49	9.62	133	53
7	92	656	797	1520	6.16	11.1	154	61
8	107	730	886	1711	6.83	12.5	175	70
9	122	805	978	1903	7.50	14.0	196	78
10	136	881	1070	2094	8.17	15.4	217	87
11	151	956	1158	2284	8.84	16.9	238	95
12	160	1030	1250	2474	9.50	18.3	259	103
13	176	1101	1341	2664	10.1	19.8	280	112
14	190	1176	1432	2855	10.8	21.2	301	120
15	200	1251	1518	3044	11.5	22.7	322	129
16	215	1322	1609	3235	12.1	24.1	343	137
17	230	1397	1699	3425	12.8	25.6	364	145
18	245	1472	1792	3616	13.5	27.0	385	154
19	255	1546	1880	3805	14.1	28.5	406	162
20	265	1616	1970	3994	14.7	29.9	427	171
21	280	1687	2057	4182	15.4	31.4	448	179

Energy = energy; SAreaA = surface area approximation; SAreaG = surface area grid; Volume = volume; Refr = refractivity;
HydE = hydration energy; LogP = octanol-water partition coefficient in logarithmic scale; Polar = Polarizability.

Table 28. qSAR Models for $P_Y(C)$: Property = f(energy/entropy)

Property	**n**	**v**	**r^2**	**SError**	**Equation**	**F (p)**
Property = f(energy)						
Energy	18	1	0.9999	0.02	$=-1.99(\pm0.03) + 2.69(\pm0.006)\cdot HE_1(P_6)$	$1.02\cdot10^{6}$ $(7.06\cdot10^{-40})$
SAreaA	18	1	0.9999	1.20	$=94.52(\pm1.56) + 108.30(\pm0.35)\cdot HE_1(P_6)$	$4.42\cdot10^{5}$ $(5.79\cdot10^{-37})$
SAreaG	18	1	0.9989	5.38	$=135.17(\pm6.31) + 44.94(\pm0.78)\cdot HE_1(P_5)$	$1.50\cdot10^{4}$ $(3.25\cdot10^{-25})$
Volume	18	1	0.9999	0.86	$=54.98(\pm1.13) + 162.45(\pm0.25)\cdot HE_1(P_6)$	$1.90\cdot10^{6}$ $(4.97\cdot10^{-42})$
HydE	18	1	0.9999	0.01	$=1.51(\pm0.013) + 0.56(\pm0.002)\cdot HE_1(P_5)$	$5.21\cdot10^{5}$ $(1.56\cdot10^{-37})$
LogP	18	1	0.9999	0.003	$=0.11(\pm0.004) + 1.19(\pm0.001)\cdot HE_1(P_6)$	$8.64\cdot10^{6}$ $(2.71\cdot10^{-47})$
Refr	18	1	0.9999	0.003	$=-2.80(\pm0.003) + 13.80(\pm0.001)\cdot HE_1(P_6)$	$1.46\cdot10^{9}$ $(4\cdot10^{-65})$
Polar	18	1	0.9999	0.003	$=1.69(\pm0.0031) + 2.75(\pm0.0004)\cdot HE_1(P_5)$	$2.34\cdot10^{8}$ $(9.42\cdot10^{-59})$
MeltP	18	1	0.9999	0.003	$=78.49(\pm0.04) + 33.81(\pm0.01)\cdot HE_1(P_6)$	$6.67\cdot10^{7}$ $(2.16\cdot10^{-54})$
BoiP	18	1	0.9999	0.03	$=176.74(\pm0.04) + 68.64(\pm0.01)\cdot HE_1(P_6)$	$2.16\cdot10^{8}$ $(1.75\cdot10^{-58})$
Property = f(entropy)						
Energy	18	2	0.9914	0.473	$=6.88(\pm2.63) - 25.13(\pm5.72)\cdot H_0(P_5) + 34.91(\pm6.65)\cdot H_\infty(P_5)$	$8.64\cdot10^{2}(3.26\cdot10^{-16})$
SAreaA	18	2	0.9913	19.11	$=470.50(\pm106.22) - 1051.97(\pm231.06)\cdot H_0(P_5) + 1451.14(\pm268.37)\cdot H_\infty(P_5)$	$8.57\cdot10^{2}(3.43\cdot10^{-16})$
SAreaG	18	2	0.9917	15.54	$=379.05(\pm86.38) - 824.33(\pm187.90)\cdot H_0(P_5) + 1148.54(\pm218.24)\cdot H_\infty(P_5)$	$8.94\cdot10^{2}$ $(2.51\cdot10^{-16})$
Volume	18	2	0.9915	28.41	$=597.83(\pm157.96) - 1533.15(\pm343.61)\cdot H_0(P_5) + 2125.29(\pm399.08)\cdot H_\infty(P_5)$	$8.72\cdot10^{2}$ $(3.02\cdot10^{-16})$
HydE	18	2	0.9912	0.20	$=4.84(\pm1.11) - 10.88(\pm2.42)\cdot H_0(P_5) + 15.02(\pm2.81)\cdot H_\infty(P_5)$	$8.45\cdot10^{2}$ $(3.81\cdot10^{-16})$
LogP	18	2	0.9914	0.21	$=4.11(\pm1.16) - 11.27(\pm2.52)\cdot H_0(P_5) + 15.61(\pm2.93)\cdot H_\infty(P_5)$	$8.66\cdot10^{2}$ $(3.18\cdot10^{-16})$
Refr	18	2	0.9915	2.42	$=43.69(\pm13.43) - 131.04(\pm29.22)\cdot H_0(P_5) + 181.47(\pm33.94)\cdot H_\infty(P_5)$	$8.71\cdot10^{2}$ $(3.06\cdot10^{-16})$
Polar	18	2	0.9915	0.96	$=17.48(\pm5.36) - 52.26(\pm11.65)\cdot H_0(P_5) + 72.37(\pm13.53)\cdot H_\infty(P_5)$	$8.71\cdot10^{2}$ $(3.04\cdot10^{-16})$
MeltP	18	2	0.9915	5.92	$=192.38(\pm32.91) - 321.02(\pm71.59)\cdot H_0(P_5) + 444.55(\pm83.15)\cdot H_\infty(P_5)$	$8.71\cdot10^{2}$ $(3.07\cdot10^{-16})$
BoilP	18	2	0.9914	12.03	$=407.80(\pm66.86) - 651.37(\pm145.44)\cdot H_0(P_5) + 902.09(\pm168.92)\cdot H_\infty(P_5)$	$8.69\cdot10^{2}$ $(3.10\cdot10^{-16})$

