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COMBINED IN SILICO AND EXPERIMENTAL INVESTIGATIONS OF VITAMIN D_3 ENCAPSULATION BY STARCH β-OLIGOSACCHARIDE

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Abstract

The relevance of the research lies in the need to develop methods for encapsulating fat-soluble vitamins with natural oligosaccharides to increase their water solubility and use in the production of functional foods. The production of nanostructured encapsulated vitamins is a new innovative direction in the food industry. This article presents the results of theoretical and experimental studies on the production of a clathrate complex of fat-soluble vitamin D3 (ViD_3, cholecalciferol) with β-cyclodextrin (β-CD). The interaction of fat-soluble ViD_3 with β-oligosaccharide was carried out by microwave activation. Encapsulation of ViD_3 in the β-CD: ViD_3 clathrate complex led to a change in the aggregate state of the ViD_3 oil solution. The resulting supramolecular water-soluble ViD_3 inclusion complex was investigated in silico by molecular docking and molecular modeling methods. The synthesized β-CD: ViD_3 complex belongs to host-guest inclusion compounds and has better solubility. The spectral properties of the β-CD: ViD_3 inclusion complex are characterized by the data of IR Fourier spectroscopy and the results of thermographic measurements on a differential scanning calorimeter. The activation

energy of the reaction of the thermo-oxidative destruction of the β-CD: ViD₃ inclusion complexes is calculated, the kinetic parameters of the thermal destruction of clathrates are determined. It is shown that the decisive role in the formation of the clathrate complex belongs to non-specific (hydrophobic, dispersion and van der Waals) interactions. The results obtained are promising for further understanding of the mechanism of molecular encapsulation of ViD₃ compounds.

Key words: functional foods; cholecalciferol; oligosaccharide; β-cyclodextrin; inclusion complexes; clathrate.

Introduction

Today, according to the latest available medical reports, the majority of the world's population faces ViD₃ deficiency. ViD₃ deficiency is currently recognized as a pandemic [1,2]. ViD₃ is involved in the metabolism of calcium and phosphorus in the human body. This vitamin is necessary for the formation and maintenance of healthy bones, endocrine [1] and other systems of the human body. Recent studies have clarified the role of ViD₃ in the prevention of cancer [3], cardiovascular diseases, HIV, diabetes and other diseases [4-6]. Millions of preschool-age children are deficient in ViD₃ [1]. Food does not fully cover the needs of ViD₃. In these cases, additional fortification of food with vitamin is necessary. The ViD₃ molecule has many olefin bonds, so it is easily oxidized during food processing and storage due to environmental conditions such as temperature, oxygen and light. In production conditions, the lipophilicity and low solubility of the native form of ViD₃ in an aqueous medium (less than 1 мкg/100 ml) also creates certain difficulties. For this reason, there is a need to develop technological methods for obtaining water-soluble forms of vitamin with improved biopharmaceutical and nutritional properties. In this paper, we have studied and presented the results of encapsulation of an oil (in olive oil) solution of ViD₃ (cholecalciferol) with β-cyclodextrin (β-CD).The use of an oil solution of the ViD₃ molecule should promote the penetration of vitamin into the cylindrical hydrophobic cavities of β-CD molecules with the formation of a guest-host complex [7] (Fig.1).

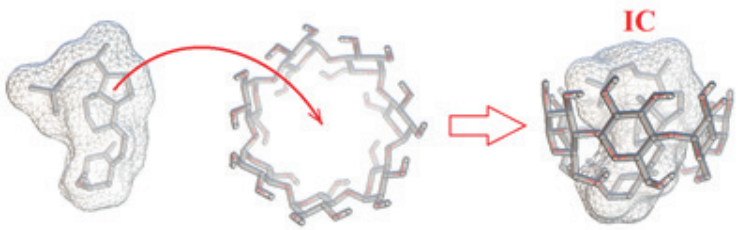


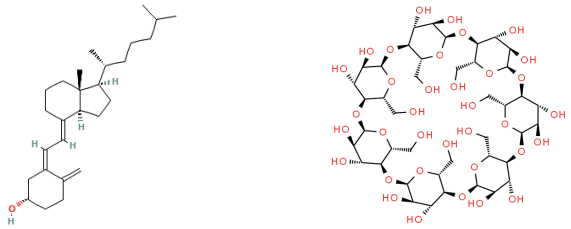
Figure 1 – Schematic representation of the formation of the inclusion complex of ViD with β-CD

