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METHOD OF OBTAINING HIGH-MOLECULAR INULIN

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It is known that inulin is a fructose polysaccharide (polyfructosan), is a product of photosynthesis of some plants and is a mixture of structurally similar polymorphs containing about 35 fructose fragments with variable specific rotation $[\alpha]_D$ from –32 to –40. A high molecular weight inulin polymer, which is isolated by recrystallization from water, can have $[\alpha]_D$=–40 [1]. Inulin is a good dietary product and a therapeutic and prophylactic drug for people with diabetes mellitus. the absorption of fructose is much less dependent on the hormone of the insulin pancreas than for glucose. Moderate intake of fructose does not cause significant changes in blood sugar levels [2].

We have found that crude inulin, obtained by precipitation with alcohol or after a single crystallization, contains impurities such as pectin, protein and amino acid residues, organic acids, phenolic compounds and oxidation products. Impurities are detected by paper chromatography with appropriate diagnostic reagents or in the UV light of a fluorescent lamp.

It is possible to note the shortcomings of these methods [4, 5]. The use of acetic acid lead to precipitate colloids is not justifiable from a medical point of view because of the toxicity of the metal ion. The use of ultrafiltration to purify inulin requires the presence of special filters and membranes that are not readily available for industrial use. In addition, purification of extracts from Jerusalem artichoke by ultrafiltration and filtration on membranes does not make it possible to release extracts containing inulin from high molecular weight natural polymers of proteins and pectins. Extraction with 25% alcohol will result in a partial loss of inulin, which is poorly soluble in alcohol solutions and will not be completely extracted under these conditions. Acidification of an inulin solution may result in loss of inulin. For example, 0.2 N. a solution of sulfuric acid causes hydrolysis of inulin for 10–15 minutes at 70 °C .

To produce high molecular weight inulin, juice from the raw material was extracted and the substances were extracted from the mash and from the raw material with hot water at 80 °C for 60 minutes. As a raw material, crushed tubers of Jerusalem artichoke were used. Juice was squeezed out of crushed Jerusalem artichoke tubers using a juicer. Additional water extracts were obtained from the mash. The extracts were carried out with heating for 60 minutes at 80 °C. The juice was diluted with hot water (95 °C) 1 : 1, and separately, the hot aqueous extracts were treated with calcium carbonate (chalk) at 80–85 °C for 60 minutes and filtered hot through the coarse layer. This made it possible to destroy the inulin-pectin complex, to coagulate proteins, to get rid of water-soluble pectins, in part from organic acids, proteins, without destroying inulin, where the pH is kept close to neutral. The filtrate of the aqueous solution of the juice was evaporated in vacuo. Crystallization of inulin was carried out at 4 °C in a refrigerator for 5 days. To the evaporated aqueous extracts, alcohol 1 : 1 was added. The precipitated precipitates of crude inulin are gray. Further purification of inulin was carried out. To this end, the inulin solution was passed through a column with an anion exchanger in the OH form. The column is washed with water at 45 °C to a volume equal to the original solution taken. Anionite allows the removal of organic acids, phenolic acids and other acidic compounds, as well as anions of organic and inorganic salts; Further, alumina was added to the eluate and heated with constant stirring for 30 minutes at 75 °C and the coarse layer was filtered and the precipitate from the filter was washed with hot water. This allows to remove impurities that are sorbed on aluminum oxide (phenols, polyphenols, products of their oxidation). 96% alcohol 1 : 3 was added to the resulting solution and inulin in the refrigerator crys-

tallized at 4 °C for 1 day. As a result, a white powder with a humidity of 10 % and a specific rotation $[\alpha]_D = -36.5°$ was obtained. The purity of inulin was monitored by chromatography on paper in a solvent system of butanol-acetic acid-water 4 : 1 : 2.

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HYDROGEN BONDS BETWEEN PYRIDINE AND HALOFORMS – NEW INSIGHTS

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Pyridine has not only been recognized as an important solvent in the organic synthesis, but also an essential building block of most drugs [1, 2]. Understand of the pyridine involved hydrogen bond, its strength under various conditions, its impact on the vibrations of the participating molecules is critical in the organic synthesis, molecular scaffold study in drug design, as well as in the study of the properties of pyridine containing biological ligands [3–5]. In nearly all the hydrogen bonding relationship that pyridine has ever involved, it is mainly considered as the electron lone pair donor, in other word, hydrogen bonding acceptor [6, 7].

With the formation of the hydrogen bond, the electron density on the pyridine ring will naturally experience redistribution in different degrees depending on the strength of the hydrogen bond. This electron density redistribution generally leads to a frequency shift of the ring related vibrations [8–10]. Among 27 vibrational normal modes of pyridine, ring breathing vibration ν_1 and triangle vibration ν_{12} have been extensively investigated with respect of their response to the hydrogen bonding [11–14].

In the present work hydrogen bond between pyridine (Py) and haloforms (CHX_3, X = F, Cl, Br, I) was studied using a combination of solution phase FTIR and quantum mechanical ab initio calculations. All FTIR measurements were performed at room temperature (298±2 K) and cyclohexane used to record the background spectra. The infrared absorption spectra of solutions with concentration of 1 M and mixtures with different volumetric ratios were recorded on a ThermoScientific Nicolet iS5 FT-IR Spectrometer using KBr windows with a 1 cm^{-1} resolution over the range of 400–4000 cm^{-1}. Calculations were performed in Gaussian09 with DFT ωB97X-D/6-311++G** (H, C, N) / DGDZTP (X) functional. While the calculation indicates other than the hydrogen bond formed between pyridinyl nitrogen ([Py–]N) and the H atom on haloform ([CX_3–]H), a ring structure is established based on both the [Py–]N involved hydrogen bond and the interaction between the alpha H on pyridine ([Py–]H) and the halogen atom on haloform ([CHX_2–]X). The formation of the ring makes the entire ring structure more rigid on one hand, and weakens the ([Py–]N involved hydrogen bond on the other hand. As a result, no significant shift was observed for ν_{12}, and ν_1 only experiences a moderate blue shift. The magnitude of the shift in ν_1 is in an order of $CHI_3 > CHBr_3 > CHCl_3 > CHF_3$ according to calculation (Tables 1 and 2). The FTIR experiments with pyridine and $CHCl_3$/$CHBr_3$ in solution of cyclohexane showed a consistent sequence (Figures 1 and 2). A strong correlation was observed between the values of ν_1 and various interatomic distances among [Py–]N, [Py–]H, [CHX_2–]X and [CX_3–]H, as well as the two bond critical points (BCP1 and BCP2) and the ring critical point (RCP). The percentage of the contribution from the internal coordinate