Table 29. qSAR Models for $G_{3,Y}(C)$: Property = f(energy/entropy)

Property	**n**	**v**	**r^2**	**SError**	**Equation**	**F (p)**
Property=f(energy)						
Energy	20	4	0.9999	0.01	$=-5.29(\pm0.051) + 13.73(\pm0.005)\cdot HE_1(P_{11}) + 0.68(\pm0.072)\cdot HE_1(P_{12}) + 0.002(\pm0.0004)\cdot E_1(P_{12}) + 0.32(\pm0.021)\cdot \log_2(E_2(P_{14}))$	$1.32\cdot10^{5}$ $(6.71\cdot10^{-34})$
SAreaA	20	4	0.9999	0.34	$= 125.89(\pm1.32) + 8.52(\pm0.14)\cdot HE_1(P_{11}) - 1.95(\pm1.86)\cdot HE_1(P_{12}) - 0.02(\pm0.01)\cdot E_1(P_{12}) - 1.05(\pm0.54)\cdot \log_2(E_2(P_{14}))$	$6.23\cdot10^{5}$ $(5.94\cdot10^{-39})$
SAreaG	20	4	0.9999	3.17	$=148.35(\pm12.33) + 20.71(\pm1.32)\cdot HE_1(P_{11}) + 6.60(\pm17.28)\cdot HE_1(P_{12}) - 0.05(\pm0.10)\cdot E_1(P_{12}) - 1.50(\pm5.01)\cdot \log_2(E_2(P_{14}))$	$5.00\cdot10^{4}$ $(9.85\cdot10^{-31})$
Volume	20	4	0.9999	6.51	$=79.37(\pm25.34) + 42.28(\pm2.71)\cdot HE_1(P_{11}) - 101.03(\pm35.51)\cdot HE_1(P_{12}) + 0.35(\pm0.21)\cdot E_1(P_{12}) + 27.00(\pm10.30)\cdot \log_2(E_2(P_{14}))$	$4.16\cdot10^{4}$ $(3.88\cdot10^{-30})$
HydE	20	4	0.9999	0.006	$=1.38(\pm0.02) + 0.08(\pm0.003)\cdot HE_1(P_{11}) - 0.02(\pm0.03)\cdot HE_1(P_{12}) -0.0003(\pm0.0002)\cdot E_1(P_{12}) - 0.02(\pm0.01)\cdot \log_2(E_2(P_{14}))$	$1.42\cdot10^{5}$ $(3.86\cdot10^{-34})$
LogP	20	1	0.9995	0.003	$=0.925(\pm0.003) + 0.008(\pm0.0001)\cdot HE_1(P_{11})$	$3.58\cdot10^{4}$ $(3.83\cdot10^{-31})$
Refr	20	1	0.9999	0.27	$=5.79(\pm0.265) + 3.72(\pm0.008)\cdot HE_1(P_{11})$	$8.99\cdot10^{5}$ $(9.56\cdot10^{-44})$
Polar	20	1	0.9999	0.06	$=2.28(\pm0.061) + 1.49(\pm0.002)\cdot HE_1(P_{11})$	$2.71\cdot10^{6}$ $(4.73\cdot10^{-48})$