ViD_3 will be better preserved in an oily shell from the effects of oxidants and will have better bioavailability [7,8]. Therefore, it is important to understand the nature of the inclusion of ViD_3 in the complex with β-CD. In this paper, we obtained the β-CD: ViD₃ inclusion complex by the microwave method [9]. The resulting complex was studied using methods of molecular docking and modeling, IR-Fourier spectroscopy, thermografimetry and differential scanning calorimetry.

Materials and methods

The following reagents were used: β-cyclodextrin (99.5%, purchased from Fluka), ViD₃ (in olive oil (here inafter vitamin ViD₃, 250 mcg (10,000 IU), cholecalciferol, C27H44O, (Aldrich company). All measurements of 1H NMR were carried out in solutions of DMSO-d6 (Aldrich), other chemicals had analytical purity of the reagent class. Molecular docking of ViD_3 with cyclodextrins was carried out using Autodesk 4.2.6, MGLTools 1.5.7 [10] and the Lamarckian Genetic Algorithm (LGA) [11] implemented in AutoDock 4.2.6. A semi-flexible docking method was used, where the receptor was considered as a solid, and the ligand rotated and moved in a given cubic region. As binding energy, Autodoc uses an empirical estimation function based on the free binding energy, including electrostatic, hydrophobic and solvation effects, as well as

configuration entropy. The Autodoc approach uses a Monte Carlo annealing simulation method with rapid energy estimation using grid-based molecular affinity potentials. The chemical structures were taken from the PubChem Substance and Compound database (pubchem.ncbi.nlm.nih.gov) [12]. Unique chemical structure identifiers: 444041 (β-CD), 5280795 (cholecalciferol) (Fig.2).



(a) Cholecalciferol (ViD_3) (b) β-CD

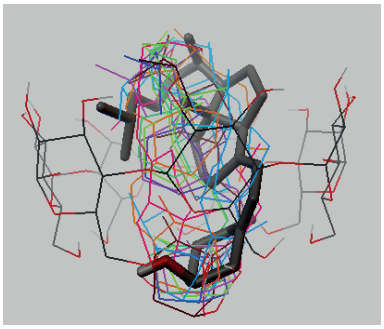
Figure 2 – Structural formulas of research objects

ViD_3 inclusion complexes with β-CD (1:1; 1:2; 1:3) obtained in an aqueous-alcoholic medium. A mixture of ViD3 and β-CD (mmol) it reacted for 600 seconds in the Anton Paar Monowave 300 microwave oven at an irradiation power of 200W in 2-minute increments at 70°C. After the procedure, the solvents were removed, and the products were washed with acetone and dried in a CaCl2 desiccator to a constant mass. The yields of β-CD: ViD_3 clathrate complexes were 52,2 (1:1), 64.3 (1:2), 63,1 (1:3) %. The resulting complexes were white crystalline substances soluble in water with the formation of a colloidal solution of milky white color (m.p. 310-320oC). The solubility of the β-CD: ViD_3 complex (2:1) in distilled water was 0.20mg ± 0.05/100 ml. The surface morphology of β-CD: ViD_3 clathrate samples was studied using a scanning electron microscope (SEM) from TesconMira3 LMN (Czech Republic). IR spectra were taken on a Cary600 series IR-Fourier spectrometer manufactured by Agilent Technologies (USA) in the range of 4000-400 cm^{-1}. Thermal properties of clathrate complexes β-CD:ViD_3 were studied on a Labsys Evolution DTA/DTS differential scanning calorimeter in a dynamic mode in the temperature range of 30-500oC when heated at a rate of 10 degrees/min in a nitrogen atmosphere in an Al2O3 crucible, temperature range 30-800 °C, sample heating rate from 5 to 20 k/min, sample weight 12-16 mg. All calculations were carried out using the Mathcad program [13].

