STUDY ON THE FORMATION OF CYCLODEXTRIN AND THIOBARBITURATE COMPLEXES

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STUDY ON THE FORMATION OF CYCLODEXTRIN AND THIOBARBITURATE COMPLEXES

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ABSTRACT

STUDY ON THE FORMATION OF CYCLODEXTRIN AND THIOBARBITURATE COMPLEXES

The aim of this M.Sc. study was to increase transport ability of 5-substituted-1-(*o*-aryl)-2-thiobarbituric acids in aqueous media by complexing them with cyclodextrin. Many derivatives of barbituric and thiobarbituric acids are drugs that act as central nervous system antidepressants and can therefore produce a wide spectrum of effects, from mild sedation to total anesthesia. Cyclodextrins have been called as cyclic oligosaccharides that can react with different molecules and form complex compounds. They are used to improve drug solubilization in aqueous medium. Therefore they have found many applications as pharmaceutical excipients. In this study, first of all *o*-substituted-2-thiobarbituric acid derivatives were synthesized from the corresponding *o*-substituted phenylthioureas. After that thiobarbituric acid and cyclodextrin derivatives were complexed in different solvents such as distilled water and phosphate buffer. Several factors were investigated for their effects on the complexation rate. One of them is thiobarbituric acid (TBA):cyclodextrin (CD) ratio. One derivative 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid was found to have the highest solubility in distilled water and phosphate buffer when TBA:CD ratio is 1:4 at the studied temperatures 25ºC and 37ºC. Another derivative, 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid has been found to have the highest solubility in distilled water when TBA:CD ratio is 1:1 at 25°C and 37°C. In phosphate buffer, highest concentration of TBA can be obtained at 25°C when TBA:CD ratio is 1:2, and at 37°C highest concentration of TBA was obtained, when TBA:CD ratio is 1:1. The effect of the structure of cyclodextrin on the complexation was also studied by using two cyclodextrin derivatives. Among them, β-CD causes to form a more stable complex than 2-hydroxypropyl-β-CD. Additionally, temperature effect was studied and it has been observed, that the complexation rate is higher at 25ºC than that at 37ºC. Results related to temperature effect study were also used to calculate the standard free energy change (ΔG^o), the standard enthalpy change (ΔH^o) and the standard entropy change (ΔS^o) values for complexation process.

ÖZET

SİKLODEKSTRİN VE TİYOBARBİTURATLARIN KOMPLEKS OLUŞUMU ÜZERİNE ÇALIŞMA

Bu tezin amacı, 5-sübsitüe-1-(*o*-aril)-2-tiyobarbitürik asitlerin siklodekstrin ile kompleks oluşturarak sulu ortam içinde taşınma yeteneğinin arttırılmasıydı. Birçok barbitürik ve tiyobarbitürik asitleri türevleri merkezi sinir sistemi antidepresanı olarak etkin olan ilaçlardır, bu sebeple, hafif sedasyondan tüm anesteziye kadar geniş yelpazede etkileri vardır. Siklodekstrinler farklı moleküllerle reaksiyona girip kompleks bileşikler oluşturabilen halkalı oligosatkaritler olarak adlandırılırlar. Bunlar sulu bir ortam içinde ilaç çözünürlüğünü arttırmak için kullanılmaktadırlar. Bu yüzden, farmasötikte yardımcı maddeler olarak birçok uygulamada kullanılmışlardır.

Bu çalışmada ilk olarak ilgili *o*-sübsitüe-feniltiyoüre türevlerinden *o*-sübsitüe-2-tiyobarbitürik asit türevleri sentezlenmiştir. Sonra bunlar tanımlanmış ve saflıkları NMR ve HPLC gibi farklı tekniklerle control edilmiştir. Çeşitli faktörlerin kompleksleşme oranı üzerindeki etkileri araştırılmıştır. Bunlardan biri, tiyobarbitürik asit(TBA):siklodekstrin (SD) oranıdır.. Bir türev, 5-metil-1-(*o*-florofenil)-2-tiyobarbitürik asitin en yüksek konsantrasyonu damıtılmış su ve fosfat tampon ortamında çalışılan 25ºC ve 37ºC sıcaklıklarda TBA:SD 1:4 oranında olduğunda bulunmuştur. 5,5-dimetil-1-(*o*-tolil)-2-tiyobarbitürik asitin en yüksek konsantrasyonu damıtılmış su ortamında 25ºC ve 37ºC sıcaklıklarda TBA:SD 1:1 oranında yüksek çözünürlüğe sahip olduğu bulunmuştur. Ve fosfat tampon ortamında 25ºC sıcaklıkta en yüksek konsantrasyonu TBA:SD 1:2 oranında iken, 37ºC sıcaklıkta en yüksek konsantrasyonu TBA:SD 1:1 oranında iken bulunmuştur. İki siklodekstrin yapısının kompleks oluşturma üzerindeki etkilerini incelenmiştir. Bunlar arasında beta-siklodekstrin, 2-hidrosipropil-betasiklodekstrine göre daha kararlı yapıya sahip kompleksin oluşmasını sağlamaktadır. Ayrıca, ısı etkisi araştırılmış ve kompleksleşme oranının 25ºC sıcaklıkta 37ºC sıcaklığa göre daha yüksek olduğu gözlemiştir.. Isı etkisi ile ilgili çalışmanın sonuçları ayrıca kompleksleşme sürecinin standard serbest enerji değişimi (ΔG^o), standard entalpi (ΔH^o), standard entropi (ΔS^o) değerlerinin hesaplanmasında kullanılmıştır.