Table 29. Continuation

Property=f(entropy)						
Energy	20	5	0.9988	8.96	$=-1186(\pm 320) - 763(\pm 360)\cdot H_0(P_{12}) - 3433(\pm 406)\cdot H_\infty(P_{12}) - 476(\pm 219)\cdot H_\infty(P_{13}) + 151(\pm 356)\cdot H_\infty(P_{14}) + 1666(\pm 387)\cdot H_1(P_{14})$	$2.27\cdot 10^3$ $(7.74\cdot 10^{-20})$
SAreaA	20	5	0.9987	5.16	$=-529(\pm 185) - 419(\pm 207)\cdot H_0(P_{12}) - 1949(\pm 234)\cdot H_\infty(P_{12}) - 265(\pm 126)\cdot H_\infty(P_{13}) + 92(\pm 205)\cdot H_\infty(P_{14}) + 919(\pm 223)\cdot H_1(P_{14})$	$2.17\cdot 10^3$ $(1.06\cdot 10^{-19})$
SAreaG	20	5	0.9988	13.21	$=-1550(\pm 473) - 1069(\pm 531)\cdot H_0(P_{12}) - 5040(\pm 599)\cdot H_\infty(P_{12}) - 668(\pm 324)\cdot H_\infty(P_{13}) + 180(\pm 524)\cdot H_\infty(P_{14}) + 2409(\pm 570)\cdot H_1(P_{14})$	$2.30\cdot 10^3$ $(7.05\cdot 10^{-20})$
Volume	20	5	0.9989	23.41	$=-3198(\pm 837) - 2111(\pm 940)\cdot H_0(P_{12}) - 9909(\pm 1061)\cdot H_\infty(P_{12}) - 1476(\pm 573)\cdot H_\infty(P_{13}) + 316(\pm 929)\cdot H_\infty(P_{14}) + 4889(\pm 1010)\cdot H_1(P_{14})$	$2.58\cdot 10^3$ $(3.17\cdot 10^{-20})$
HydE	20	5	0.9987	0.05	$=-4.24(\pm 1.62) - 3.54(\pm 1.82)\cdot H_0(P_{12}) - 17.07(\pm 2.06)\cdot H_\infty(P_{12}) - 2.25(\pm 1.11)\cdot H_\infty(P_{13}) + 0.82(\pm 1.80)\cdot H_\infty(P_{14}) + 7.83(\pm 1.96)\cdot H_1(P_{14})$	$2.10\cdot 10^3$ $(1.33\cdot 10^{-19})$
LogP	20	4	0.9981	0.006	$=0.25(\pm 0.16) - 0.42(\pm 0.14)\cdot H_0(P_{12}) - 2.06(\pm 0.27)\cdot H_\infty(P_{12}) - 0.26(\pm 0.09)\cdot H_\infty(P_{13}) + 1.01(\pm 0.25)\cdot H_1(P_{14})$	$1.93\cdot 10^3$ $(3.80\cdot 10^{-20})$
Refr	20	4	0.9986	2.46	$=-285(\pm 65) - 169(\pm 55)\cdot H_0(P_{12}) - 920(\pm 111)\cdot H_\infty(P_{12}) - 107(\pm 37)\cdot H_\infty(P_{13}) + 430(\pm 100)\cdot H_1(P_{14})$	$2.68\cdot 10^3$ $(3.26\cdot 10^{-21})$
Polar	20	4	0.9987	0.95	$=-114(\pm 25) - 68(\pm 21)\cdot H_0(P_{12}) - 368(\pm 43)\cdot H_\infty(P_{12}) - 43(\pm 14)\cdot H_\infty(P_{13}) + 172(\pm 39)\cdot H_1(P_{14})$	$2.86\cdot 10^3$ $(2.05\cdot 10^{-21})$

Table 30. qSAR Models for $G_{3,Y}(O,N,C)$: Property = f(energy/entropy)