Results

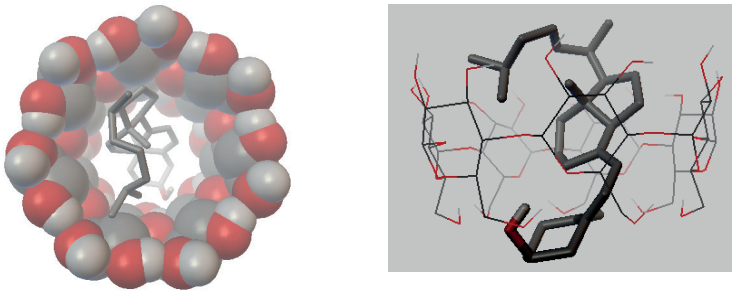
Recent advances in molecular docking methods make it possible to reasonably predict the preferred configuration of one molecule relative to another in the formation of a stable complex. The binding energy between the receptor molecule and the ligand is used as a quantitative estimate. Initially, we performed molecular docking of β-CD with a cholecalciferol molecule to determine the binding energy of their inclusion complexes in a ratio of 1:1 (Fig. 3).

Based on the docking, 10 conformations of the cholecalciferol ligand with β-CD were obtained and their binding energy was estimated. At the same time, the best binding was demonstrated by conformation number 4, its binding energy was -2.7 kcal/mol.



Conformation number	Binding energy, kcal/mol
4	-2.70
7	-0.17
10	+1.70
6	+4.22
3	+7.45
8	+17.43
1	+17.68
5	+27.93
9	+8.98
2	+23.00

(a) 10 possible conformations of the ViD3 molecule inside the β-CD cavity;



Top view Side view

(b) conformation with the best binding (binding energy = -2.7 kcal/mol)

Figure 3 – Results of ViD_3 docking with β-cyclodextrin

The negative value of the binding energy indicates the successful complexation between the molecules of cholecalciferol with β-CD, at the same time, a sufficiently low value suggests the need for special conditions for the complexation reaction. A small amount of binding energy between cholecalciferol and β-CD is noteworthy, so it seemed interesting to find out the presence of hydrogen bonds between receptor and ligand molecules using AutoDock tools (Figure 4). As can be seen from the data presented in Figure 4, a system of 14 intramolecular hydrogen bonds between OH groups is formed in the β-CD molecule. At the same time, hydrogen bonds between the receptor and ligand molecules are not observed. The absence of intermolecular hydrogen bonds between the receptor and the ligand may be the reason for the low binding energy between them.

The next step was the modeling of ViD3 and β-CD complexes in a molar ratio of 1:2. For convenience, the wider side of β-CD was designated as "Head", and the opposite edge – "Tail" (Figure 5a).

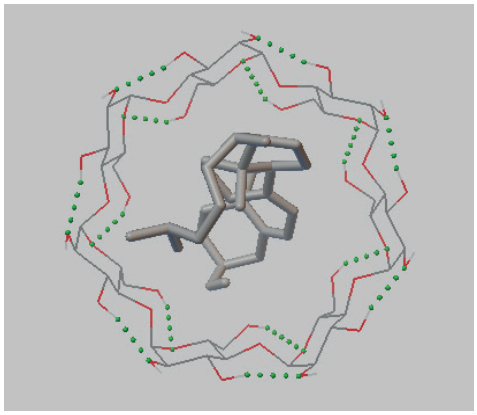
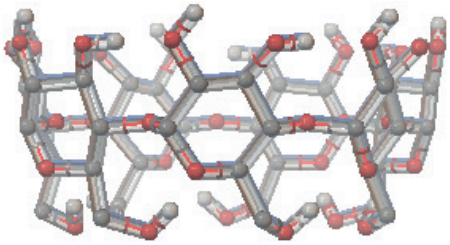


