QSR and Estimated Biological and Physicochemical Properties Study of Paraffin-base Petroleum (C_1-C_{40})

Kh. Kheradmand*[1], F. Kheradmand[2], M. Kheradmand[3] and Gh. Habibi Dehfouli[4]

Abstract:

The hydrocarbon compounds in petroleum have different structures. Some of them are linear and normal. This homolog series sometimes have attracted the notice for chemical and biochemical studies. The structural parameters are useful indices for examination of structure-property relationship. Graph theory is a delightful ground for the exploration of proof techniques in Discrete Mathematics and its results have applications in many areas of sciences. Topological indices are the numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. In this study the quantitative structural relationship (QSR) between the number of carbon atoms in the structures of normal hydrocarbon C_1 to C_{40}, logarithm of calculated Octanol-Water partitioning coefficients and total biodegradation ($logK_{ow}$ and TB_d (mol/h), respectively), median lethal concentration 50 (LC_{50}), water solubility (S_w, mg.L^{-1}/25ºC) and some of the other calculated chemical and biochemical data in the normal hydrocarbon C_1 to C_{40} (**1-40**) is represented. The results would be extended for some of the other members of these compounds. The interesting results of concerning among $logK_{ow}$, LC_{50}, S_w, TB_d (g/h) and some of the other data with the descriptors for these compounds are presented and discussed.

Keywords: Octanol-Water partitioning coefficient; Biodegradation; Molecular topology; LC_{50}; Water solubility; Topological index; Normal hydrocarbon.

1- Islamic Azad University- Arak Branch, Member of Young Researchers Club (YRC)

2- Chemistry Department, Faculty of Science, Islamic Azad University- Arak Branch, Arak, Iran

3- Physics Department, Faculty of Science, Esfahan University, Esfahan, Iran

4- Chemistry Department, Faculty of Science, Islamic Azad University- Arak Branch, Arak, Iran

Introduction:

Liquid geologically-extracted hydrocarbons are referred to petroleum (literally "rock oil") or mineral oil, while gaseous geologic hydrocarbons are referred to natural gas. All of them are significant sources of fuel and raw materials as a feedstock for organic chemicals production and they are commonly found in the Earth's subsurface using the tools of petroleum geology. The extraction of liquid hydrocarbon fuel from a number of sedimentary basins has been integral to modern energy development. Hydrocarbons are mined from tar sands, oil shale and potentially extracted from sedimentary methane hydrates. These reserves require distillation and upgrading to produce synthetic crude and petroleum. Reserved oil in sedimentary rocks is the source of hydrocarbons for energy, transport and petrochemical industries. Hydrocarbons are of prime economic importance because they encompass the constituents of the major fossil fuels (coal, petroleum, natural gas, etc.) and their derivatives plastics, paraffin, waxes, solvents and oils. Hydrocarbons are one of the Earth's most important energy resources. The predominant use of hydrocarbons is as a combustible fuel source. In their solid form, hydrocarbons take the form of asphalt [1-4] Mixtures of volatile hydrocarbons are now used in preference to the chlorofluorocarbons as a propellant for aerosol sprays, due to chlorofluorocarbons impact on the ozone layer. Methane and ethane C_2 are gaseous at ambient temperatures and they cannot be readily liquefied by pressure alone. Propane C_3 is however easily-liquefied, and exists in 'propane bottles' mostly as a liquid. Butane C_4 is so easily-liquefied that it provides a safe, volatile fuel for small pocket lighters. Pentane C_5 is a clear liquid at room temperature, commonly used in chemistry and industry as a powerful nearly odorless solvent of waxes and high molecular weight organic compounds, including greases. Hexane C_6 is also a widely used non-polar, non-aromatic solvent, as well as a significant fraction of common gasoline.[1-4] C_6 through C_{10} alkanes, alkenes and isomeric cycloalkanes is the top components of gasoline, naptha, jet fuel and specialized industrial solvent mixtures. With the progressive addition of carbon units, the simple non-ring structured hydrocarbons have higher viscosities, lubricating indices, boiling points, solidification temperatures, and deeper color. At the opposite extreme from C_1 methane lie the heavy tars that remain as the *lowest fraction* in a crude oil refining retort. They are collected and widely utilized as roofing compounds, pavement composition, wood preservatives (the creosote series) and as extremely high viscosity sheer-resisting liquids.[1-4] Investigation of the different useful applications of graph theory shows obviously that this aria is an exploration of techniques in Discrete Mathematics and its results can be applied in various fields of sciences. Graph theory has been found to be an effective tool in *QSAR* and *QSPR* [5-10]. A graph is a topological concept rather than a geometrical concept of fixed geometry, and hence Euclidean metric lengths, angles and three-dimensional spatial configurations have no meaning. Numerous studies have been made relating to these mentioned fields by using what are called topological indices (TI) [10]. All of the applications proved that we can utilize the topological indices as very useful for molecular structure studies like description and suggestion of chemical and structural properties, biological and toxicological characters of compounds. One of the stages of topological indices (TI) started when M. Randić introduced the molecular branching index.[11] In 1975, Randić proposed a topological index that has become one of the most widely used in both *QSAR* and *QSPR* studies. However, the most important contribution of this stage is probably the great number of applications of *TI*s in several fields of chemistry. The *TI*s are based on the original idea of Randić of molecular branching but extended to account for contributions coming from path clusters, clusters and chains of different lengths [12-19]. The new jump of research in TIs probably has started on 1990's. At the middle of the 1990 decade the number of studies and applications of TIs in chemistry was increased.[20,27] Among the successful TIs in these applications, it is worth to mention the molecular connectivity indices [20,21], including the Randic index [11], Randić index[22,30,34,35], the indices of Kier[24], elecro topological state indices[25], Balaban index[26] and Wiener index [23]. *N. Trinajstić* and coworkers reported that 39 topological indices are presently available in the literatures.[28] Estrada has made important studies in terms of generalized TIs with several topological indices in the graph invariant.[29] In 1993 and 1997 a related complex of application of the Wiener and Harary indices was reported in fullerene science.[36,37] The use of the effective mathematical methods for making good correlations between several data properties of chemicals and the indices were reported.[36-39]

It needs to use the effective and useful mathematical methods for making good concern between several data of chemical properties, medicinal chemistry and biological activity of chemicals. The octanol-water partition coefficient (K_{ow}) is a measure of the equilibrium concentration of a compound between octanol and water that indicates the potential for partitioning in to soil organic matter (i.e., a high K_{ow} indicates a compound which will preferentially partition into soil organic matter rather than water). This coefficient is inversely related to the solubility of a compound in water. The $logK_{ow}$ is used in models to estimate plant and soil invertebrate bioaccumulation factors. LogK_{ow} is commonly used in QSAR studies and drug design, since this property is related to drug absorption, bioavailability, metabolism, and toxicity. This parameter is also used in many environmental studies to help determine the environmental fate of chemicals [31-33].

Biodegradation (TB_d) is a useful and important factors in chemical and biochemical studies [32].

In this study the relationship of the number of carbon atoms in the structures of normal hydrocarbon C_1 to C_{40} (**1-40**) as an important class of the saturated hydrocarbons as molecular descriptions of structure-property relationship studies, logarithm of calculated Octanol-Water partitioning coefficients and total biodegradation, $logK_{ow}$ and TB_d (mol/h and g/h), respectively, median lethal concentration 50 (LC_{50}), water solubility (S_w, mg.L^{-1}/25ºC), HLC (in atm.m^3/mol), EC_{50} green algae (in ppm), logarithm values of bioconcentration factor as log[BCF], Bio half-life, logarithm values of bioaccumulation factor as log[BAF], adsorption coefficient (K_{oc}), fugacity in air and soil, reaction air (kg/hr) and advection percent sediment in C_1 to C_{40} compounds **1-40** (see Table-1) will be considered [31-33,40,41].

Graphing and Mathematical Method:

The number of carbon atoms in the normal hydrocarbon C_1 to C_{40} (**1-40**), "n" factor, is a favored value in the structures. For modeling operations linear (MLR) and nonlinear (ANN) models was used and investigated in this study. To calculate the scales that were not reported previously the equations 1-10 of this study were utilized. Some of the other indices were examined and the best results and equations for extending the physicochemical data were chosen. All graphing operations were performed using the *Microsoft Office Excel-2003* program. The data of Octanol-Water partitioning coefficients and total biodegradation ($logK_{ow}$ and TB_d (g/h), respectively), median lethal concentration 50 (LC_{50}) and water solubility (S_w, mg.L^{-1}/25ºC) were calculated by EPI-suit v3.12 package.[41].