Property	n	v	r^2	SError	Equation	F (p)
Property=f(energy)						
Energy	19	2	0.9999	15.74	$= -187.63(\pm 28.462) + 0.01(\pm 0.003)\cdot E_2(P_{11}) + 282.91(\pm 3.841)\cdot HE_1(P_{13})$	$9.96\cdot 10^4$ $(1.73\cdot 10^{-33})$
SAreaA	19	2	0.9751	11.73	$= 9.34(\pm 25.24) + 69.27(\pm 8.26)\cdot HE_1(P_{12}) - 0.01(\pm 0.002)\cdot E_2(P_{12})$	$3.13\cdot 10^2$ $(1.49\cdot 10^{-13})$
SAreaG	19	2	0.9961	15.74	$= 35.05(\pm 28.08) - 0.013(\pm 0.003)\cdot E_2(P_{12}) + 56.80(\pm 3.69)\cdot HE_1(P_{13})$	$2.04\cdot 10^3$ $(5.39\cdot 10^{-20})$
Volume	19	2	0.9981	20.99	$= -146(\pm 58.93) + 212(\pm 18.58)\cdot HE_1(P_{12}) + 19(\pm 11.93)\cdot \log_2(E_2(P_{12}))$	$4.29\cdot 10^3$ $(1.46\cdot 10^{-22})$
HydE	19	2	0.9372	1.50	$= -11.39(\pm 2.72) + 0.0011(\pm 0.0003)\cdot E_2(P_{11}) - 2.19(\pm 0.37)\cdot HE_1(P_{13})$	$1.19\cdot 10^2$ $(2.42\cdot 10^{-10})$
LogP	19	1	0.9999	0.02	$= -0.55(\pm 0.02) + 0.27(\pm 0.0006)\cdot HE_1(P_{11})$	$1.05\cdot 10^6$ $(3.55\cdot 10^{-42})$
Ref	19	1	0.9999	0.19	$= 0.45(\pm 0.21) + 2.74(\pm 0.006)\cdot HE_1(P_{11})$	$8.37\cdot 10^5$ $(2.49\cdot 10^{-41})$
Polar	19	1	0.9999	0.04	$= 1.12(\pm 0.0005)\cdot HE_1(P_{11})$	$4.05\cdot 10^6$ $(3.78\cdot 10^{-47})$
Property=f(entropy)						
Energy	19	3	0.99918	51.86	$= -4823(\pm 239) - 18646(\pm 2073)\cdot H_2(P_{11}) + 7280(\pm 959)\cdot H_1(P_{13}) - 1824(\pm 652)\cdot H_\infty(P_{13})$	$6.11\cdot 10^3$ $(2.26\cdot 10^{-23})$
SAreaA	19	1	0.9153	20.97	$= -40.00(\pm 47.04) + 95.49(\pm 14.86)\cdot H_\infty(P_{13})$	$3.13\cdot 10^2$ $(1.49\cdot 10^{-13})$
SAreaG	19	1	0.99308	20.34	$= -420(\pm 45.62) + 337(\pm 14.41)\cdot H_\infty(P_{13})$	$2.44\cdot 10^3$ $(8.41\cdot 10^{-20})$
Volume	19	2	0.9996	10.28	$= -1094(\pm 27.05) - 3175(\pm 137.67)\cdot H_2(P_{11}) + 1190(\pm 29.11)\cdot H_1(P_{13})$	$1.79\cdot 10^4$ $(1.60\cdot 10^{-27})$
HydE	19	1	0.8166	2.42	$= -32.33(\pm 1.27)\cdot H_2(P_{11})$	$8.0\cdot 10^1$ $(7.65\cdot 10^{-8})$
LogP	19	3	0.9989	0.15	$= -12.17(\pm 0.68) - 44.09(\pm 5.88)\cdot H_2(P_{11}) + 17.09(\pm 2.72)\cdot H_1(P_{13}) - 3.95(\pm 1.85)\cdot H_\infty(P_{13})$	4597 $(1.91\cdot 10^{-22})$
Refr	19	3	0.9989	1.50	$= -116.80(\pm 6.92) - 442.86(\pm 59.99)\cdot H_2(P_{11}) + 171.92(\pm 27.75)\cdot H_1(P_{13}) - 39.71(\pm 18.87)\cdot H_\infty(P_{13})$	$4.48\cdot 10^3$ $(2.30\cdot 10^{-22})$
Polar	19	3	0.9990	0.59	$= -47.96(\pm 2.71) - 180.99(\pm 23.48)\cdot H_2(P_{11}) + 70.20(\pm 10.86)\cdot H_1(P_{13}) - 16.11(\pm 7.39)\cdot H_\infty(P_{13})$	$4.91\cdot 10^3$ $(1.17\cdot 10^{-22})$

Table 31 qSAR Models for $G_{4,Y}(C)$: Property = f(energy/entropy)