Figure 4 – A system of 14 hydrogen bonds in complexes of cholecalciferol with β-CD

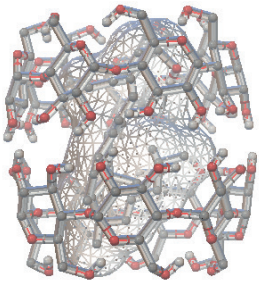
In this case, three types of mutual orientation between two β-CD molecules are possible: «head to head» (HH), «head to tail» (HT) and "tail to tail" (TT) (Figure 5b-d).

«Head»

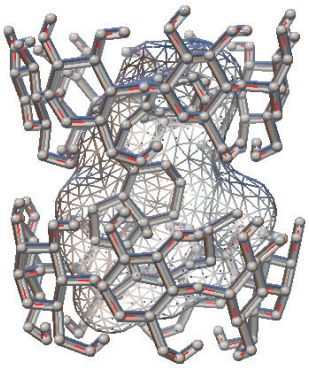


«Tail»

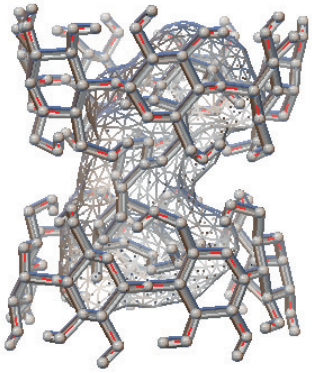
(a) the head and tail of the β-cyclodextrin molecule



(b) type of head-to-head complex (HH) (binding energy = -4.71 kcal/mol)



(c) type of head-to-tail complex (HT), (binding energy = -7.32 kcal/mol)



(e) tail-to-tail complex type (TT), (binding energy = +3.85 kcal/mol)

Figure 5 – The β-CD (a) molecule and three types of its complexes with ViD_3 (2:1)

As can be seen from Figure 5, two types of the «head-to-head» (HH) and «head-to-tail» (HT) complexes demonstrate more effective binding (-4.71 and -7.32 kcal/mol, respectively) compared to the 1:1 complex (-2.7 kcal/mol).

Figure 6 shows scanned electron micrographs of the β-CD: ViD_3 inclusion complex (2:1) (m.p. 310-320°C). The magnification on panels Figure 6a-i is from 931 to 7560x.The photos of the samples show the layered crystal structure of β-CD (Figure 6a-f), a physical mixture and β-CD:ViD_3 clathrate (Figure 6e,f). Photos of clathrate show a sharp change in the morphology of the crystals of the initial and final substances. The crystalline forms of the clathrate inclusion complex are covered with a film. Similar results were described in [13,14].