Results and Discussion:

It is reported and accepted that the toxicity property of organic compounds can be predicted on the basis of the $logK_{ow}$.[38] The QSAR results hold true for quite a lot of organic compounds, the most commonly used for test organism, follows this standard pattern. [39] Biodegradation is usually quantified by incubating a chemical compound in presence of a degrader, and measuring some factors like oxygen or production of CO_2. The biodegradation QSAR studies demonstrate that microbial biosensors are a viable alternative means of reporting on potential biotransformation. However, a few chemicals are tested and large data sets for different chemicals need for QSAR modeling.[30-39] This study shows the structural relationship between the number of carbon atoms in the structures of normal hydrocarbon C_1 to C_{40} (**1-40**) as an important class of the saturated hydrocarbons as molecular descriptions of structure-property relationship studies, logarithm of calculated Octanol-Water partitioning coefficients and total biodegradation, $logK_{ow}$ and TB_d (mol/h and g/h), respectively, median lethal concentration 50 (LC_{50}), water solubility (S_w, mg.L^{-1}/25ºC), HLC (in atm.m^3/mol), EC_{50} green algae (in ppm), log[BCF], Bio half-life, log[BAF], K_{oc}, fugacity in air and soil, reaction air (kg/hr) and advection percent sediment in C_1 to C_{40} compounds **1-40**.

An LC_{50} value is the concentration of a material in air that will kill 50% of the test subjects (animals, typically mice or rats) when administered as a single exposure (typically 1 or 4 hours). Also called the median lethal concentration and lethal concentration 50, this value gives an idea of the relative acute toxicity of an in halable material. Other variants that are occasionally used are LC_{25} and LC_{75} which refer to the lethal concentration that kills 25% and 75% of test subjects, respectively. Both LC_{50} and LD_{50} values state the animal used in the test. This is important because animal toxicity studies do not necessarily extrapolate (extend) to humans. For example, dioxins are highly toxic to guinea pigs and ducklings at extremely low levels, but have never been conclusively linked to a single human death even at very high levels of acute (short term) exposure. However, it is best to err on the safe side when evaluating animal toxicity studies and assume that most chemicals that are toxic to animals are toxic to humans. Typical units for LC_{50} values are parts per million (ppm) of material in air, micrograms (10^{-6} = 0.000001 g) per liter of air and milligrams (10^{-3} = 0.001 gr) per cubic meter of air.[36] There are two

types of the fishes that were often considered in the more of veterinary studies: Carassius auratus (Gold fish) and Perca fluviatilis (the sea fish).
The biological half-life of water in a human is about 7 to 10 days. It can be altered by behavior. Drinking large amounts of alcohol will reduce the biological half-life of water in the body. This has been used to decontaminate humans who are internally contaminated with tritiated water T_2O (tritium). Drinking the same amount of water would have a similar effect, but many would find it difficult to drink a large volume of water. The basis of this decontamination method is to increase the rate at which the water in the body is replaced with new water.
An effective dose in pharmacology is the amount of drug that produces a therapeutic response in 50% of the people taking it, sometimes also called ED-50. In radiation protection it is an estimate of the stochastic effect that a non-uniform radiation dose has on a human. In pharmacology, effective dose is the median dose that produces the desired effect of a drug. The effective dose is often determined based on analysing the dose-response relationship specific to the drug. The dosage that produces a desired effect in half of the test population is referred to as the ED-50, for "Effective dose, 50%".

Bioconcentration factor (BCF) used to describe the accumulation of chemicals in organisms, primarily aquatic, that live in contaminated environments. According to EPA guidelines, "the BCF is defined as the ratio of chemical concentration in the organism to that in surrounding water. Bioconcentration occurs through uptake and retention of a substance from water only, through gill membranes or other external body surfaces. In the context of setting exposure criteria it is generally understood that the terms "BCF" and "steady-state BCF"' are synonymous. A steady-state condition occurs when the organism is exposed for a sufficient length of time that the ratio does not change substantially." Bioconcentration factors (BCFs) are used to relate pollutant residues in aquatic organisms to the pollutant concentration in ambient waters.[42-50] The bioconcentration factor (BCF) is related to biomagnification efects. Many chemical compounds, especially those with a hydrophobic component partition easily into the lipids and lipid membranes of organisms and bioaccumulate. If the compounds are not metabolized as fast as they are consumed, there can be significant magnification of potential toxicological effects up the food chain. The concern about bioaccumulation and biomagnification comes mainly from experience with chlorinated compounds, especially pesticides and PCBs, and their deleterious effects on vulnerable species, especially birds, frogs, and fish. Only minimal experimental and monitoring information has been gathered on the bioaccumulation properties of many other currently used chemical compounds. In fact, the biomagnification of many widely available chemicals has not been observed or predicted in aquatic systems. BCF or BAF (bioaccumulation factor) values are based on U.S. Environmental Protection Agency publications pursuant to Section 304(a) of the Federal Water Pollution Control Act as amended, literature values, or site-specific bioconcentration data. Current EPA guidelines for the derivation of human health water quality criteria use BCFs as well. [42-50]

The organic carbon adsorption coefficient, K_{OC}, is crucial for estimating a chemical compound's mobility in soil and the prevalence of leaching from soil. The adsorption of a compound increases with an increase in organic content, clay content, and surface area of the soil. The presence of a chemical compound can also be detected in ground water, and inference can be made about its residence time in the soil and the degradation period before reaching the water table. The presence of continuous pores or channels in soil will increase the mobility of a chemical compound in the soil.[51-55]

Fugacity is a measure of a chemical potential in the form of 'adjusted pressure.' It reflects the tendency of a substance to prefer one phase (liquid, solid, or gas) over another, and can be literally defined as "the tendency to flee or escape". At a fixed temperature and pressure, a homogeneous substance will have a different fugacity for each phase. The phase with the lowest fugacity will be the most favorable, and will have the lowest Gibbs free energy. Fugacity has the same units as pressure (e.g., atm, psia, bars, etc.) As well as predicting the preferred phase of a single substance, fugacity is also useful for multi-component equilibrium involving any combination of solid, liquid and gas equilibrium. It is useful as an engineering tool for predicting the final phase and reaction state of multi-component mixtures at various temperatures and pressures without doing the actual lab test. Fugacity is not a physical property of a substance; rather it is a calculated property which is intrinsically related to chemical potential. When a system approaches the ideal gaseous state (very low pressure), chemical potential approaches negative infinity, which for the purposes of mathematical modeling is undesirable. Under the same conditions, fugacity approaches the ideal pressure of the substance and the fugacity coefficient (defined below) approaches 1. Thus, fugacity is much easier to manipulate mathematically.[1, 42-55]

In Fig.-1 to Fig.-8 two dimensional diagrams of the relationship between the values of $logK_{ow}$, TB_d, log(*BCF*), log(*BCF*), bio-half life, soil fugacity and estimated log(K_{oa}) with number of carbon atoms in the normal hydrocarbon C_1 to C_{40} **1-40** (n-factor) were shown. In some figures, the logarithmic values of these amounts were demonstrated. The values of the relative structural coefficients of the logarithm of calculated Octanol-Water partitioning coefficients and total biodegradation, $logK_{ow}$ and TB_d (mol/h and g/h), respectively, median lethal concentration 50 (LC_{50}), water solubility (S_w, mg.L^{-1}/25ºC), HLC (in atm.m^3/mol), EC_{50} green algae (in ppm), log[BCF], Bio half-life, log[BAF], K_{oc}, fugacity in air and soil, reaction air (kg/hr) and advection percent sediment in C_1 to C_{40} compounds **1-40** data were shown in Table-1. Table 2 shows the equations (1-13) that indicate the relationships between the selected chemical and biochemical data logarithm of calculated Octanol-Water partitioning coefficients and total biodegradation, $logK_{ow}$ and TB_d (mol/h and g/h), respectively, median lethal concentration 50 (LC_{50}), water solubility (S_w, mg.L^{-1}/25ºC), HLC (in atm.m^3/mol), EC_{50} green algae (in ppm), log[BCF], Bio half-life, log[BAF], K_{oc}, fugacity in air and soil, reaction air (kg/hr) and advection percent sediment in C_1 to C_{40} compounds **1-40**.
Equation 1 has shown the linear relationships between log(K_{ow}) and number of carbon atoms in C_1 to C_{40} compounds **1-40**. The R-squared value (R^2) for this graph shows 0.9930. Equation 2 has shown a second order relationship between TB_d (in g/h) and number of carbon atoms in C_1 to C_{40}. The R-squared value (R^2) for this graph shows 0.9050. The equation 3 is a four-order polynomial equation between TB_d (in mol/h) and the number of carbon atoms in C_1 to C_{40}. The R-squared value (R^2) for this graph shows 0.8553. In equations 4 was demonstrated the correlations between $logS_w$ with the number of carbon atoms in C_1 to C_{40} compounds **1-40**. The value of R-squared value (R^2) for this equation and its graph is 0.9970. The relationships between *log (BCF)* and the number of carbon atoms in the linear hydrocarbons C_1 to C_{40}. The R-squared value (R^2) for this graph shows 0.8711. The exponential relationship of bio-half life (B-hl) and "n" as the number of carbon atoms of **1-40** were shown in equations 5. In this equation the R^2 value is 0.9898. Equation 6 was demonstrated the relationship of *log [BAF]* and the number of carbon atoms in the linear hydrocarbons C_1 to C_{40} (R^2=0.9111). In equations 7 the correlations between Soil Fugacity and n-values of C_1 to C_{40} compounds **1-40** was shown. The R-squared value (R^2) for this graph shows 0.9320. The equations 9 and 10 show the linear correlations of $logK_{oa}$ and $logK_{aw}$ with the number of carbon atoms in C_1 to C_{40} compounds **1-40**. The values of R-squared value (R^2) for equations 9 and 10 and their graph are 0.9920 and 0.9580, respectively. In equations 11 to 13 the exponential correlations between LC_{50}, EC_{50} and K_{oc}(Soil) with the number of carbon atoms in C_1 to C_{40} compounds **1-40** were demonstrated. The values of R-squared value (R^2) for equations 11 to 13 and their graph are 0.8108, 0.9800 and 0.9962, respectively. By the use of descriptor "n" for linear hydrocarbons C_1 to C_{40} compounds **1-40** in the Eq.-1 to -13 we can achieve a good approximation for the selected chemical and biochemical data logarithm of calculated Octanol-Water partitioning coefficients and total biodegradation, $logK_{ow}$ and TB_d (mol/h and g/h), respectively, median lethal concentration 50 (LC_{50}), water solubility (S_w, mg.L^{-1}/25ºC), HLC (in atm.m^3/mol), EC_{50} green algae (in ppm), log[BCF], Bio half-life, log[BAF], K_{oc}, fugacity in air and soil, reaction air (kg/hr) and advection percent sediment in C_1 to C_{40} compounds **1-40**.