Property	n	v	r^2	SError	Equation	F (p)
Property=f(energy)						
Energy	20	1	0.9990	7.73	$= 9.79(\pm7.49) + 26.69(\pm0.42)\cdot HE_1(P_{15})$	$1.76\cdot10^4$ $(2.19\cdot10^{-28})$
SAreaA	20	1	0.9999	2.40	$= 145.26(\pm2.32) + 33.71(\pm0.13)\cdot HE_1(P_{15})$	$2.92\cdot10^5$ $(2.36\cdot10^{-39})$
SAreaG	20	1	0.9996	7.51	$= 165.27(\pm7.28) + 40.41(\pm0.41)\cdot HE_1(P_{15})$	$4.28\cdot10^4$ $(7.57\cdot10^{-32})$
Volume	20	1	0.9999	8.10	$= 179.42(\pm7.84) + 80.18(\pm0.44)\cdot HE_1(P_{15})$	$1.45\cdot10^5(1.28\cdot10^{-36})$
HydE	20	1	0.9998	0.03	$= 1.60(\pm0.03) + 0.28(\pm0.002)\cdot HE_1(P_{15})$	$1.15\cdot10^5$ $(1.02\cdot10^{-35})$
LogP	20	1	0.9999	0.04	$= 0.99(\pm0.04) + 0.44(\pm0.002)\cdot HE_1(P_{15})$	$1.72\cdot10^5$ $(2.77\cdot10^{-37})$
Ref	20	1	0.9999	0.73	$= 7.77(\pm0.71) + 7.92(\pm0.04)\cdot HE_1(P_{15})$	$1.73\cdot10^5$ $(2.72\cdot10^{-37})$
Polar	20	1	0.9999	0.28	$= 3.08(\pm0.27) + 3.17(\pm0.02)\cdot HE_1(P_{15})$	$1.94\cdot10^5$ $(9.42\cdot10^{-38})$
Property=f(entropy)						
Energy	20	3	0.9597	50.01	$= 1101.07(\pm379)\ H_0(P_{15}) + 460.22(\pm219)\cdot H_\infty(P_{15})$ - $1524.61(\pm360)\cdot H_2(P_{15})$	$1.35\cdot10^2$ $(1.43\cdot10^{-11})$
SAreaA	20	3	0.9661	57.93	$= 1389.83(\pm439)\cdot H_0(P_{15}) + 401.26(\pm254)\cdot H_\infty(P_{15})$ + - $1743.27(\pm417)\cdot H_2(P_{15})$	$1.61\cdot10^2$ $(3.60\cdot10^{-12})$
SAreaG	20	3	0.9696	65.76	$= 1609.32(\pm499)\cdot H_0(P_{15}) + 516.69(\pm289)\cdot H_\infty(P_{15})$ - $2056.97(\pm473)\cdot H_2(P_{15})$	$1.81\cdot10^2$ $(1.50\cdot10^{-12})$
Volume	20	3	0.9696	65.76	$= 3264.11(\pm1013)\cdot H_0(P_{15}) + 1209.12(\pm586)\cdot H_\infty(P_{15})$ + $-4350.51(\pm961)\cdot H_2(P_{15})$	$1.72\cdot10^2$ $(2.20\cdot10^{-12})$
HydE	20	3	0.9613	0.51	$= 11.61(\pm3.86)\cdot H_0(P_{15}) + 2.67(\pm2.23)\cdot H_\infty(P_{15})$ - $13.93(\pm3.66)\cdot H_2(P_{15})$	$1.41\cdot10^2$ $(1.04\cdot10^{-11})$
LogP	20	3	0.9674	0.74	$= 17.88(\pm5.62)\cdot H_0(P_{15}) + 6.63(\pm3.25)\cdot H_\infty(P_{15})$ - $23.82(\pm5.33)\cdot H_2(P_{15})$	$1.68\cdot10^2$ $(2.60\cdot10^{-12})$
Ref	20	3	0.9670	13.43	$= 323.64(\pm101.80)\cdot H_0(P_{15}) + 133.37(\pm58.90)\cdot H_\infty(P_{15})$ - $445.08(\pm96.55)\cdot H_2(P_{15})$	$1.66\cdot10^2$ $(2.89\cdot10^{-12})$
Polar	20	3	0.9670	5.38	$= 129.64(\pm40.76)\cdot H_0(P_{15}) + 53.36(\pm23.59)\cdot H_\infty(P_{15})$ - $178.25(\pm38.66)\cdot H_2(P_{15})$	$1.66\cdot10^2$ $(2.90\cdot10^{-12})$

Table 32. qSAR Models for $G_{5,Y}(C)$: Property = f(energy/entropy)