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LIST OF SYMBOLS/ABBREVIATIONS

A	Absorbance
C(mol/L)	Concentration (mole/Liter)
K	Stability constant
K_c	Complexation constant
L	Quartz cuvette dimension
M	Molarity
n	Mole
R	Universal gas constant
T	Temperature
V	Volume
ε	Absorptivity
α-CD	Alpha-cyclodextrin
β-CD	Beta-cyclodextrin
β-CD-TBA	Beta-cyclodextrin –thiobarbituric acid
°C	Centigrade degress
δ	Chemical shift
ΔH°	Enthalpy change
ΔS°	Entropy change
ΔG°	Free energy change
γ-CD	Gamma-cyclodextrin
µL	Microliter
µm	Micrometer
λ	Wavelength
Bf	Buffer
cm	Centimeter
CMV	Cytomegalovirus
d	Doublet
D. water	Distilled/deionized water

DNA	Deoxyribonucleic acid
ES	Ethyl salicylate
FDA	Food and Drug Administration
G	Gram
GRAS	Generally recognized as safe
h	Hour
HCl	Hydrochloric acid
HP β-CD	Hydroxpropyl-beta cyclodextrin
Hz	Heartz
H NMR	Proton nuclear magnetic resonance
HPLC	High performance liquid chromotography
IUPAC	International Union of Pure and Applied Chemistry
IV	Intravenous
J	Joule
JP	Japanese Pharmacopoeia
L	Liter
m	Multiplet
mg	Milligram
MHz	Megahertz
min	Minute
mL	Milliliter
mm	Millimeter
mM	Millimolar
mmol	Millimole
mmol/L	Millimole per liter
molK	Mole kelvin
MS	Methyl salicylate
nm	Nanometer
NMR	Nuclear magnetic resonance
q	Quartet
PAN	Polyacrylonitrile
PES	Polyamide
Ph. Eur.	European Pharmacopoeia

PP	Polypropylene
ppm	Parts per million
RNA	Ribonucleic acid
RP	Reversed phase
rpm	Revolutions per minute
s	Singlet
TBA	Thiobarbituric acid
TEA	Triethylamine
US	United States
UV	Ultra viole
vs	Versus

1. INTRODUCTION

Barbiturates are a class of drugs that are utilized as anesthetics and sleeping agents and are used for the treatment of anxiety, epilepsy and other psychiatric disorders, and possess effects on the motor and sensory functions. Compounds containing nitrogen and sulphur, have an important role to be used as anticancer and antiviral agents, so barbiturates and thiobarbiturates are also used as anticancer and antiviral. Currently, barbiturates are used in specific therapeutic applications. [4].

Cyclodextrins are a group of structurally related natural products and are formed during bacterial digestion of cellulose [14]. Cyclodextrin molecule is a toroidal form, a small cylinder with a hydrophilic outer surface and a well-defined hydrophobic central cavity. α-, β- and γ-cyclodextrins, are formed of six, seven and eight α-(1,4)-linked glycosyl units, respectively. The inside is nonpolar and the outside is polar, because the hydroxyl groups, both primary and secondary, face outward [22]. The hydrophobic cavity can act as a host for a hydrophobic guest molecule. This property becomes useful for solubilising and stabilising highly hydrophobic molecules in solvents such as water. Therefore cyclodextrin is a good auxiliary in drug delivery by solving and transporting sparingly soluble drug in aqueous solutions. No hydrogen bonds are formed or broken during the formation of such host guest complexes [19].

The aim of this thesis is to synthesize different types of 5-substitued 1-(*o*-aryl)-2 thiobarbituric acid. Then, in order to synthesize 5-methyl-1-(*o*-aryl)-2-thiobarbituric acids and 5,5-dimethyl-1-(*o*-aryl)-2-thiobarbituric acids. The aim of this study, was to increase transport abilities of 5-substitued 1-(*o*-aryl)-2 thiobarbituric acids in aqueous medium by forming complex with cyclodextrin.For this reason, 5-methyl-1-(*o*-aryl)-2-thiobarbituric and 5,5-dimethyl-1-(*o*-aryl)-2-thiobarbituric acids were synthesized from the reaction of the corresponding *ortho*-substituted phenylthioureas and methylmalonic acid or dimethylmalonic acid in the presence of acetyl chloride.

In this thesis, first of all different derivatives of all 5-substituted-1-(*o*-aryl)-2-thiobarbituric acid derivatives were synthesized, they were characterized by NMR and their purities were checked by HPLC. After that, the derivatives were mixed with commercially available cyclodextrin molecules and the complex formation were determined using different

techniques such as UV-Spectroscopy and HPLC. Then, the thiobarbituric acid derivative and cyclodextrin derivative were mixed in aqueous solution and complex formation between thiobarbiturates and cyclodextrin is followed by UV spectroscopy. The effects of factors such as solvent, mixing time, period, ratio between thiobarbiturate and cyclodextrin, temperature and cyclodextrin structure on the complexation ratio were determined by UV-spectroscopy.

The Guest-host complex formation of thiobarbituric acid drug derivatives with beta-cyclodextrin in aqueous medium was investigated using "Phase solubility results" obtained from UV-vis spectrophotometer. Solubility curves of thiobarbituric acid drugs were developed by mixing of beta-cyclodextrin with thiobarbituric acid at two temperatures: (25°C and 37°C) and pH 2.4. The free energy change (ΔG°), the enthalpy (ΔH°) and the entropy (ΔS°) values were calculated using data of the phase solubility.

The theory part of this thesis includes general information about barbituric acids and thiobarbituric acids, cyclodextrins and literature survey about cyclodextrin used in drug delivery. In the Materials and Methods part, experimental procedures and experimental techniques used such as HPLC and UV-Spectroscopy analyses were explained in detail. Then, obtained results and their related discussions were given in the results and discussions parts. Finally, conclusions and future works were presented.

2. THEORETICAL BACKGROUND

2.1. BARBITURIC AND THIOBARBITURIC ACIDS

Barbituric acid or malonylurea or 6-hydroxyuracil is an organic compound containing a pyrimidine heterocyclic structure. Barbituric acid is the major complex of barbiturate drugs, in spite of that barbituric acid itself is not pharmacologically active. Barbituric acids have the specific character of biological activity, particularly when aromatic or alkyl groups are substituted to fifth carbon of the ring. Barbituric acid is used by combining malonic acid (left, Figure 2.1) with urea (right, Figure 2.1), with the elimination of two water molecules (shown in red rectangle) as shown in Figure 2.1 [1].