Conclusion:

The chemical, biochemical and environmental factors as the important points have high importance for predicting the useful models in the chemical and biochemical, medical and drug structure designs studies of the compounds. The toxicity property of organic compounds can be predicted on the basis of the $logK_{ow}$. The biodegradation QSAR studies demonstrate that microbial biosensors are viable alternative means of reporting on potential biotransformation. Here the relationship of the structural relationship between the number of carbon atoms in the structures of normal hydrocarbon C_1 to C_{40} (**1-40**) as an important class of the saturated hydrocarbons as molecular descriptions of structure-property relationship studies, logarithm of calculated Octanol-Water partitioning coefficients and total biodegradation, $logK_{ow}$ and TB_d (mol/h and g/h), respectively, median lethal concentration 50 (LC_{50}), water solubility (S_w, mg.L^{-1}/25ºC), HLC (in atm.m^3/mol), EC_{50} green algae (in ppm), log[BCF], Bio half-life, log[BAF], K_{oc}, fugacity in air and soil, reaction air (kg/hr) and advection percent sediment in C_1 to C_{40} compounds **1-40** was considered. The structural parameters (n) show good differences between the values of the selected calculated data which they were computed by EPI-suit v3.12 package, as important factors in chemical and biochemical studies in these compounds.

References:

1. a) McMurry, J. *Organic Chemistry* 5th ed. Brooks/Cole: **2000**, Thomson Learning. b) Hydrocarbon - Wikipedia, the free encyclopedia.htm.
2. Clayden, J., Greeves, N., et al. *Organic Chemistry* Oxford , **2000**.
3. Silberberg, Martin. Chemistry the Molecular Nature Of Matter And Change. New York: McGraw-Hill Companies, **2004**.
4. Meierhenrich, Uwe. Amino Acids and the Asymmetry of Life. Springer, **2008**.
5. P. J. Hansen and P. Jurs, *J. Chem. Edu.*, **1988**, 65, 574-580. (and the literature cited therein).
6. H. Hosoya, *Bull. Chem. Soc. Jpn*., **1971**, 44, 2332-2339.
7. M. Randić , *Acta Chim. Slov.*, **1998**, 45, 239-252.
8. G. Rücker and C. Rücker, *J. Chem. Inf. Cmput. Sci.*, **1999**, 39, 788-802.
9. H. Wiener, *J. Am. Chem. Soc.*, **1947**, 17-20.
10. Y. P. Du, Y. Z. Liang, B. Y. Li and C. J. Xu, *J. Chem. Inf. Cmput. Sci.*, **2002**, 42, 1128-1138.
11. M. Randić , *J. Am. Chem. Soc.*, **1975**, 97, 6609-6615.
12. A. Sabljić and N. Trinajstić, *Acta Pharm. Ugosl.* , **1981**, 31, 189-214.
13. P. G. Sybold, M. May and U. A. Bagal, *J. Chem. Edu.*, **1987**, 64, 575-582.
14. L. B. Kier and L. H. Hall, *Molecular Connectivity in Chemistry and Drug Research*, Academic Press, New York, **1976**.
15. M. Randić , *J. Math. Chem.*, **1991**, 7, 155-168.
16. M. Randić and D. Mills and S. C. Basak, *Int. J. Quantum Chem.*, **2000**, 80, 1199-1209.
17. M. Randić, D. Plavšić and N. Lerš, *J. Chem. Inf. Cmput. Sci.*, **2001**, 41, 657-662.
18. M. Randić and S. C. Basak, *J. Chem. Inf. Cmput. Sci.*, **2001**, 41, 614-618.
19. M. Randić and M. Pompe , *J. Chem. Inf. Cmput. Sci*., **2001**, 41, 575-581.
20. L. B. Kier and L. H. Hall, *Molecular Connectivity in Chemistry and Drug Research*, Academic Press, New Yourk, **1976**.
21. L. B. Kier and L. H. Hall, *Molecular Connectivity in Structure-Activity, Research Studies Press*, Letchwork, 1986.
22. I. Gutman and M. Randic, *Chem. Phys. Lett.*, **1977**, 47, 15-19.
23. H. Wiener, *J. Am. Chem. Soc.*,**1947**,69,17-20.
24. L. B. Kiere, *Quant. Struc.-Act. Relat.*, **1985**,4,109-116.
25. L. B. Kiere and L. H. Hall, *Molecular Structure Description: The Electrotopological State*, Academic Press, New York, **1999**.
26. A. Balaban, *Chem. Phys. Lett.*, **1982**, 89, 399-404.
27. Quin-Nan Hu and Yi-Zeng Liang, *Internet Electron. J. Mol. Des.*, **2004**, 3(6), 335-349.
28. M. Barysz, D. Plavšić and N. Trinajstić, *Match,* **1986,** 19, 89-116.
29. E. Estrada, *Chem. Phys. Lett.*, **2000**, 336, 284-252.
30. J. G. Leahy and R. R. Colwell, *Microbiol Mol Biol Rev.*, **1990**, 54(3), 305-315
31. C. Hansch, A. Leo and D. Hoekman, *Exploring QSAR: Hydrophobic, Electronic, Steric Constants*, ACS, Washington, DC, USA, **1995**.
32. J. G. Bundy, A. W. J. Morriss, D. G. Durham, C. D. Campbell and G. I. Paton, *Chemosphere*, **2001**, 42, 885-892. (and the literature cited there in).
33. A. Li and S.H. Yalkowsky, *Ind. Eng. Chem. Res.*, **1998**, 37, 4470 -4475.
34. A. A. Taherpour, F. Shafiei, *J. Mol. Struct. THEOCHEM*, **2005**, *726*, 183-188.
35. S. D. Bolboaca and L. Jantschi, *Int. J. Mol. Sci.*, **2007**, *8,* 335-345.
36. Z. Slanina, M.-C. Chao, S.-L. Lee and I. Gutman, *J. Serb. Chem. Soc.*, **1997**, 62(3) 211-217.
37. D. Plavšić, S. Nikolić, N. Trinajstić and Z. Mihalić, *J. Math. Chem.*, **1993**, 12, 235-250.
38. A. A. Taherpour, *Fullerenes, Nanotubes and Carbon Nanostructures,* **2007**, 15, 405-415.
39. A. A. Taherpour, *Fullerenes, Nanotubes and Carbon Nanostructures,* **2008**, 16(2), 142-153.
40. For answering to some questions about the LC_{50} was used: http://www.ilpi.com/msds/ref/lc50.html.
41. For study about the EPI-suit v3.12, See US *Environmental Protection Agency* site: http://www.epa.gov/epahome/docs

42. Davis J.W. Carpenter C.L., "Environmental assessment of the alkanolamines.", Reviews of Environmental Contamination & Toxicology. 149:87-137, 1997.

43. Svendsen C. Weeks J.M. "Relevance and applicability of a simple earthworm biomarker of copper exposure. II. Validation and applicability under field conditions in a mesocosm experiment with Lumbricus rubellus.", Ecotoxicology & Environmental Safety. 36(1):80-8, 1997 Feb.

44. Svendsen C. Weeks J.M. "Relevance and applicability of a simple earthworm biomarker of copper exposure. I. Links to ecological effects in a laboratory study with Eisenia andrei." Ecotoxicology & Environmental Safety. 36(1):72-9, 1997 Feb.