Property	n	v	r^2	SError	Equation	F (p)
Property=f(energy)						
Energy	19	3	0.9999	0.57	$= -1.87(\pm1.91) + 6.58(\pm0.34)\cdot HE_1(P_{16})$ - $0.03(\pm0.01)\cdot E_1(P_{16}) + 2.22\cdot10^{-4}(\pm1.05\cdot10^{-4})\cdot E_2(P_{16})$	$6.26\cdot10^4$ $(5.98\cdot10^{-31})$
SAreaA	19	3	0.9979	11.09	$= 153.96(\pm36.84) + 32.23(\pm6.64)\cdot HE_1(P_{16})$ - $0.28(\pm0.18)\cdot E_1(P_{16}) + 2.78\cdot10^{-3}(\pm2.03\cdot10^{-3})\cdot E_2(P_{16})$	$2.37\cdot10^3$ $(2.73\cdot10^{-20})$
SAreaG	19	3	0.9982	11.69	$= 167.28(\pm38.80) + 43.56(\pm6.99)\cdot HE_1(P_{16})$ - $0.44(\pm0.18)\cdot E_1(P_{16}) + 3.89\cdot10^{-3}(\pm2.14\cdot10^{-3})\cdot E_2(P_{16})$	$2.74\cdot10^3$ $(9.28\cdot10^{-21})$
Volume	19	3	0.9998	11.15	$= 184.39(\pm37.02) + 85.42(\pm6.67)\cdot HE_1(P_{16})$ - $0.47(\pm0.18)\cdot E_1(P_{16}) + 4.20\cdot10^{-3}(\pm0.002)\cdot E_2(P_{16})$	$2.41\cdot10^4$ $(7.80\cdot10^{-28})$
HydE	19	3	0.9961	0.12	$= 1.74(\pm0.39) + 0.27(\pm0.07)\cdot HE_1(P_{16}) - 2.64\cdot10^{-3}$ $(\pm0.002)\cdot E_1(P_{16}) + 2.65\cdot10^{-5}(\pm2.15\cdot10^{-5})\cdot E_2(P_{16})$	$1.27\cdot10^3$ $(2.84\cdot10^{-18})$
LogP	19	1	0.9999	0.03	$= 1.15(\pm0.03) + 0.53(\pm1)\cdot HE_1(P_{16})$	$8.27\cdot10^5$ $(2.76\cdot10^{-41})$
Refr	19	1	0.9999	0.35	$= 10.00(\pm0.38) + 8.23(\pm0.02)\cdot HE_1(P_{16})$	$1.24\cdot10^6$ $(8.67\cdot10^{-43})$
Polar	19	1	0.9999	0.18	$= 3.97(\pm0.19) + 3.29(\pm0.008)\cdot HE_1(P_{16})$	$7.73\cdot10^5$ $(4.90\cdot10^{-41})$
Property=f(entropy)						
Energy	19	2	0.9258	16.96	$= -239.09(\pm104.35) + 637.46(\pm555.33)\cdot H_0(P_{16})$ - $603.25(\pm570.99)\cdot H_2(P_{16})$	$9.98\cdot10^1$ $(9.22\cdot10^{-10})$
SAreaA	19	2	0.9326	60.77	$= -665.34(\pm373.89) + 2177.07(\pm1989.66)\cdot H_0(P_{16})$ - $2041.01(\pm2045.75)\cdot H_2(P_{16})$	$1.11\cdot10^2$ $(4.25\cdot10^{-10})$
SAreaG	19	2	0.9522	57.90	$= -651.41(\pm356.22) + 2032.94(\pm1895.66)\cdot H_0(P_{16})$ - $1863.57(\pm1949.10)\cdot H_2(P_{16})$	$1.59\cdot10^2$ $(2.71\cdot10^{-11})$
Volume	19	2	0.9285	200.31	$= -2608.62(\pm1232.33) + 7481.67(\pm6557.96)\cdot H_0(P_{16})$ - $7063.55(\pm6742.82)\cdot H_2(P_{16})$	$1.04\cdot10^2$ $(6.85\cdot10^{-10})$
HydE	19	1	0.9136	0.52	$= -1.87(\pm1.21) + 1.49(\pm0.23)\cdot H_0(P_{16})$	$1.80\cdot10^2$ $(1.80\cdot10^{-10})$
LogP	19	2	0.9136	1.85	$= -24.42(\pm11.37) + 69.99(\pm60.49)\cdot H_0(P_{16})$ - $66.75(\pm62.19)\cdot H_2(P_{16})$	$8.46\cdot10^1$ $(3.11\cdot10^{-9})$
Polar	19	2	0.9134	11.53	$= -155.43(\pm70.94) + 436.34(\pm377.50)\cdot H_0(P_{16})$ - $416.12(\pm388.14)\cdot H_2(P_{16})$	$8.44\cdot10^1$ $(3.16\cdot10^{-9})$

Table 33. qSAR Models for $G_{6,Y}(C)$: Property = f(energy/entropy)