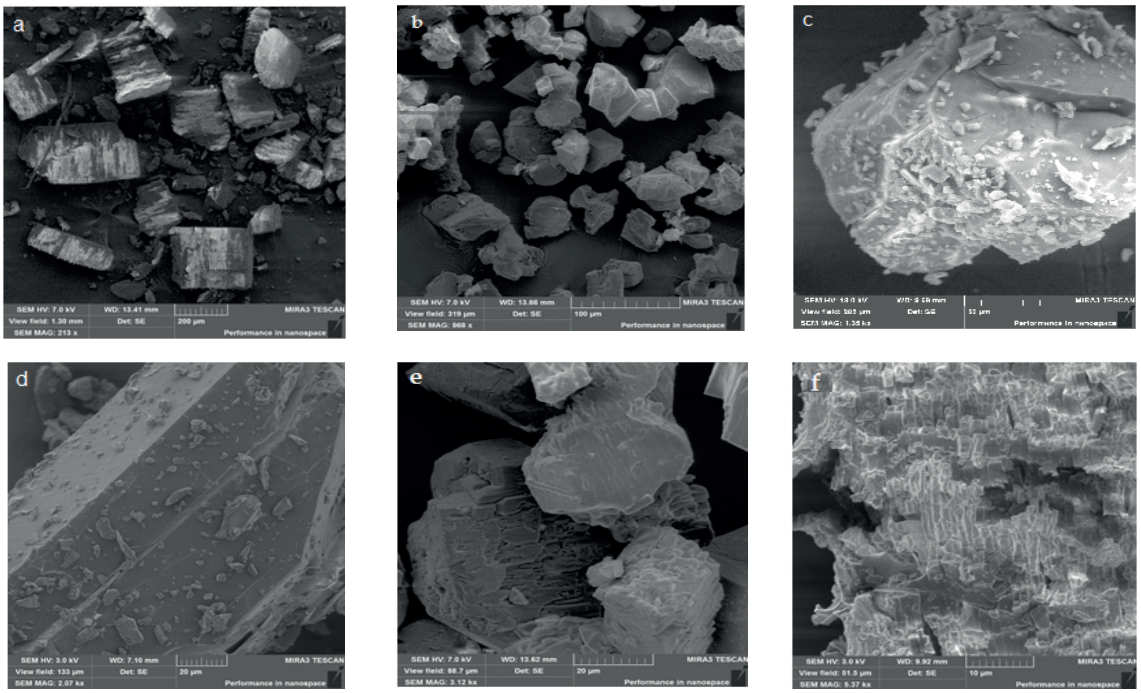


Figure 6 – Electron micrographs of β-CD (a, b), a physical mixture of β-CD with ViD_3 (c, d) and clathrate β-CD:ViD3 (2:1) (e, f) at various magnifications

In the IR spectra (Figure 7), and valence oscillations of the O-H bond are detected as a wide band with a maximum at 3398 (β-CD (a), 3564 (ViD_3 (b) and 3368 cm-1 (β-CD: ViD_3 (c). There is also an absorption band at 2924 cm-1, characteristic of valence vibrations of CH bonds in the CH and CH2 groups [14,15].The absorption bands C=C, OH and other groups of ViD_3 do not appear in the IR spectra of the β-CD:ViD_3 complex. This may mean that these groups are masked by very wide and intense β-CD bands in the same wavelength range. In the area of 1643 cm-1 there is an intense band C=O group belonging to the complex of the β-CD: ViD_3 complex.