45. Falandysz J. Chwir A. "The concentrations and bioconcentration factors of mercury in mushrooms from the Mierzeja Wislana sand-bar, northern Poland." Science of the Total Environment. 203(3):221-8, 1997 Sep 15.

46. Traas T.P. Luttik R. Jongbloed R.H. "A probabilistic model for deriving soil quality criteria based on secondary poisoning of top predators. I. Model description and uncertainty analysis." Ecotoxicology & Environmental Safety. 34(3):264-78, 1996 Aug.

47. Wang X. Harada S. Watanabe M. Koshikawa H. Sato K. Kimura T., "Determination of bioconcentration potential of tetrachloroethylene in marine algae by 13C." Chemosphere. 33(5):865-77, 1996 Sep.

48. Pant A. Srivastava S.C. Singh S.P. "Factors regulating methyl mercury uptake in a cyanobacterium." Ecotoxicology & Environmental Safety. 32(1):87-92, 1995 Oct.

49. Makela T.P. Oikari A.O. "Pentachlorophenol accumulation in the freshwater mussels Anodonta anatina and Pseudanodonta complanata, and some physiological consequences of laboratory maintenance." Chemosphere. 31(7):3651-62, 1995 Oct.

50. Brown D.G. Lanno R.P. van den Heuvel M.R. Dixon D.G. "HPLC determination of plasma thiocyanate concentrations in fish blood: application to laboratory pharmacokinetic and field-monitoring studies." Ecotoxicology & Environmental Safety. 30(3):302-8, 1995 Apr.

51. Vaussenat F. Bosc JY. LeBlanc M. Canaud B. "Data acquisition system for dialysis machines. A model for membrane hydraulic permeability." *ASAIO Journal.* 43(6):910-5, 1997 Nov-Dec.

52. Jop KM. Guiney PD. Christensen KP. Silberhorn EM. "Environmental fate assessment of two synthetic polycarboxylate polymers." *Ecotoxicology & Environmental Safety.* 37(3):229-37, 1997 Aug.

53. Heuman DM. Bajaj RS. Lin Q. "Adsorption of mixtures of bile salt taurine conjugates to lecithin-cholesterol membranes: implications for bile salt toxicity and cytoprotection." *Journal of Lipid Research.* 37(3):562-73, 1996 Mar.

52. Underhill DW. "The adsorption of argon, krypton, and xenon on activated charcoal." *Health Physics.* 71(2):160-6, 1996 Aug.

53. Scarpitta SC. "A new beaded carbon molecular sieve sorbent for ^{222}Rn monitoring." *Health Physics.* 70(5):673-9, 1996 May.

54. el-Kheshen S. Zia H. Badawi A. Needham TE. Luzzi LA. "Coating charcoal with polyacrylate-polymethacrylate copolymer for haemoperfusion. III: The effect of the coat thickness on the adsorption capacity of the coated charcoal and its adsorptivity to small and middle size molecules." *Journal of Microencapsulation.* 12(5):505-14, 1995 Sep-Oct.

55. Scarpitta SC. "A theoretical model for ^{222}Rn adsorption on activated charcoal canisters in humid air based on Polanyi's potential theory [see comments]." Comment in: *Health Physics* 1996 Feb;70(2):271-3 *Health Physics.* 68(3):332-9, 1995 Mar.

No. C	log K_{ow}	TBd (gr/h) 10^{-2}	TBd (mol/h) 10^{-4}	Exp. logK_{oa}	Est. logK_{oa}	Exp.HLC (atm.m3/mol)	logK_{aw}	-log WSol. (mol/lit)	LC_{50} Fish (mg/lit)	EC_{50} Green Algae(ppm)	log BCF	Biohalf life	log BAF	Soil K_{OC}	Fugacity Air 10^{-12}	Fugacity Soil 10^{-8}	ReactionAir 10^{3} (kg/hr)
1	1.09	0.177	1.1	-0.38	-0.34	0.66	1.43	0.789	147.544	19.372	0.39	0.1004	0.28	3.98	374	85.1	455
2	1.81	0.182	0.6	0.42	0.499	0.5	1.311	1.506	91.243	16.474	0.86	0.2706	0.84	13.2	186	45.4	166
3	2.36	0.191	0.43	0.97	0.899	0.71	1.461	2.077	49.472	11.888	1.22	0.3887	1.32	21.7	164	30.9	582
4	2.89	0.22	0.38	1.53	1.301	0.95	1.589	2.632	24.109	7.711	1.57	0.5954	1.79	39.6	58.9	23.4	1.22
5	3.39	0.316	0.44	1.96	1.682	1.25	1.708	3.161	11.065	4.71	1.9	0.8255	2.17	72.2	38.8	18.8	1.42
6	3.9	0.555	0.46	2.4	2.033	1.8	1.867	3.699	4.886	2.768	2.24	1.153	2.49	132	26.6	15.8	1.55
7	4.66	1.2	1.2	2.95	2.747	2.0	1.913	4.45	2.101	1.584	2.74	1.921	2.84	240	19.6	13.6	1.65
8	5.18	1.55	1.4	3.35	3.062	3.21	2.118	4.996	0.885	0.888	3.08	2.922	3.06	437	15.1	11.9	1.73
9	5.65	1.71	1.3	5.65	3.507	3.4	2.143	5.5	0.368	0.491	2.02	3.965	3.88	796	12.0	10.6	1.79
10	5.01	1.45	1	_	2.687	5.15	2.323	5.055	0.151	0.268	1.6	2.454	2.97	1450	9.8	9.53	1.83
11	5.74	1.78	1.1	_	3.843	1.93	1.897	5.784	0.061	0.145	2.08	4.013	3.3	2640	8.02	8.58	1.86
12	6.1	1.77	1	_	3.576	8.18	2.524	6.19	0.025	0.078	2.32	5.026	2.86	4820	6.94	7.93	1.85
13	6.73	2.3	1.2	_	4.659	2.88	2.071	6.827	0.01	0.041	2.73	7.617	4.6	8780	5.67	7.16	1.86
14	7.2	2.26	1.1	_	4.625	9.2	2.575	7.334	0.004	0.022	3.43	10.37	5.71	16000	4.42	6.74	1.81
15	7.71	2.84	1.3	_	4.998	12.6	2.712	7.87	0.00155	0.012	3.18	14.46	4.86	29200	3.47	6.26	1.34
16	8.2	7.47	3.3	_	6.914	0.47	1.286	8.391	0.000613	0.006	2.94	19.92	5.28	53200	2.14	2.86	1.7
17	8.69	4.21	1.7	_	5.493	38.5	3.197	8.913	0.000241	0.003	2.7	27.44	4.8	96900	3.04	5.52	1.71
18	9.18	5.46	2.1	_	5.859	51.2	3.321	9.435	0.0000942	0.00165	2.46	37.8	4.64	177000	2.71	5.25	1.71
19	9.67	6.51	2.4	_	6.227	67.9	3.443	9.956	0.0000367	0.000855	2.22	52.08	4.43	322000	2.42	4.94	1.71
20	10.16	7.1	2.5	_	6.593	90.2	3.567	10.478	0.0000143	0.000443	1.98	71.75	4.19	586000	2.17	4.65	1.71
21	10.65	7.5	2.5	_	6.959	120	3.691	10.999	0.00000555	0.000229	1.74	98.85	3.91	1070000	1.96	4.38	1.71
22	11.15	7.66	2.5	_	7.337	59	3.813	11.521	0.00000215	0.000118	1.5	136.2	3.61	1950000	1.76	4.11	1.71
23	11.64	7.73	2.4	_	7.704	211	3.936	12.042	0.00000083	0.0000606	1.26	187.6	3.29	3550000	1.60	3.84	1.7
24	12.13	7.76	2.3	_	8.071	280	4.059	12.564	0.00000032	0.0000311	1.61	258.5	2.94	6400000	1.44	3.57	1.68
25	12.62	7.78	2.2	_	8.438	372	4.182	13.085	1.23E-07	0.000016	1.37	356.1	2.57	11800000	1.30	3.3	1.65
26	13.11	7.78	2.1	_	8.805	494	4.305	13.607	4.74E-09	0.00000816	1.13	490.6	2.18	21500000	1.16	3.01	1.62
27	13.6	7.79	2	_	9.172	655	4.428	14.128	1.82E-09	0.00000417	0.89	675.9	1.77	39100000	0.969	2.77	1.57
28	14.09	7.79	2	_	9.539	870	4.551	14.65	6.97E-09	0.00000213	0.65	931.2	1.35	71300000	0.909	2.4	1.52
29	14.58	7.79	1.9	_	9.908	1150	4.672	15.171	2.67E-09	0.00000108	0.5	1283	0.94	130000000	0.798	2.08	1.46
30	15.07	7.79	1.8	_	10.274	1530	4.796	15.693	1.02E-09	5.52E-07	0.05	1767	0.57	237000000	0.692	1.76	1.39
31	15.57	7.79	1.8	_	10.649	2040	4.921	16.214	3.9E-09	0.00000028	0.05	2435	0.27	432000000	0.596	1.47	1.31
32	16.06	7.79	1.7	_	11.017	2700	5.043	16.736	1.49E-09	1.42E-07	0.5	3355	0.09	787000000	0.505	1.19	1.24
33	16.55	7.79	1.7	_	11.751	4760	5.289	17.257	5.67E-09	7.23E-08	0.5	4622	0	1430000000	0.37	0.964	1.15
34	17.04	7.79	1.6	_	12.118	6320	5.412	17.779	1.6E-09	3.66E-08	0.5	6367	-0.03	2610000000	0.42	1.35	1.3
35	17.53	7.79	1.6	_	12.485	8390	5.535	18.3	8.22E-09	1.86E-08	0.5	8772	-0.04	4760000000	0.355	1.09	1.22
36	18.02	7.79	1.5	_	12.853	1110	5.657	18.822	3.13E-09	9.39E-08	0.5	12090	-0.05	8680000000	0.157	0.917	1.1
37	18.51	7.79	1.5	_	12.853	1110	5.657	19.343	1.9E-09	4.75E-08	0.5	6550	-0.05	1E+10	0.0187	1.04	1.08
38	19	7.79	1.5	_	13.218	1480	5.782	19.856	4.51E-09	2.4E-08	0.5	22940	-0.05	1E+10	0.0128	1.23	1.15
39	19.45	7.79	1.4	_	13.586	1960	5.904	20.386	1.71E-09	1.21E-08	0.5	31600	-0.05	1E+10	0.00119	1.42	1.22
40	19.99	7.79	1.4	_	13.962	2610	6.028	20.908	6.49E-09	6.12E-08	0.5	43540	-0.05	1E+10	0.0245	1.59	1.31