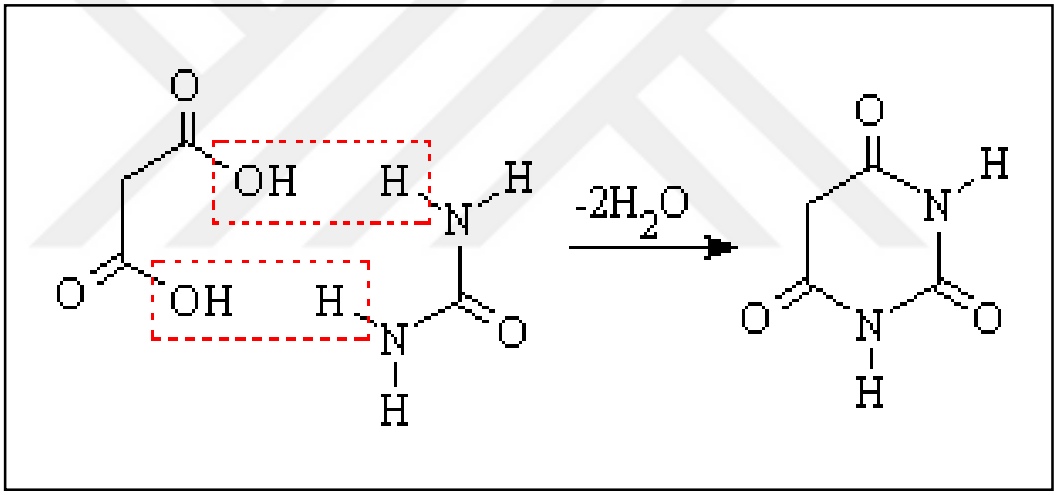


Figure 2.1. Synthesis of barbituric acid [1]

Malonic acid or propanedioic acid is a dicarboxylic acid with structure $CH_2(COOH)_2$. The ionized form of malonic acid, as well as its esters and salts, is known as malonates. For example, diethyl malonate is malonic acid's diethyl ester. The chemical structure of malonic acid is shown in Figure 2.2 [2].

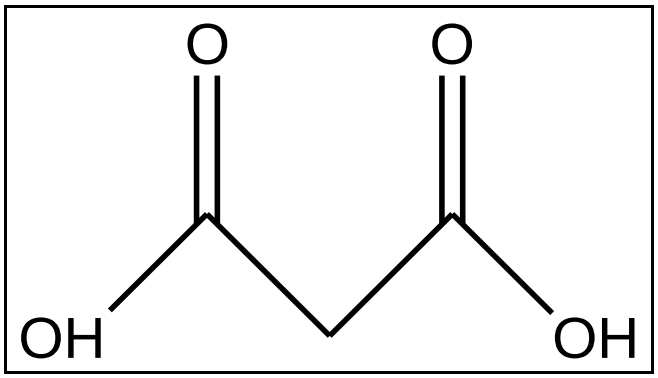


Figure 2.2. Chemical structure of malonic acid [2]

Urea or carbamide is an organic composite. It has the chemical formula $CO(NH_2)_2$. The molecule contains two $-NH_2$ groups joined by a carbonyl (C=O) functional group. The solid molecule is colourless, odourless, highly soluble in water and almost non-toxic. The chemical structure of urea can be seen in Figure 2.3 [3].

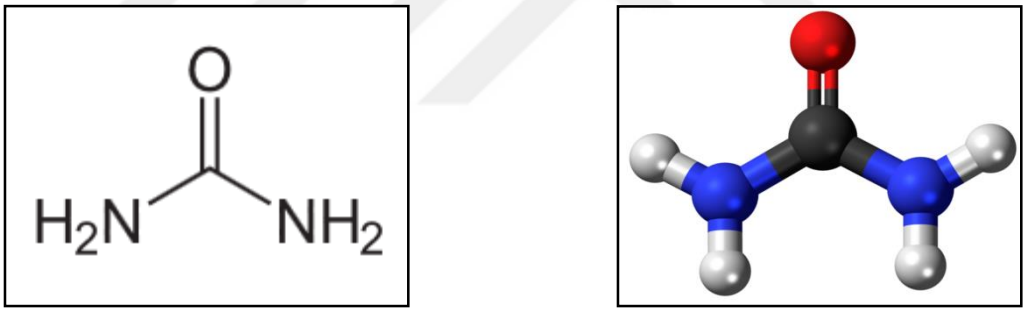


Figure 2.3. Chemical structure of urea [3]

2.1.1. History of Barbituric Acid

First of all, barbituric acid or malonylurea or 2,4,6-trioxohexahydropyrimidine was first synthesized in 1864 by German chemist Adolf von Baeyer. The structure of barbituric acid is shown in Figure 2.4.

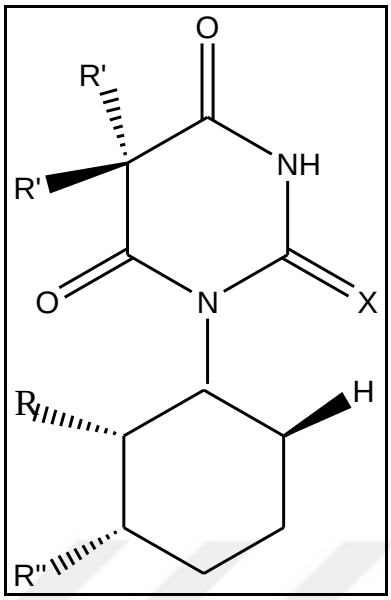


Figure 2.4. Structure of barbituric acid

Barbituric acid is produced by condensing urea (an animal waste product) with diethyl malonate (an ester, which was obtained from the acid of apples). No substance of medical value is discovered until 1903. Two German chemists working at Bayer, Emil Fischer and Joseph von Mering discovered its activity. Barbital is very influential in inducing sleep in dogs. Then, barbital was traded by Bayer under the trade name Veronal. When this discovery was declared, chemists fast produced many new medically active barbiturates, counting the sleeping pill phenobarbital, and pentobarbitone (*Nembutal*). Before full pre-operative anesthesia, this is often used to induce sleepiness. In 1955 the production of barbiturates in the US alone was made to enough to supply 10 million adults with a sleeping pill every night of the year. Chemists have derived till now over 2,500 barbiturates that do possess pharmacologically active qualities. Ultra short-acting barbiturates are generally used for anesthesia because their extremely short duration of action is allowed for greater control [46]. Some IUPAC and common names of barbituric acid are listed in Table 2.1.