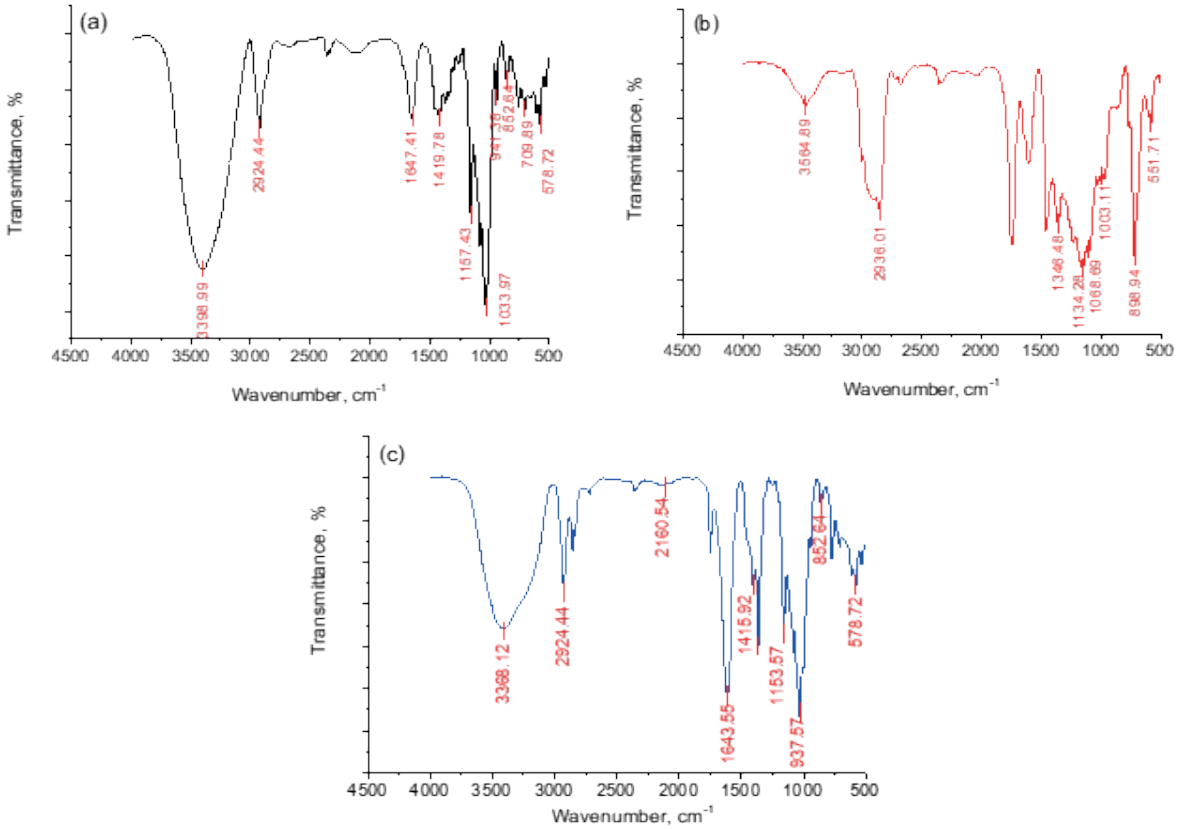


Figure 7 – IR spectra of β-CD (a), ViD₃ (b) and β-CD: ViD₃ (2:1)

The thermal properties of β-CD: ViD3 clathrates were analyzed by thermogravimetric analysis [17]. Figure 8a, b shows thermograms of TG and DTG β-CD and its clathrate β-CD: ViD3 (2:1) (heating rate 10 deg/min). The thermoanalytical parameters of the decomposition of β-CD and its clathrate β-CD: ViD3 (2:1) are represented by the TG/DTG curves (Figure 8a, b). To compare the thermal stability of β-CD and clathrate β-CD: ViD3 (2:1), the activation energies of the decomposition reaction were determined (Table).

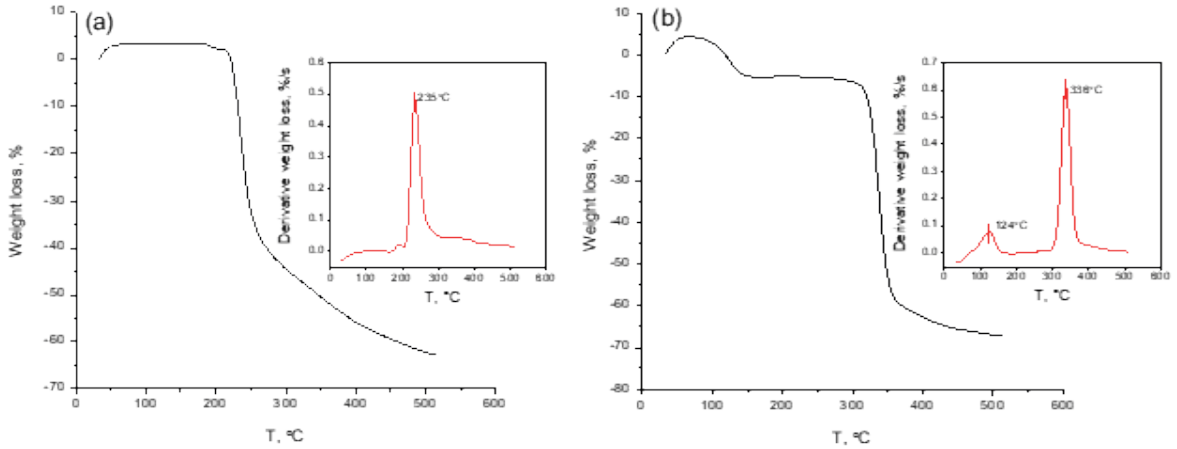


Figure 8 – TG/DTG curves for β-CD: ViD₃ with a constant heating rate of 10 deg/min in a nitrogen medium: a) β-CD; b) β-CD: ViD3 (2:1)