Table-1: The selected physicochemical properties of C_1-C_{40}.

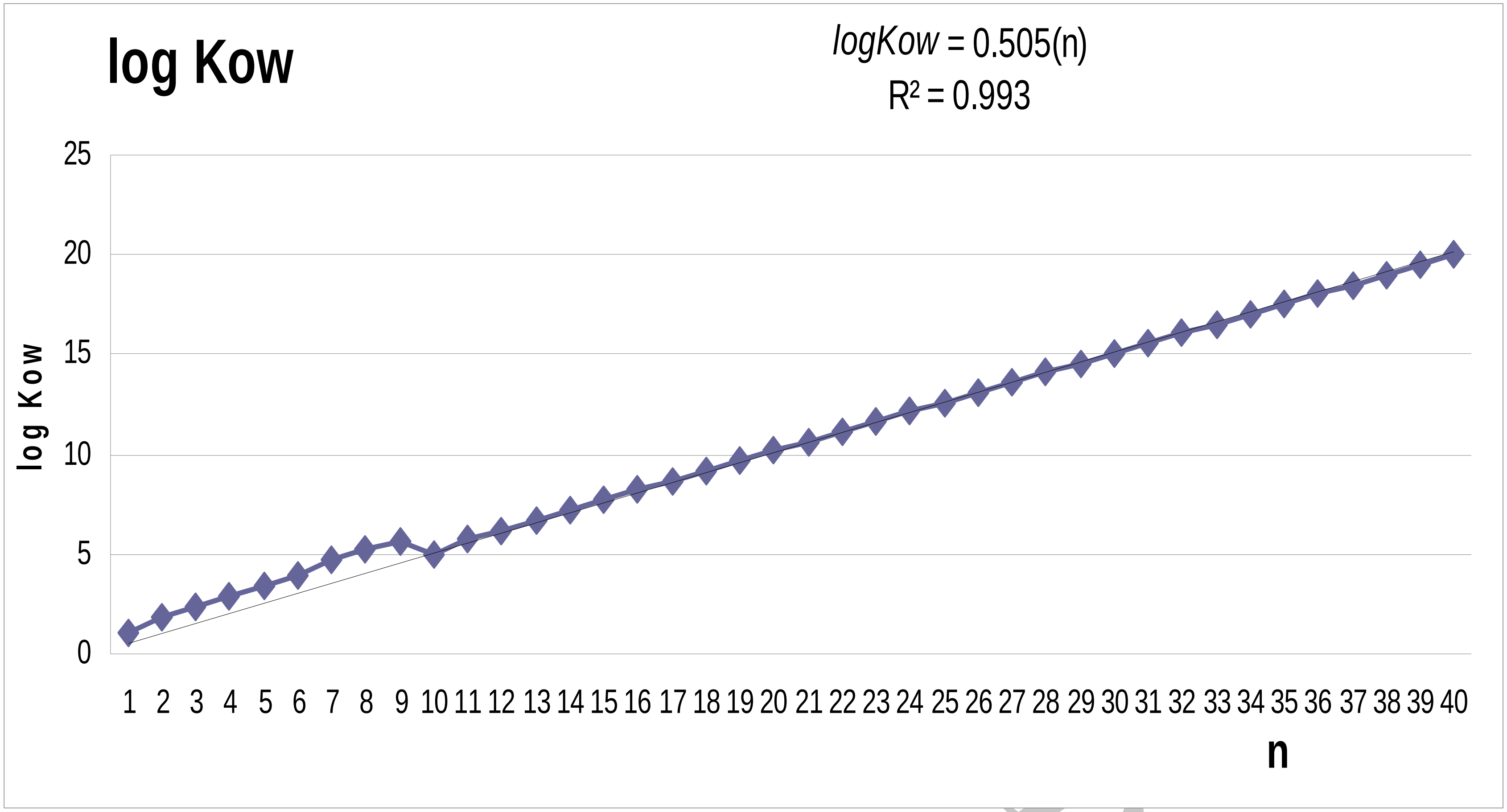

Fig.-1: The relationship between the values of log(K_{ow}) versus the number of carbon atoms in the structures of normal hydrocarbon C_1 to C_{40} (**1-40**).

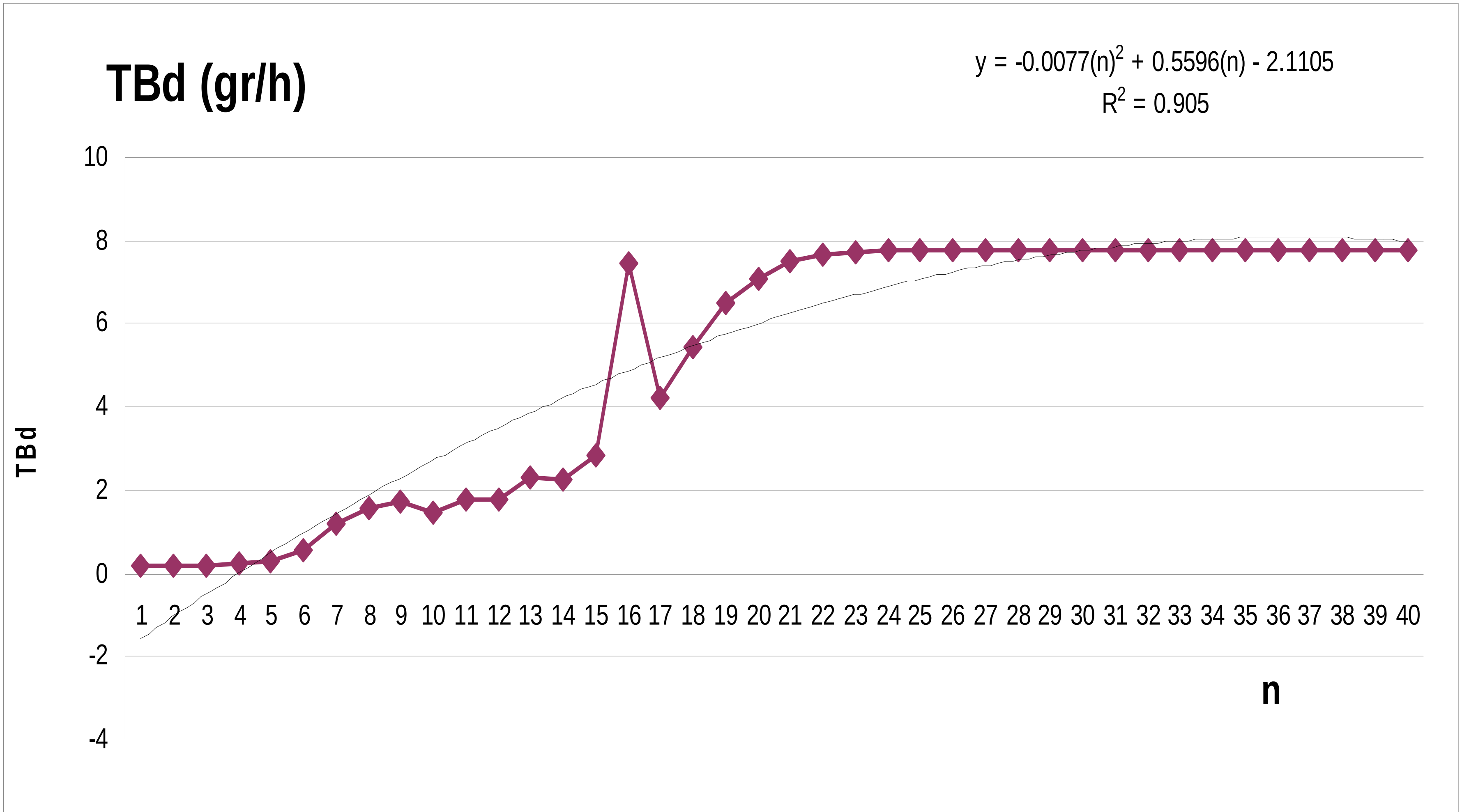

Fig.-2: A plot of the total biodegradation (TB_d) in gr/h versus the number of carbon atoms in the structures of normal hydrocarbon C_1 to C_{40} (**1-40**).