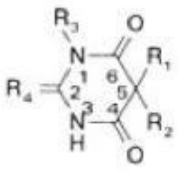
Table 2.1. Some IUPAC names of barbituric acids [5]

IUPAC names of barbituric acids	
2,4,6[1H,3H,5H]-Pyrimidinetrione	Pyrimidine-2,4,6-trione
1,3,5-trihydropyrimidine-2,4,6-trione	6-Hydroxyuracil
2,4,6-pyrimidinetriol	Pyrimidin-2,4,6[1H,3H,5H]
2,4,6-Pyrimidinetrione	Barbitursäure
Malonylurea	Malonylharnstoff
N,N'-Malonylurea	Hydrouracil,6-hydroxy-

Beside the anesthetic activities barbiturates possess different activities, too. They are also used for the cure of anxiety, epilepsy and other psychiatric disorders and dominate effects on the motor and sensory functions [6]. Barbiturates can in most conditions be used as the free acid or as salts of sodium, calcium, potassium, magnesium, lithium, and so on [6].

Different types of drugs based on barbituric acids have been developed. Another barbituric acid derivative, which was phenobarbital, was introduced as a sedative-hypnotic under the trade name Luminal by Bayer in 1912 [7].

Greatest used types of barbiturates are barbital (veronal), phenobarbital (Luminal) and pentrobarbital (Nembutal). Their chemical structures are seen in Figure 2.5 [8].



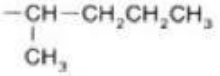
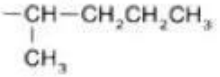
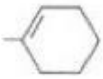
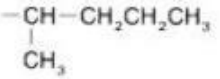
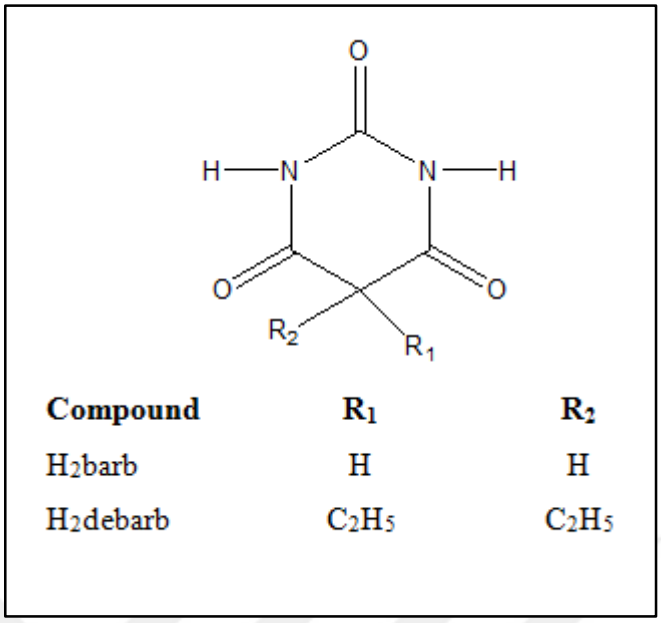
	R_1	R_2	R_3	R_4
Barbital	$-C_2H_5$	$-C_2H_5$	H	O
Phenobarbital	$-C_2H_5$		H	O
Pentobarbital	$-C_2H_5$		H	O
Secobarbital	$-CH_2-CH=CH_2$		H	O
Hexobarbital	$-CH_3$		$-CH_3$	O
Thiopental	$-C_2H_5$		H	S

Figure 2.5. Structures of mostly used barbiturates [8]

In spite of sedative-hypnotic activity of many barbiturates, only a few have anticonvulsant properties. Many barbiturates cause convulsions at larger doses. Phenobarbital (5-ethyl-5-phenylbarbituric acid) (Figure 2.5) is the drug used most commonly for convulsive disorders [9]. Although 5,5-diethylbarbituric acid (**2**) (Figure 2.6) was found to be sedative-hypnotic, low lipid/water partition coefficient of 5,5-diethylbarbituric acid made it difficult to be used in biological systems [10]. Veronal is usually used as its sodium salt (**3**) which is derived from its tautomeric form and is water-soluble. It is more readily sucked than its parent compound **2** (Figure 2.6) [11].



Compound	R_1	R_2
H_2barb	H	H
H_2debarb	C_2H_5	C_2H_5

Figure 2.6. Barbituric acid (1) and its derivatives (2, 3) [11]

2.1.2. Synthesis of Barbituric Acid and Thiobarbituric Acid Derivatives

Barbiturates are cyclic ureides and are produced when a dicarboxylic acid reacts with urea. The acids are used generally in the form of ester and are condensed in the presence of sodium ethoxide [12].

A lot of cyclic ureides are derived from malonic acid or malonic esters. They are collectively known as ‘barbiturates’ because of their relationship with malonyl urea or barbituric acid. Barbituric acid is prepared by the interaction of urea and malonyl dichloride or diethyl malonate. These details are displayed in Figure 2.7. Many cyclic ureides are obtained from malonic acid or malonic esters. They are together known as “barbiturates” owing to their relationship of malonyl urea or barbituric acid [12].