Table. Activation energy values of β-CD and clathrate β-CD: ViD3 (2:1) in nitrogen atmosphere

Sample	E_a, kJ/mol	A, c^{-1}
β-CD	164.58	$1.10 \cdot 10^{17}$
β-CD:ViD₃ (2:1)	103.50	$8.96 \cdot 10^{10}$

Discussion

The results of molecular modeling of the mechanism of formation of the encapsulation process showed that the «tail-to-tail» complex demonstrates positive binding energy, which indicates the absence of complex formation of this type. At the same time, the head-to-tail complex (c) in the β-CD: ViD₃ complex demonstrates the maximum binding energy, which indicates greater stability of such a complex [11,12].

Morphology of the surface of β-CD crystals and binary systems β-CD: ViD₃ was analyzed using SEM. SEM is an important tool for visualizing the surface texture of clathrate complexes. This is a qualitative method used to study the structural aspects of the studied objects and helps to assess the presence of another component in the obtained preparations. Changes in the morphology of the crystal surface indicate the formation of the β-CD: ViD₃ clathrate complex.

One of the informative methods for confirming the formation of inclusion complexes is the IR spectroscopy method. The β-CD molecule has the shape of a truncated cone [7,8]. When the guest molecule is placed in the hydrophobic cavity of the CD, a pronounced chemical shift should occur in the vibrational absorption spectra of the ViD3 molecules. In the IR spectra (Figure 7), the valence vibrations of the O-H bond are recorded as a wide band with a maximum at 3398 (β-CD (a), 3564 (ViD₃ (b) and 3368 (β-CD: ViD₃ (c) cm-1. There is also an absorption band at 2924 cm-1, characteristic of valence vibrations of CH bonds in the CH and CH_2 groups [15-17]. However, the absorption bands of C=C, OH and other ViD3 groups in the complex do not appear in the IR spectra of the β-CD: D_3 complex.

Comparing the thermogravimetric curves of β-CD and clathrate β-CD: ViD₃ (Figure 8a, b), we conclude that for β-CD: ViD₃ clathrate in the temperature range ~124° ...~235°C, there is an intense decrease in the mass of the sample (~77.27%). This section of the TG curve corresponds to the maximum change in the rate of mass loss on the DTG curve at a temperature of ~ 235°C (Figure 8b). Mass loss at low temperatures (~124oC) in clathrates β-CD: ViD3 is associated with the removal of moisture, which is also confirmed by the data of DTG (Figure 8b). The resulting clathrates β-CD: ViD₃ contained bound water, as did the original β-CD. Based on the data obtained, the kinetic parameters of the thermal decomposition of clathrate β-CD: ViD3 were calculated (2:1) (Table) [14,17]. To compare the thermal stability of β-CD and β-CD: ViD₃ (2:1) clathrate the activation energies of the decomposition reaction were determined. Comparing the calculations of the thermal destruction of β-CD and clathrate β-CD: ViD_3 (2:1), it can be argued that the activation energies of β-CD and clathrate β-CD: ViD₃ (2:1) are different at the same degrees of transformation (α).

Conclusion

The interaction of fat-soluble vitamin ViD3 with β-oligosaccharide under microwave activation in an aqueous alcohol medium leads to the formation of a water-soluble supramolecular inclusion complex. Encapsulation of ViD3 in a clathrate complex β-CD: ViD3 led to a change in the aggregate state of the oil solution ViD3. The synthesized complex β-CD: ViD3 (2:1) belongs to «host-guest» inclusion compounds and has a better solubility. The decisive role in the formation of the clathrate complex belongs to non-specific (hydrophobic, dispersion and van der Waals) interactions. The results obtained are promising for further understanding of the molecular encapsulation of vitamin D3 compounds.