Property	n	v	r^2	SError	Equation	F (p)
Property=f(energy)						
Energy	20	1	0.9990	2.60	$= 5.42(\pm 0.04)\cdot HE_1(P_{17})$	$1.84\cdot 10^4$ ($1.54\cdot 10^{-28}$)
SAreaA	20	1	0.9999	2.52	$= 151.81(\pm 2.44) + 29.53(\pm 0.08)\cdot HE_1(P_{17})$	$5.67\cdot 10^5$ ($6.12\cdot 10^{-42}$)
SAreaG	20	1	0.9999	2.86	$= 176.71(\pm 2.77) + 36.14(\pm 0.09)\cdot HE_1(P_{17})$	$6.61\cdot 10^5$ ($1.53\cdot 10^{-42}$)
Volume	20	1	0.9999	7.24	$= 206.35(\pm 7.01) + 76.37(\pm 0.24)\cdot HE_1(P_{17})$	$4.60\cdot 10^5$ ($3.97\cdot 10^{-41}$)
HydE	20	1	0.9998	0.05	$= 1.68(\pm 0.045) + 0.26(\pm 0.002)\cdot HE_1(P_{17})$	$1.35\cdot 10^5$ ($2.52\cdot 10^{-36}$)
LogP	20	1	0.9999	0.06	$= 1.07(\pm 0.057) + 0.58(\pm 0.02)\cdot HE_1(P_{17})$	$4.08\cdot 10^5$ ($1.18\cdot 10^{-40}$)
Ref	20	1	0.9999	0.79	$= 93.10(\pm 0.77) + 8.42(\pm 0.03)\ HE_1(P_{17})$	$4.66\cdot 10^5$ ($3.56\cdot 10^{-41}$)
Polar	20	1	0.9999	0.43	$= 3.38(\pm 0.42) + 3.37(\pm 0.01)\cdot HE_1(P_{17})$	$2.49\cdot 10^5$ ($1.01\cdot 10^{-38}$)
Property=f(entropy)						
Energy	20	3	0.9851	10.47	$= 527.08(\pm 102.48)\cdot H_0(P17_2) - 1011.88(\pm 124.02)\cdot H_1(P_{17}) + 488.05(\pm 176.30)\cdot H_2(P_{17})$	$3.74\cdot 10^2$ ($5.11\cdot 10^{-15}$)
SAreaA	20	3	0.9829	62.03	$= 285.38(\pm 236.05) + 3253.43(\pm 1153.36)\cdot H_0(P17_2) - 5803.63(\pm 926.62)\cdot H_1(P_{17}) + 2492.04(\pm 1210.20)\cdot H_2(P_{17})$	$3.07\cdot 10^2$ ($2.39\cdot 10^{-14}$)
SAreaG	20	3	0.9824	76.98	$= 312.69(\pm 292.95) + 3891.40(\pm 1431.37)\cdot H_0(P17_2) + - 6977.06(\pm 1149.98)\cdot H_1(P_{17}) + 3028.34(\pm 1501.92)\cdot H_2(P_{17})$	$2.99\cdot 10^2$ ($2.98\cdot 10^{-14}$)
Volume	20	3	0.9796	170.23	$= 6198(\pm 1666.55)\cdot H_0(P17_2) -13542(\pm 2016.97)\cdot H_1(P_{17}) + 7602(\pm 2867.02)\cdot H_2(P_{17})$	$2.72\cdot 10^2$ ($6.22\cdot 10^{-14}$)
HydE	20	3	0.9831	0.55	$= 2.97(\pm 2.09) + 29.30(\pm 10.23)\cdot H_0(P17_2) - 52.25(\pm 8.22)\cdot H_1(P_{17}) + 22.39(\pm 10.73)\cdot H_2(P_{17})$	$3.10\cdot 10^2$ ($2.20\cdot 10^{-14}$)
LogP	20	3	0.9801	1.28	$= 49.23(\pm 12.51)\cdot H_0(P17_2) - 104.24(\pm 15.14)\cdot H_1(P_{17}) + 56.58(\pm 21.53)\cdot H_2(P_{17})$	$2.79\cdot 10^2$ ($5.01\cdot 10^{-14}$)
Ref	20	3	0.9807	18.25	$= 739.60(\pm 178.65)\cdot H_0(P17_2) - 1525.31(\pm 216.22)\cdot H_1(P_{17}) + 803.48(\pm 307.34)\cdot H_2(P_{17})$	$2.88\cdot 10^2$ ($3.97\cdot 10^{-14}$)
Polar	20	3	0.9804	7.37	$= 298.30(\pm 72.15)\cdot H_0(P_{17}) -609.92(\pm 87.32)\cdot H_1(P_{17}) + 318.25(\pm 124.12)\cdot H_2(P_{17})$	$2.83\cdot 10^2$ ($4.57\cdot 10^{-14}$)

The investigation of the results obtained in structure-property relationships analysis revealed the followings:

- All investigated formulas of entropies and energies appear in the simple- or multivariate linear regression models with best performances (see Tables 28 - 33).
- The goodness-of-fit of all models varied from 0.9134 (see $G_{5,Y}(C)$, Table 32) to 0.9999.
- The highest determination coefficient was obtained for the structure with carbon atoms (see Tables 28 - 33).
- A determination coefficient very close to the highest possible value ($r^2 = 1$) was systematically obtained for $P_Y(C)$, $G_{4,Y}(C)$, $G_{5,Y}(C)$, $G_{6,Y}(C)$ when the investigated properties proved to be almost perfect linear with energy.
- Almost systematically, the goodness-of-fit of the linear regression models have lower values when the property of interest was investigated as function of entropy compared with the situation when the property of interest was investigated as a function of energy.
- All obtained simple- and multivariate linear regression models were significantly statistic, proving that the proposed formulas for entropies and energies are useful descriptors in investigation of the linear relationship with investigated properties on regular structures (see Tables 28 - 33).
- The investigated properties revealed to be linear dependent by the same entropies and energies parameters for the following structures: $P_Y(C)$, $G_{3,Y}(C)$, $G_{4,Y}(C)$, $G_{6,Y}(C)$.
- The descending classification of entropy parameters used by the identified models is as follows (see Table 13): Hartley's entropy (appear in 40 out of 49 models, ~ 82%); min entropy (32 out of 49 models, 65%); Simpson diversity index (appear in 27 out of 49 models, ~ 55%); and Shannon's entropy (21 out of 49 models, ~43%).
- The descending classification of energy parameters used by the identified models are: HE_1 (Eq(28), 50 out of 50 models, ~ 100%); E_2 (Eq(27), 15 out of 50 models, ~ 30%); E_1 (Eq(26), 10 out of 50 models, ~ 20%). The HE_2 (Eq(29) was not identified in any SAR model (see Table 34).