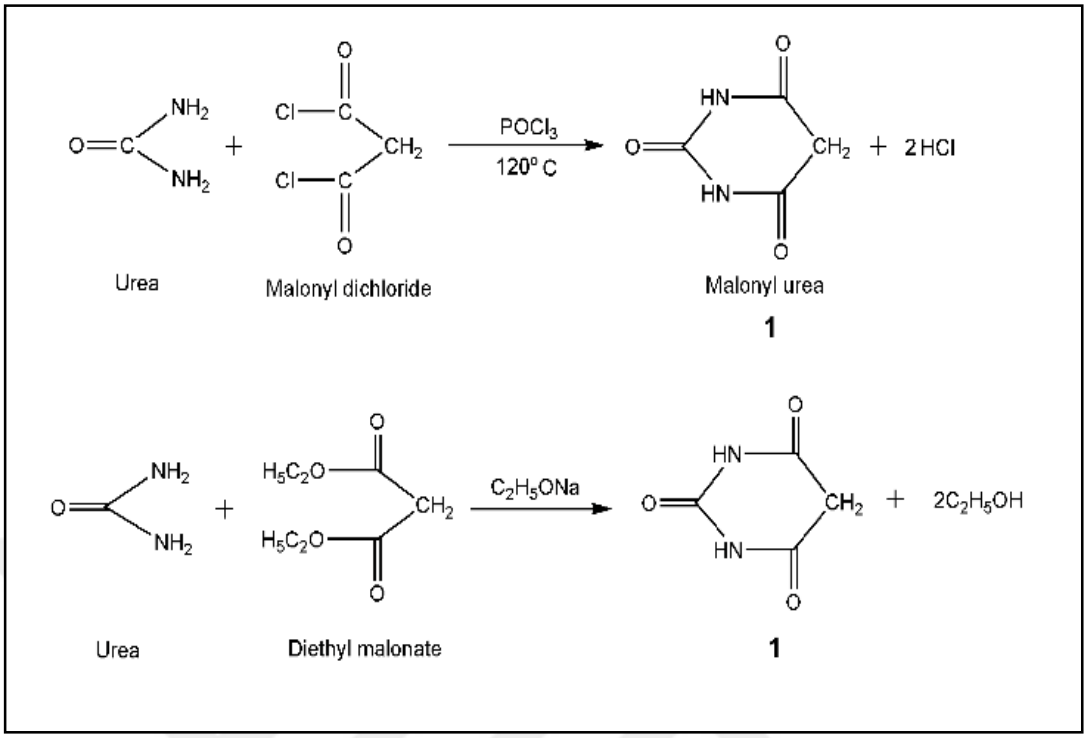


Figure 2.7. Synthesis of barbituric acid [12]

2.1.3. Physical Properties of Barbituric Acids

Firstly, barbituric acids and barbiturate derivatives are regarded as hydrophilic and lipophilic because of 2,4,6-pyrimidinetrione ring system and 5,5'-substituents respectively. The pKa value of barbituric acid in water is 4.01, that is, it is highly strong acid and soluble in polar solvents [13].

Barbiturate derivatives having at least one unchangeable NH hydrogen retain their acidic properties, but the relative acidity of barbituric acid derivatives is not dependent only on the N-substitution, but also the C-5 substitution separately. In Figure 2.8, the effect of N-substitution and C-5 substitution on the pH of barbituric acid can be seen [13].

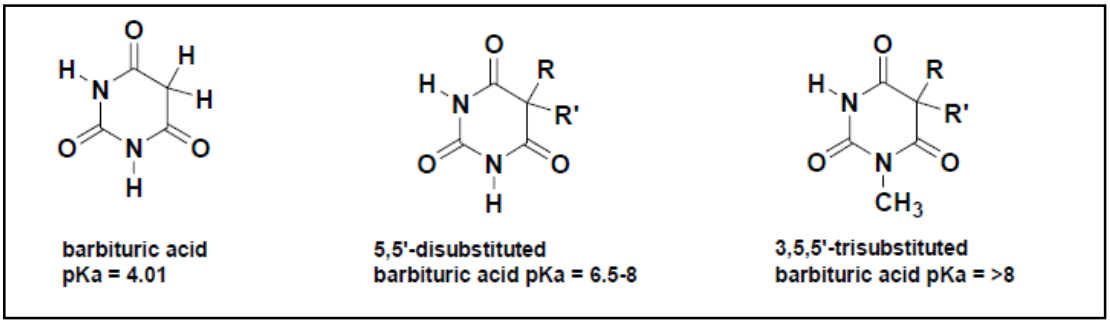


Figure 2.8. Acidic properties of barbituric acids [13]

2.2. CYCLODEXTRIN

Cyclodextrins are a group of compounds structurally associated with natural products and they are formed through bacterial digestion of cellulose. In addition, cyclodextrins have a cyclic oligosaccharide structure. They contain (α-1,4)-linked α-D-glucopyranose units and consist of rather lipophilic central cavity and a hydrophilic outer surface [14].

Owing to the chain conformation of the glucopyranose units, the cyclodextrins are shaped like a truncated cone somewhat perfect cylinders. The central cavity is lined by the skeletal carbons and ethereal oxygens of the glucose residues, which give cyclodextrin a lipophilic character [14].

Types of cyclodextrins (CDs) are α-CD, β-CD and γ-CD, which include six, seven and eight glucopyranose units, respectively (Figure 2.9) [14].

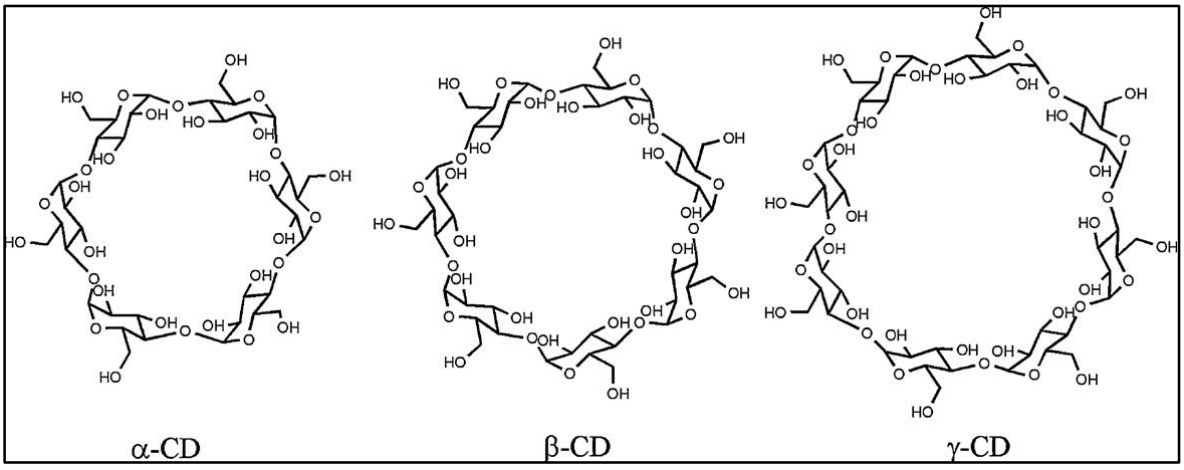


Figure 2.9. Chemical structures of types of cyclodextrins [15]

Food products, cosmetics and other products consist of cyclodextrins. They are especially used as solubilizing agents to grow water-solubility of lipophilic compounds. Besides, cyclodextrins can be used to enhance both chemical and physical stability of various compounds and to advance taste or bioavailability of drugs, to decrease local irritation and to convert liquids to solid powders. Cyclodextrins also can be used as process aids to extract or isolate specific compounds from a mixture [16].