Information about financing

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$Д_3$ ВИТАМИНІНІҢ КРАХМАЛДЫҢ β-ОЛИГОҚАНТЫМЕН ҚАПТАЛУЫН БІРІКТІРІЛГЕН IN SILICO ЖӘНЕ ТӘЖІРИБЕЛІК ТҰРҒЫДА ЗЕРТТЕУ

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Түйін

Табиғи олигоқанттан алынған β-циклодекстринмен (β-ЦД) майда еритін Д3 дәруменін (холекальциферол) қаптау зерттеулерінің нәтижелері ұсынылған. Майда еритін Д3 дәруменінің β-олигоқантпен өзара әрекеттесуі сулы-спиртті ортада микротолқынды белсендіру кезінде суда еритін супрамолекулалық β-ЦД:$Д_3$ қосу кешенінің пайда болуына әкелді. Холекальциферолды клатрат кешеніне қаптау осы дәруменнің май ерітіндісінің агрегаттық күйінің өзгеруіне әкелді. Синтезделген β-ЦД:$Д_3$ кешені «қожайн-қонақ» қосылыстарына жатады және ол суда жақсы ериді. β-ЦД:$Д_3$ қосу кешенінің спектрлік қасиеттері ИҚ-Фурье спектроскопиясының деректерімен сипатталды. Дифференциалды сканерлеу калориметріндегі термографиялық өлшеулердің нәтижелері келтірілді. β-ЦД:Д3 клатратты қосу кешендерінің термототығу деструкциясы реакциясының белсену энергиясын есептеу жүргізілді, клатраттардың термиялық ыдырауының кинетикалық көрсеткіштері анықталды. Алынған нәтижелер Д3 дәрумені қосылыстарының молекулалық қапталу механизмін одан әрі түсінуге мүмкіндік береді. Клатрат кешенінің түзілу механизмі спецификалық емес (гидрофобты, дисперсиялық және ван-дер-Ваальс) өзара әрекеттесулерге жатады.

Кілт сөздер: функционалды тағам; холекальциферол; олигоқант; β-циклодекстрин; қосылған кешен; клатрат.

КОМБИНИРОВАННЫЕ IN SILICO И ЭКСПЕРИМЕНТАЛЬНЫЕ ИССЛЕДОВАНИЯ ИНКАПСУЛЯЦИИ ВИТАМИНА Д₃ β-ОЛИГОСАХАРИДОМ КРАХМАЛА

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Аннотация

Представлены результаты исследований инкапсуляции жирорастворимого витамина Д3 (cholecalciferol) с β-циклодекстрином (β-ЦД), получаемым из натурального олигосахарида. Взаимодействие жирорастворимого витамина Д₃ с β-олигосахаридом при микроволновой активации в водно-спиртовой среде приводит к образованию водорастворимого супрамолекулярного комплекса включения. Инкапсуляция Д₃ в клатратный комплекс β-ЦД: Д₃ привела к изменению агрегатного состояния витамина Д₃. Синтезированный комплекс β-ЦД: Д3 относится к соединениям включения «хозяин-гость» и обладает лучшей растворимостью. Спектральные свойства комплекса включения β-ЦД: Д₃ охарактеризованы данными ИК-Фурье спектроскопии. Приведены результаты термографических измерений на дифференциальном сканирующем калориметре. Проведен расчет энергии активации реакции термоокислительной деструкции клатратных комплексов включения β-ЦД: Д₃, определены кинетические параметры термической деструкции клатратов. Комплексообразование витамина Д3 с бета-циклодекстрином способствовало сохранению антиоксидантной активности. Полученные результаты являются многообещающими для дальнейшего понимания механизма молекулярной инкапсуляции соединений витамина Д₃. Решающая роль в образовании клатратного комплекса принадлежит неспецифическим (гидрофобным, дисперсионным и вандерваальсовым) взаимодействиям.

Ключевые слова: функциональная пища; холекальциферол; олигосахарид; β-циклодекстрин; комплекс включения; клатрат.