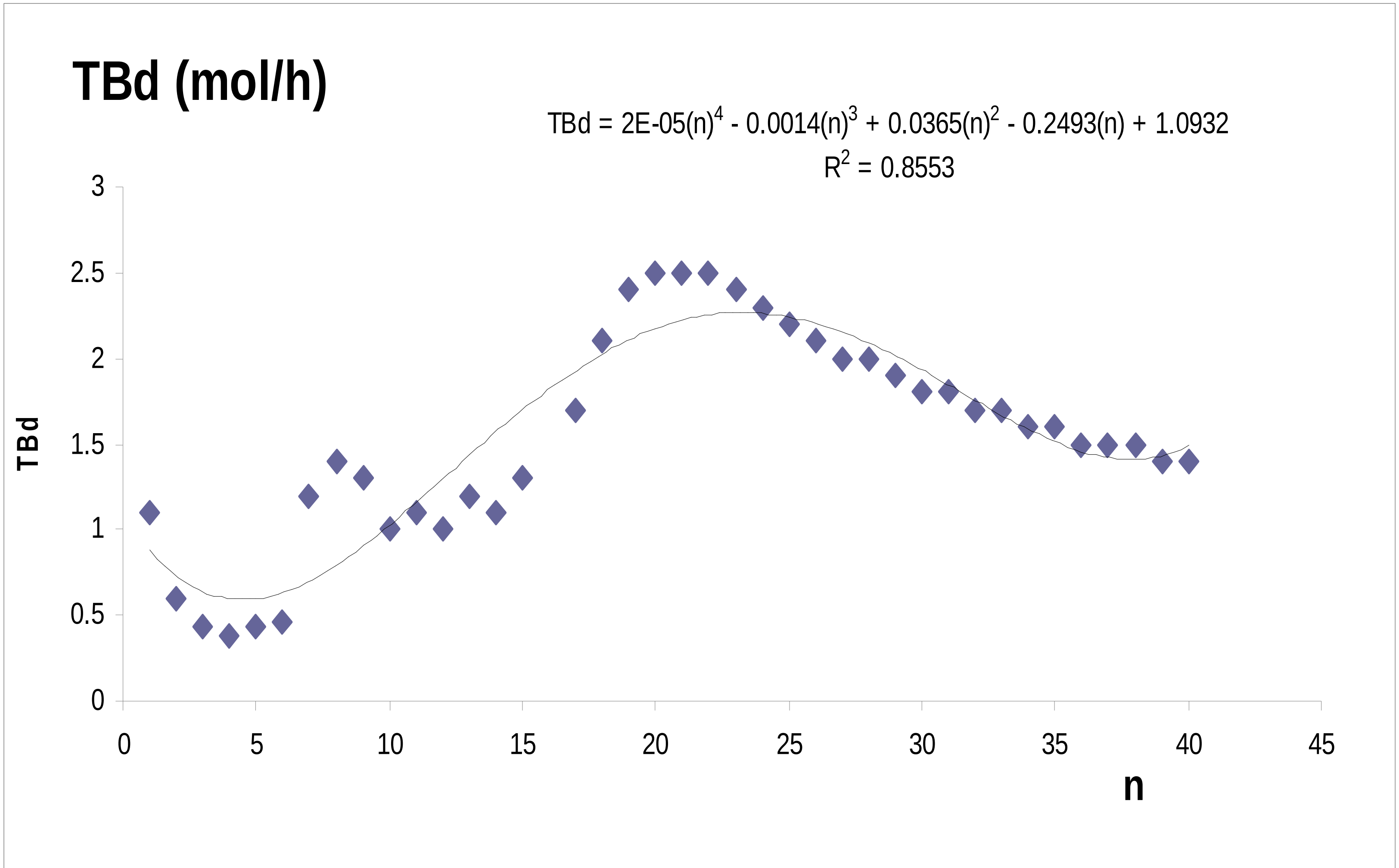

Fig.-3: A plot of the total biodegradation (TB_d) in mol/h versus the number of carbon atoms in the structures of normal hydrocarbon C_1 to C_{40} (**1-40**).

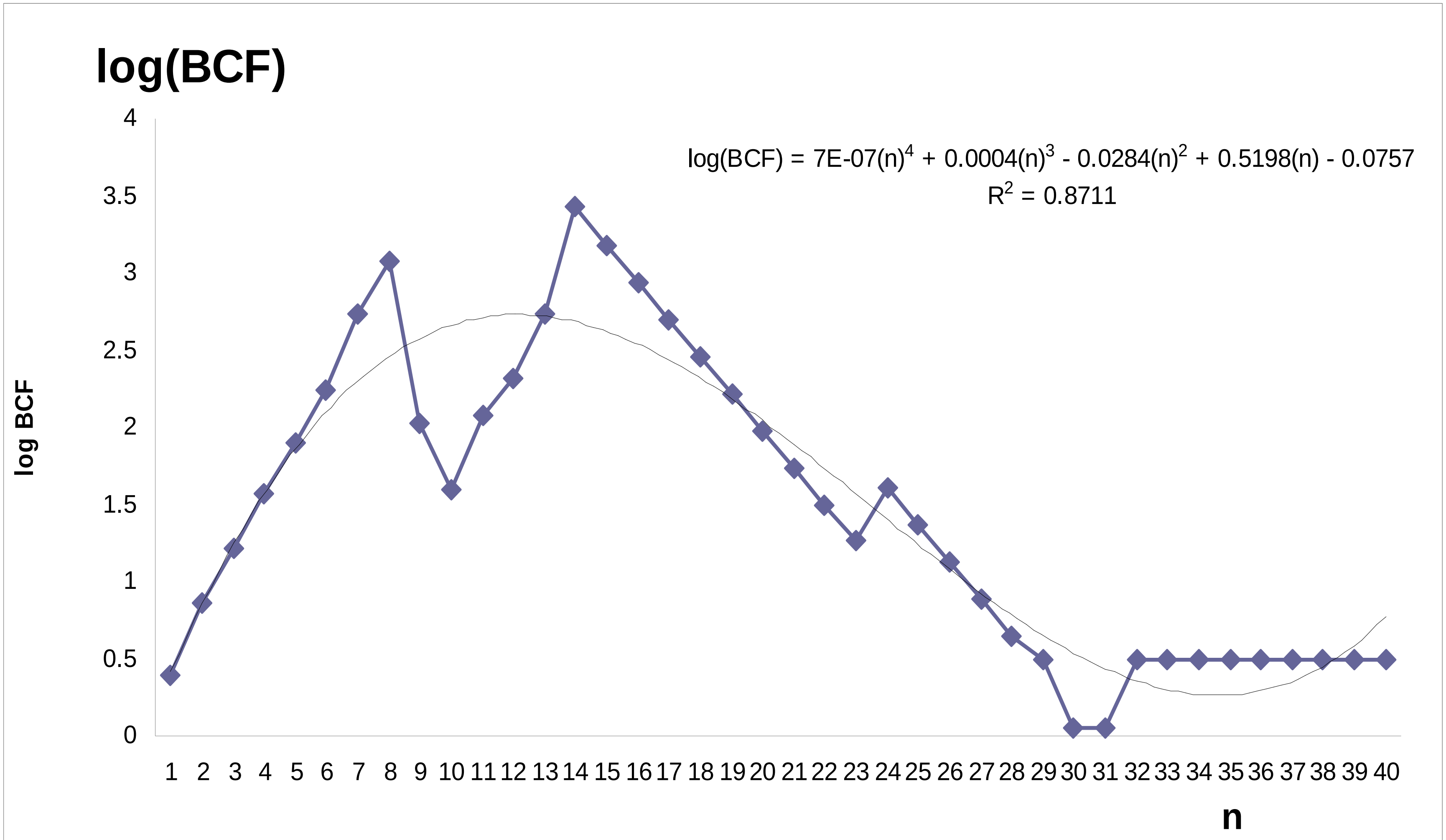

Fig.-4: The relationship between the values of log(*BCF*) versus the number of carbon atoms in the structures of normal hydrocarbon C_1 to C_{40} (**1-40**).