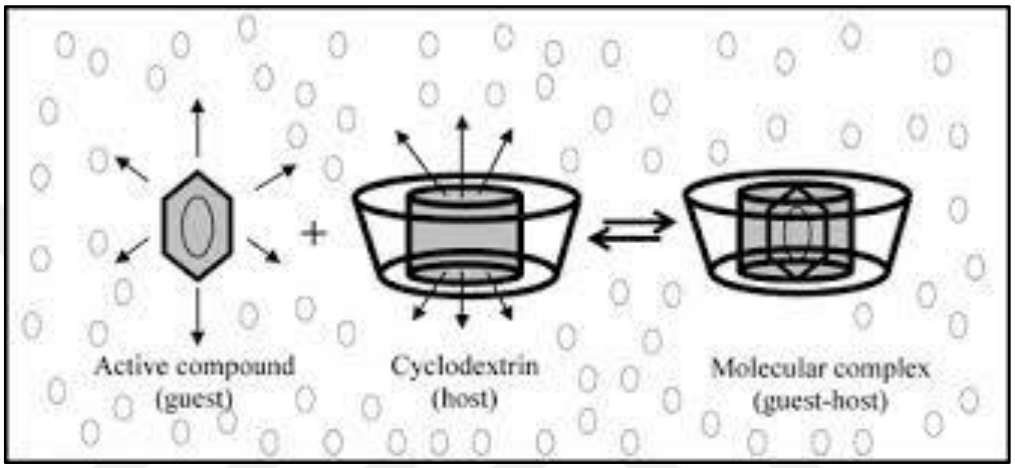


Figure 2.10. Schematic representation of cyclodextrin [19]

Considerable properties of CDs are that cyclodextrins have hydrophobic cavities of different sizes enabling the complexation of hydrophobic guest molecules (Figure 2.11). These complexes provide a solution for insolubility. The cyclodextrins are chemically and physically stable, and they undergo the same reactions as other carbohydrates. Cyclodextrins are not deteriorated by hot aqueous alkali and rather resistant to acid hydrolysis. The most important property of cyclodextrins are that the hydroxyl groups of the cyclodextrin can be substituted to change the solubility of cyclodextrin in water and in other solvents, and to convert the binding strength between the cyclodextrin and the guest compound. Cyclodextrins and their derivatives have a wide range of applications. Solubility of guest compounds can be changed to make them more soluble or less soluble in water. Cyclodextrins can be used to conserve compounds against the effects of light, heat, and oxygen. Volatility of compounds can be reduced by complexation with cyclodextrins to so that increased shelf life and reduced release of compounds into the environment can be achieved These are called as cyclomaltoses, cycloamyloses and Schardinger dextrins [17].

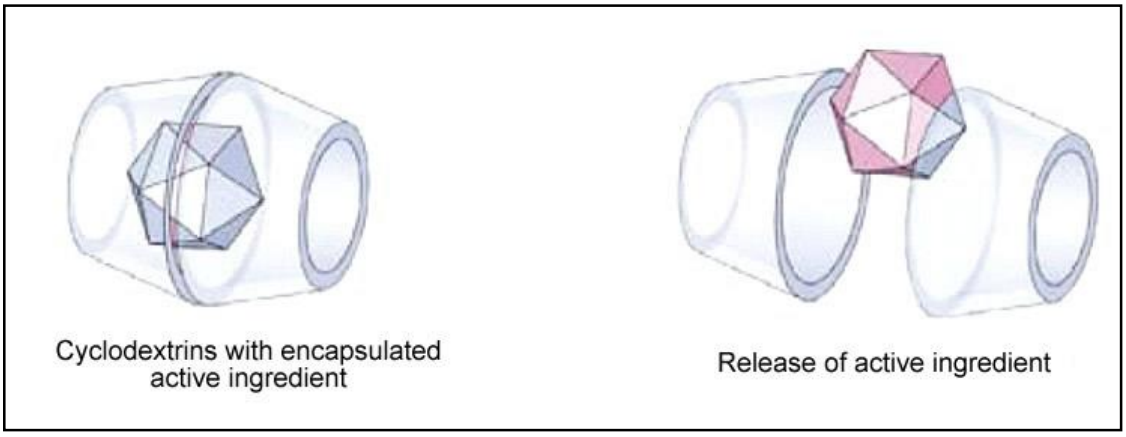


Figure 2.11. Cyclodextrin encapsulation

Cyclodextrins (CDs) have been known as useful pharmaceutical excipients. Owing to their exhaustive studies, they can be used widely in pharmaceutical industry. Their molecular structures give them a feature like hydrophilic exterior and a hydrophobic central cavity. This allows them to form non-covalent inclusion complexes by entrapping the drug into their central cavities. These non-covalent inclusion complexes propose a variety of physicochemical advantages over unmanipulated drugs [18].

2.2.1. History of Cyclodextrin

In 1903, the bacterial strain capable of producing these products from starch was not maintained. In 1904, Schardinger separated a new organism that was able to produce acetone and ethyl alcohol from starch and sugar. In 1911, Schardinger described the strain as Bacillus macerans, which produce enormous amount of crystalline dextrins that have 25-30 per cent starch. He named the crystalline products as ‘crystalline dextrins α’ and ‘crystalline dextrin β’ [18].

In the years following these explorations, large ring cyclodextrins (LR-CDs) were discovered. Presently only α-CD, β-CD and γ-CD, as well as some of their derivatives have been introduced to the market [19].

The physical, chemical and biological properties of parent drug and/or CDs are dramatically modified. Cyclodextrins are safe when administered through various routes. The formation

of inclusion complexes of a drug with non-toxic agents are a promising approach used to develop the dissolution properties of drug [19].

Today, more than 30 different pharmaceutical products containing cyclodextrins are on the market worldwide. Some of them are given in Table 2.2. More and more cyclodextrin based on dosage forms are under development [20].