Table 34. Summary of entropy and/or energy formulas used in best performing qSAR models

Structure \ Prop	Energy	SAreaA	SAreaG	Volume	HydE	LogP	Refr	Polar	MeltP	BoilP
$P_Y(C)$	HE_1 H_0; H_∞	HE_1 H_0; H_∞	HE_1 H_0; H_∞	HE_1 H_0; H_∞	HE_1 H_0; H_∞	HE_1 H_0; H_∞	HE_1 H_0; H_∞	HE_1 H_0; H_∞	HE_1 H_0; H_∞	HE_1 H_0; H_∞
$G_{3,Y}(C)$	HE_1; E_1; E_2 H_0; H_1; H_∞	HE_1; E_1; E_2 H_0; H_1; H_∞	HE_1; E_1; E_2 H_0; H_1; H_∞	HE_1; E_1; E_2 H_0; H_1; H_∞	HE_1; E_1; E_2 H_0; H_1; H_∞	HE_1 H_0; H_1; H_∞	HE_1 H_0; H_1; H_∞	HE_1 H_0; H_1; H_∞	n.a. n.a	n.a. n.a
$G_{3,Y}(O,N,C)$	E_2; HE_1 H_1; H_2; H_∞	HE_1; E_2 H_1; H_2; H_∞	E_2; HE_1 H_∞	HE_1; E_2 H_∞	E_2; HE_1 H_1; H_2	HE_1 H_2	HE_1 H_1; H_2; H_∞	HE_1 H_1; H_2; H_∞	n.a. n.a.	n.a. n.a.
$G_{4,Y}(C)$	HE_1 H_0; H_2; H_∞	HE_1 H_0; H_2; H_∞	HE_1 H_0; H_2; H_∞	HE_1 H_0; H_2; H_∞	HE_1 H_0; H_2; H_∞	HE_1 H_0; H_2; H_∞	HE_1 H_0; H_2; H_∞	HE_1 H_0; H_2; H_∞	n.a. n.a.	n.a. n.a.
$G_{5,Y}(C)$	HE_1; E_1; E_2 H_0; H_2	HE_1; E_1; E_2 H_0; H_2	HE_1; E_1; E_2 H_0;	HE_1; E_1; E_2 H_2	HE_1; E_1; E_2 H_0; H_2	HE_1 H_0	HE_1 n.a.	HE_1 H_0; H_2	n.a. n.a.	n.a. n.a.
$G_{6,Y}(C)$	HE_1 H_0; H_1; H_2	HE_1 H_0; H_1; H_2	HE_1 H_0; H_1; H_2	HE_1 H_0; H_1; H_2	HE_1 H_0; H_1; H_2	HE_1 H_0; H_1; H_2	HE_1 H_0; H_1; H_2	HE_1 H_0; H_1; H_2	n.a. n.a.	n.a. n.a.

HE_1 = Eq(28); HE_2 = Eq(29); E_1 = Eq(26); E_2 = Eq(27);
H_0 = Hartley's entropy; H_1 = Shannon's entropy; H_2 = Simpson diversity index; H_∞ = min entropy.

Counting polynomials found applications in biochemistry, genetics and molecular medicine. Rocha et al. [16] introduced new family of metrics for graphs applied on protein secondary and three-dimensional (3D). Srba developed and applied a polynomial time algorithm for analysis of genotype information in pedigrees [17]. Some studies were conducted in investigation of the structure-activity relationships by using counting and characteristic polynomials [7]. Moreover, counting polynomials found their application also on correlation studies [2]. The investigation of counting polynomials of regular iterative structures and the approach of using the information entropy and energy in investigation of structure-activity relationships could open new pathway in drug discovery.

Conclusions

New theoretical results on fragment's size and order based on sizes were obtained by using four square matrices (Szeged, Cluj, MaxF, and CMaxF). The obtained matrices were used to obtain the counting polynomials for a series of regular structures (star, complete, and path). The obtained counting polynomials formulas are general and are parameterized by the type of repeated structure and the number of iterations.

A series of exact formulas were obtained for entropies and energies of counting polynomials on investigated repeated structures. Some exceptions of this rule are observed on the Shannon's entropy, where the exact formulas were obtained just for the first four counting polynomial formulas. The Shannon entropy for other than first four counting polynomials are just approximations of the exact formulas and are given with associated significance levels obtained through comparison with the exact formula obtained based on counting polynomial formulas of first twenty representative.

The informational entropy and energy proved to be useful descriptors in investigation of linear relationship with investigated regular structure properties. The EH_1 energy proved to be able to explain the linear relationship between structure and almost all investigated properties. The preferred entropy by the most identified models was Hartley's entropy. Even if the atoms of the investigated repeated structures are changed, the investigated informational parameter proved their ability in explaining the relationship between structure and investigated properties.

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