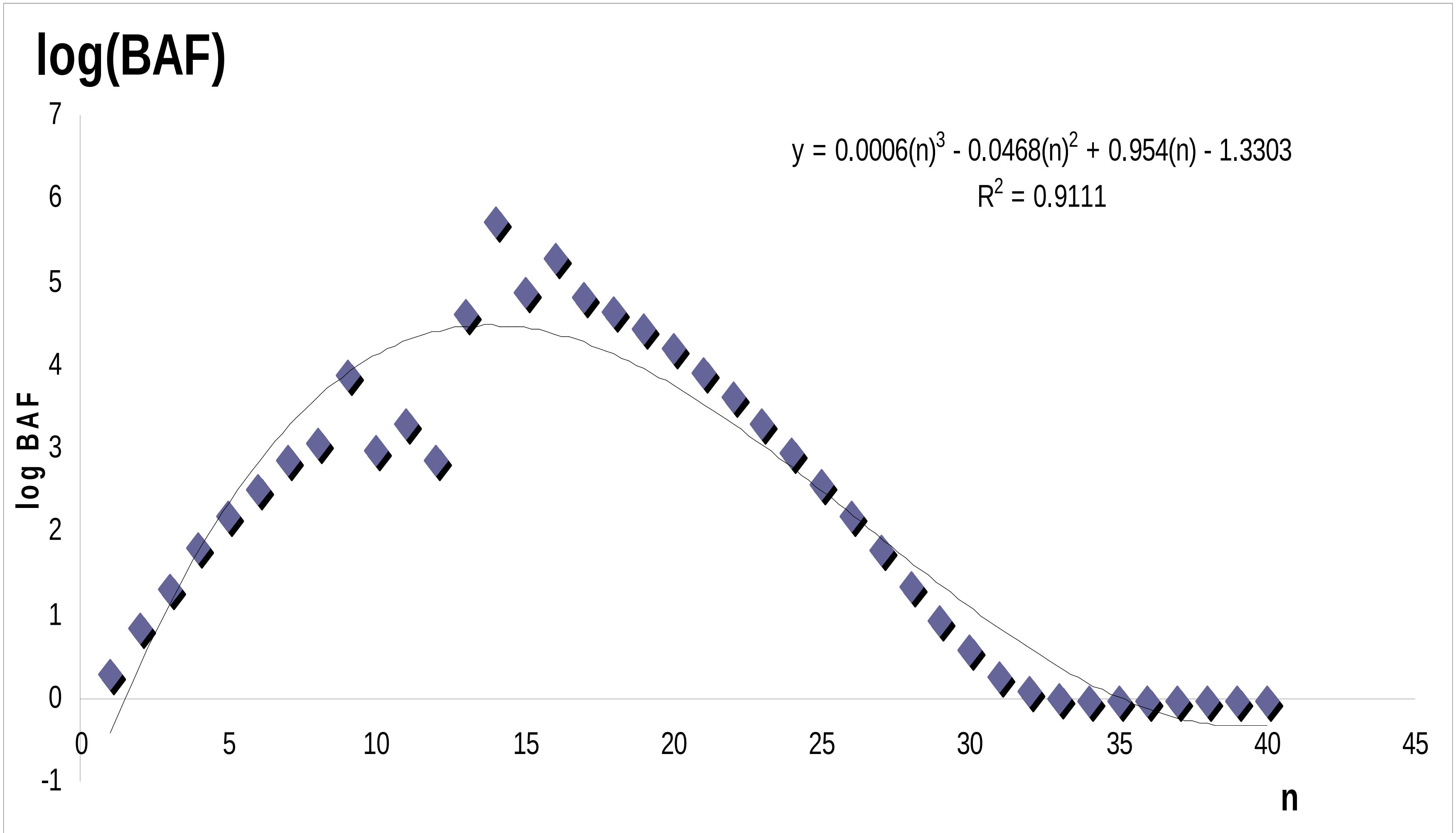

Fig.-5: The relationship between the values of log(*BAF*) versus the number of carbon atoms in the structures of normal hydrocarbon C_1 to C_{40} (**1-40**).

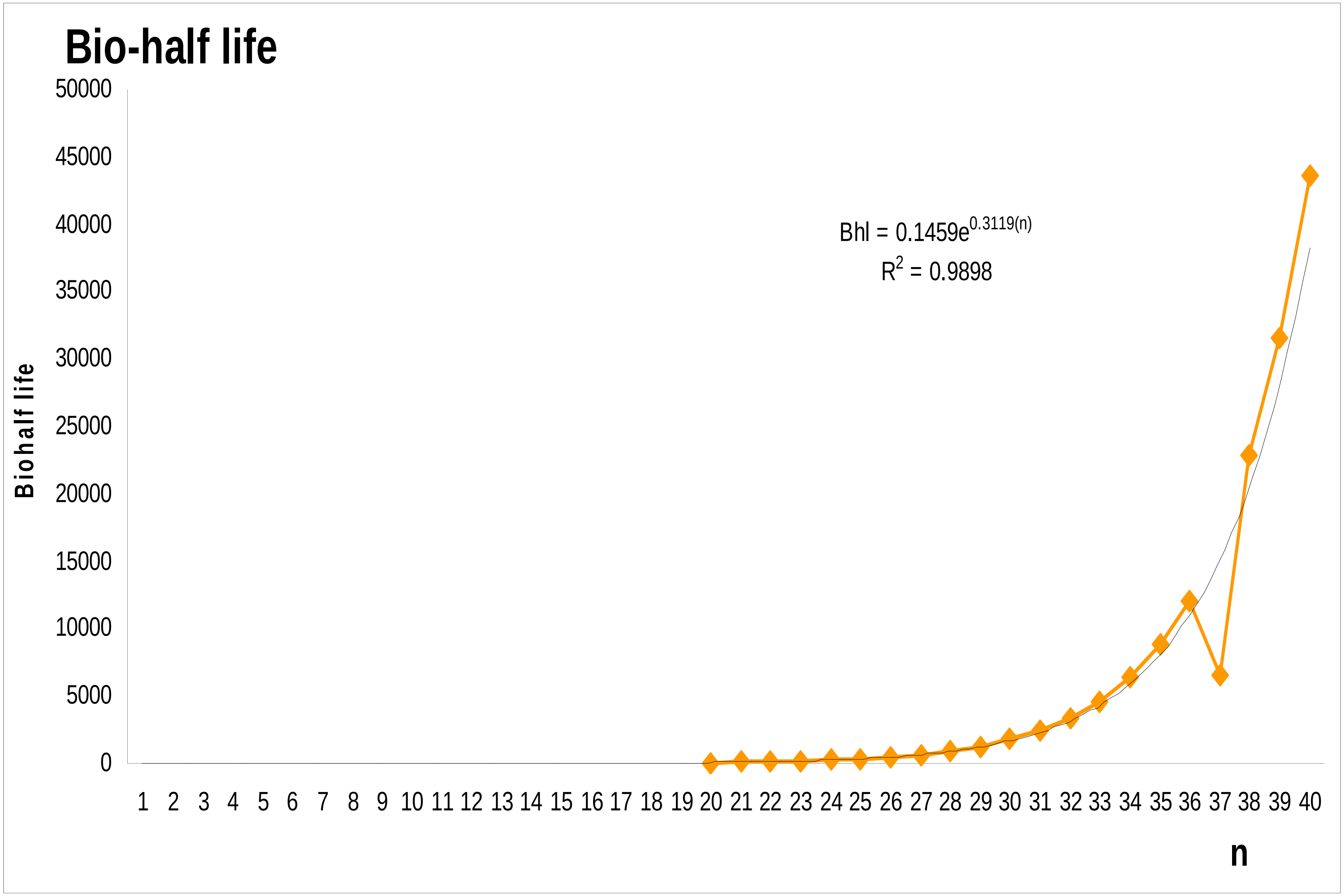

Fig.-6: The relationship between the values of Bio-half life (B-hl) versus the number of carbon atoms in the structures of normal hydrocarbon C_1 to C_{40} (**1-40**).