Table 2.2. Some beta-CD containing pharmaceutical products on the market [20]

Brand Name	**Drug/Cyclodextrin**	**Formulation**	**Company**
Prostarmon E	PGE2 / βCD	Sublingual tablet	Ono (Japan)
Caverject Dual	Alprostadil / αCD	i.v. solution	Pfizer (USA)
Aerodiol	17-β-Estradiol / MβCD	Nasal spray	Servier (France)
Cetirizin	Cetirizine / βCD	Chewable tablet	Losan Pharma (Switzerland)
Fluner	Flunarizine / βCD	Tablet	UCB Pharma (USA)
Vitaseptol	Thiomersal / βCD	Eye drop	Europhta (Monaco)
Mobitil	Meloxicam / βCD	Tablet, suppository	Medical Union Pharmaceutical (Egypt)
Abilify	Aripiprazole / sulfobutyl- βCD	i.m. solution	Bristol-Myers Squibb (USA)
Cerenia	Maropitant / sulfobutyl-βCD	Parental solution	Pfizer Animal Health (USA)
Vfend	Voriconazole / sulfobutyl ether -βCD	i.v. solution	Pfizer (USA)
MitoExtra	Mitomycin / HPβCD	i.v. infusion	Novartis (Switzerland)
Voltaren OPHTHA	Diclofenac (INN) sodium / HPβCD	Eye drop	Novartis (Switzerland)
Dexocort	Hydrocortisone / HPβCD	Solution	Actavis (EU)
Nicorette	Nicotine / Bcd	Subligual tablet	Pfizer (USA)

More than 1500 different CD derivatives have been defined in the literature [19].Types of cyclodextrins:

- α -cyclodextrin: six membered sugar ring molecule
- β -cyclodextrin: seven membered sugar ring molecule
- γ -cyclodextrin: eight membered sugar ring molecule.

Due to the chair formation of the glucopyranose units, cyclodextrin molecules are formed like cones with secondary hydroxyl groups spreading from the wider edge and the primary groups from the narrow edge. This gives cyclodextrin molecules a hydrophilic outer surface, whereas the lipophilicity of their central cavity is comparable to an aqueous ethanolic solution. The naturally occurring cyclodextrins are α, β and γ types containing six, seven and eight glucopyranose units respectively. They have restricted aqueous solubility owing to the strong intermolecular hydrogen bonding in the crystal state. Substitution of the -OH group has improved their solubility. The various derivatives that have gained pharmaceutical interest are mainly hydroxyl or propyl derivatives of β, γ and methylated β-cyclodextrins, sulfobutyl ether β-cyclodextrin, and so on [19].

As well, some characteristics belong to different cyclodextrin types, such as molecular weight, central cavity diameter, and height of torus, outer diameter, solubility in water, surface tension, melting range and water crystallization are shown in Table 2.3 [21].

Table 2.3. Some characteristics of cyclodextrins [21]

	α-cyclodextrin	**β-cyclodextrin**	**γ-cyclodextrin**
Molecular weight	972	1135	1297
Central cavity diameter (A)	4.7-5.3	6.0-6.5	7.5-8.3
Height of torus (A)	7.9	7.9	7.9
Outer diamaeter (A)	14.6	15.4	17.5
Solubility in water (w/v, per cent)	14.2	1.85	23.2
Surface tension (mN/m)	71	71	71
Melting range (ºC)	255-260	255-265	240-245
Water of crystallization (w/v, per cent)	10	13-15	8-18

Moreover, many cyclodextrin derivatives were synthesized. Animation and esterification of primary and secondary hydroxyl group of the cyclodextrins are used to produce derivatives. The solubility of these derivatives is varying and is connected to the influence of the substituent. The alteration in the volume of hydrophobic cavity and modifications in the structure can increase the rate of solubility and stability. The optimizations of reaction situation, well separation of products and regioselective reagents have critical roles in the synthesis of derivatives [21].

Cyclodextrin molecule is a toroidal form, a small cylinder with a hydrophilic outer surface and a hydrophobic central cavity of well-defined size which is displayed in Figure 2.12. The inside is nonpolar because the hydroxyl groups, both primary and secondary, face outward. When cyclodextrins form inclusion complexes, the free rotation of the primary hydroxyl groups decreases the effective cavity diameter on the side where complexation takes place. The approximate dimensions of the cyclodextrins are displayed in Figure 2.12 [22].