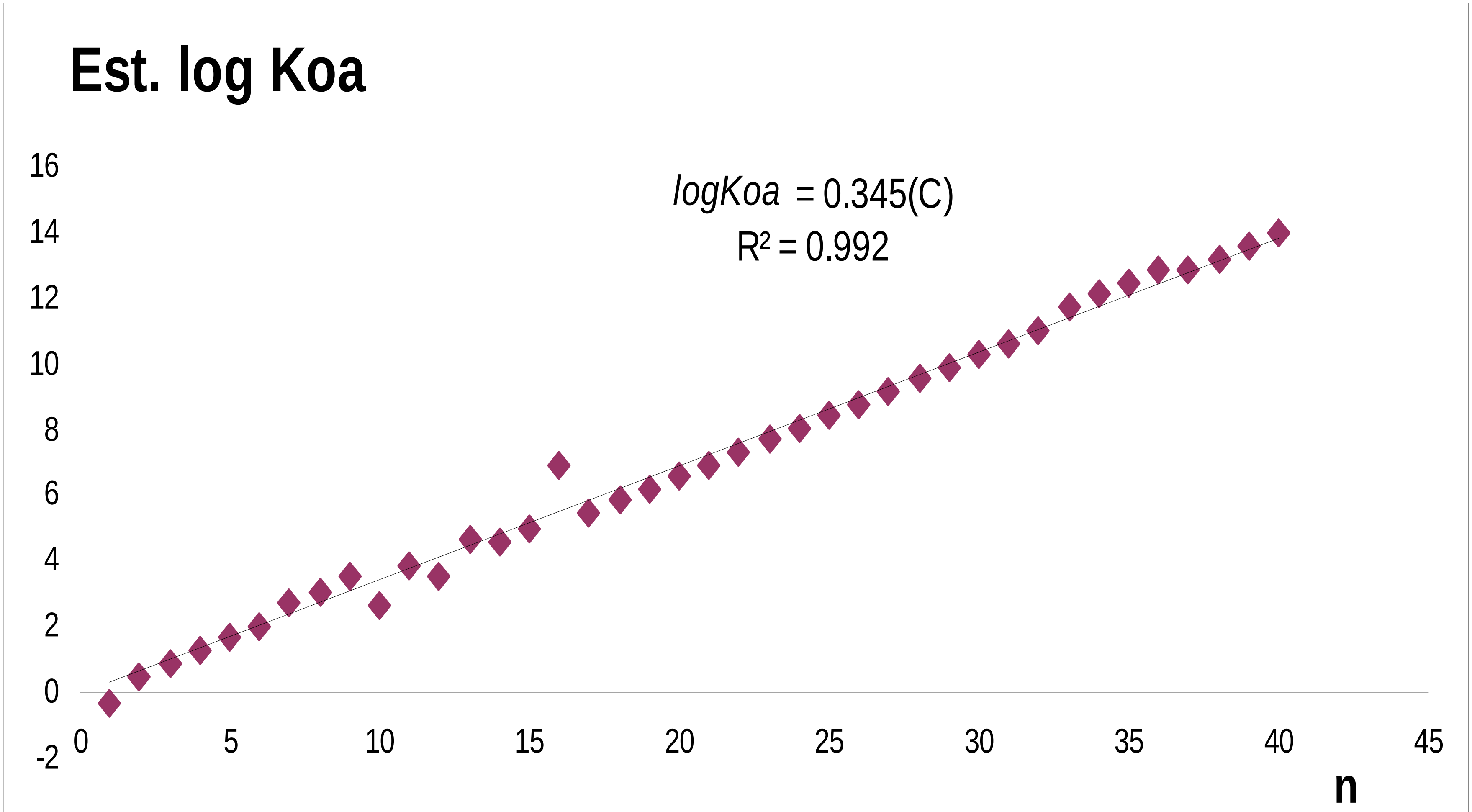

Fig.-7: The curve of the relationship between the values of estimated log(K_{oa}) versus the number of carbon atoms in the structures of normal hydrocarbon C_1 to C_{40} (**1-40**).

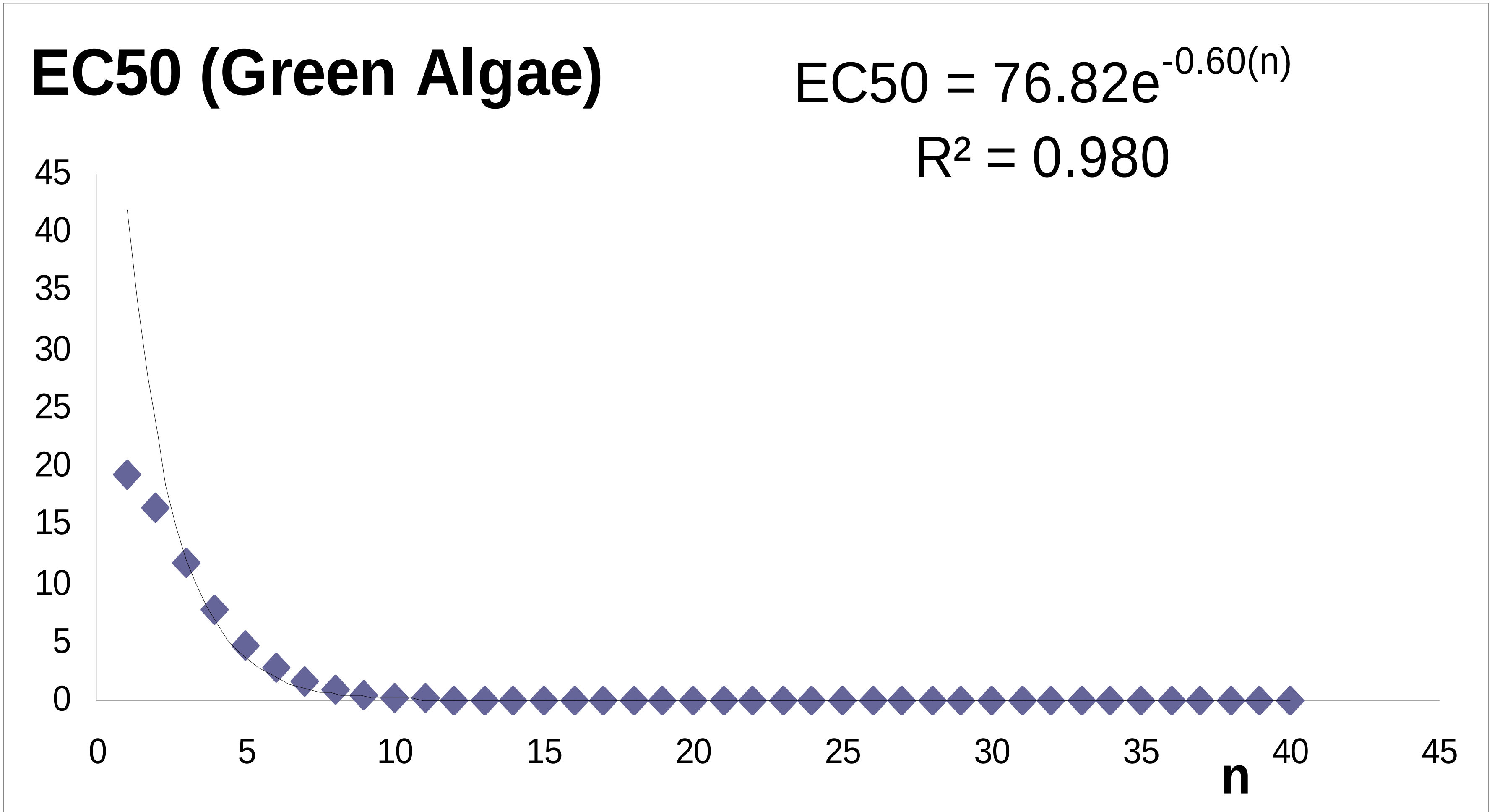

Fig.-8: The relationship between the values of EC_{50} (green algae) versus the number of carbon atoms in the structures of normal hydrocarbon C_1 to C_{40} (**1-40**).

Table-2: The equations (1-13) that indicate the relationships between the selected chemical and biochemical data logarithm of calculated Octanol-Water partitioning coefficients and total biodegradation, $logK_{ow}$ and TB_d (mol/h and g/h), respectively, median lethal concentration 50 (LC_{50}), water solubility (S_w, $mg.L^{-1}/25^oC$), HLC (in $atm.m^3/mol$), EC_{50} green algae (in ppm), log[BCF], Bio half-life, log[BAF], K_{oc}, fugacity in air and soil, reaction air (kg/hr) and advection percent sediment in C_1 to C_{40} compounds **1-40**.

No. of Equations	The Equations	R^2
1	$logK_{ow} = 0.505(n)$	0.9930
2	TB_d (g/h)= $-0.0077(n)^2+0.5596(n)-2.1105$	0.9050
3	TB_d(mol/h)= $2\times10^{-5}(n)^4-0.0014(n)^3+0.0365(n)^2 - 0.2493(n) + 1.0932$	0.8553
4	$logS_w = -0.524(n)$	0.9970
5	$log(BCF) = 7\times10^{-7}(n)^4+0.0004(n)^3-0.0284(n)^2 +0.5198(n)-0.0757$	0.8711
6	B-hl = 0.1459exp[0.3119(n)]	0.9898
7	$log[BAF] = 0.0006(n)^3-0.0468(n)^2+0.954(n) - 1.3303$	0.9111
8	Soil Fugacity = $139.2(n)^{-1.24}$	0.9320
9	$logK_{oa} = 0.345(n)$	0.9920
10	$logK_{aw}=0.128(n) + 0.927$	0.9580
11	LC_{50} = 30.417exp[-0.7402(n)]	0.8108
12	EC_{50} = 76.82exp[-0.60(n)]	0.9800
13	K_{oc}(Soil) = 4.4401exp[0.5827(n)]	0.9962