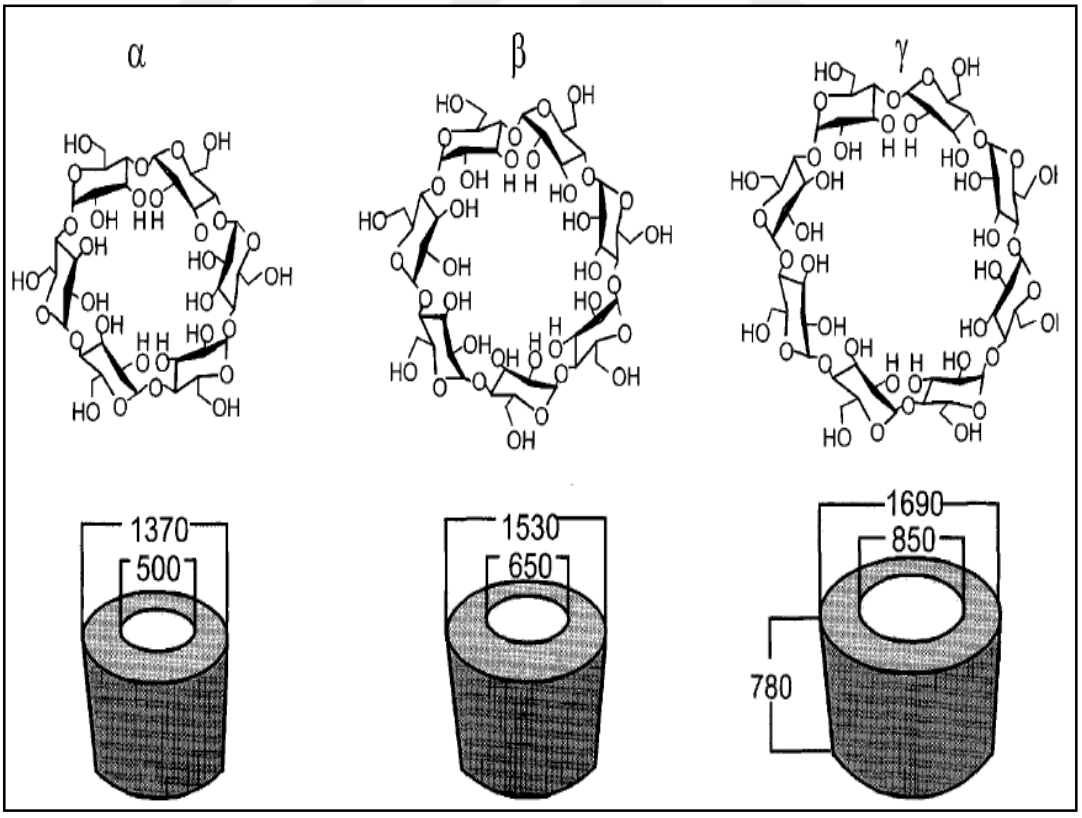


Figure 2.12. Dimensions of cyclodextrins (dimensions in pm)

The very important feature of CDs is their ability of “entrapping” hydrophobic guest molecules into their cavity in the aqueous phase as displayed in Figure 2.13. This complexation ability is owing to their chemical structure and the glucopyranose units’ conformation. In cyclodextrin molecules, the glucopyranose units are present in the chair conformation. Therefore, the hydroxyl functional groups are oriented to the cone exterior with the primary hydroxyl groups of the sugar residues at the narrow and wider edges, which is given it a hydrophilic outer surface. The central cavity is formed by the skeletal carbons and ethereal oxygens of glucose residues, which is given the CD molecules a comparatively hydrophobic inner cavity. The polarity of this cavity has appraised to be similar to that of an aqueous ethanolic or methanolic solution [20].

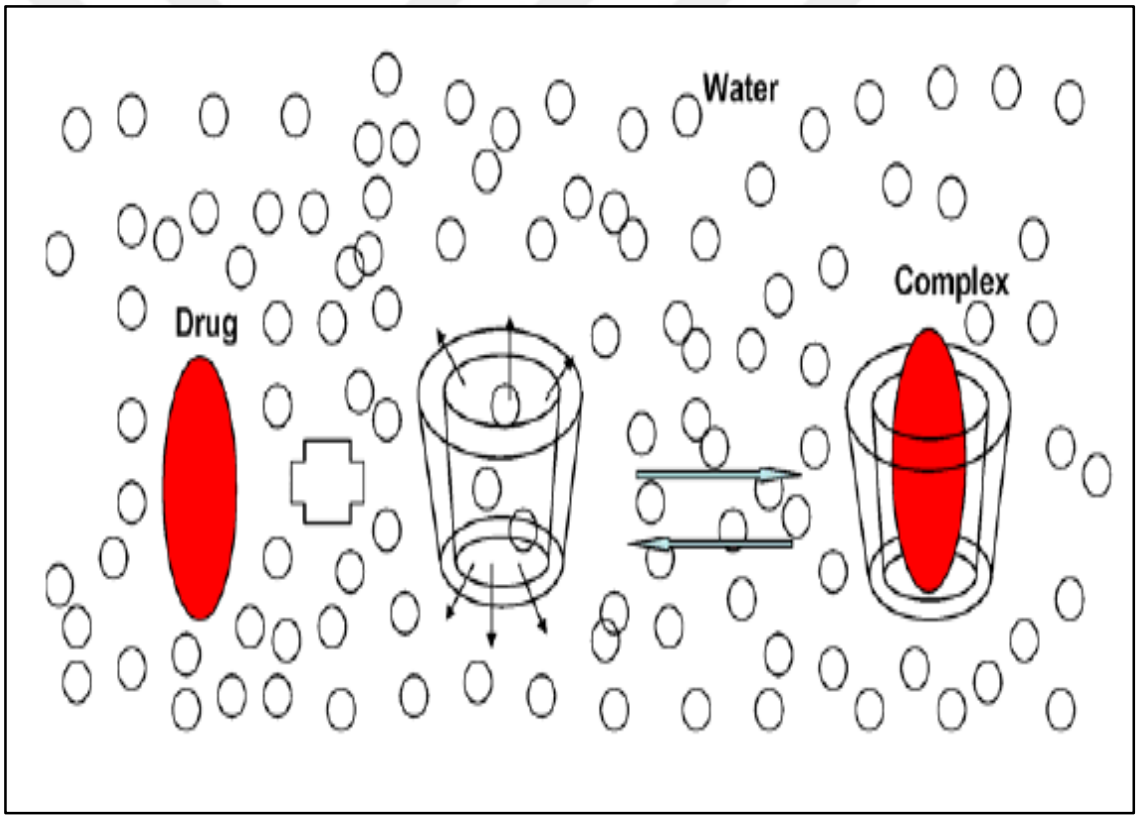


Figure 2.13. Complexation process of CDs with drugs [20]

Inclusion in CDs has an influence on the physicochemical properties of guest molecules as they are temporarily included within the host cavity. These properties are listed at the below [23]:

- Physical isolation of incompatible compounds.

- Solubility enhancement of highly insoluble guests.
- Retarding influence in dyeing and finishing.
- Chromatographic separations.
- Protection of dyes from undesired aggregation and adsorption.
- Removal of dyes and auxiliaries from dyeing effluents.
- Taste modification by masking of flavours, unpleasant odours.
- Control of volatility and sublimation.
- Stabilization of labile guests against the degradative effects of oxidation, visible or UV light and heat.
- Controlled release of drugs and flavors.

Hydrophobic molecules are incorporated into the cavity of cyclodextrins by displacing water. This process is favoured by the repulsion of the molecule by water. This effectively encapsulates the molecule of interest within the cyclodextrin, rendering water-solubility of the molecule. When the water-soluble complex is diluted in a much larger volume of aqueous solvent, the process is inverted, thereby releasing the molecule of concern into the solution [24].

2.3. APPLICATIONS OF CYCLODEXTRINS

CDs can change the physicochemical features of a guest. When a guest compound is included in the CD cavity, the guest becomes bounded by the atoms in the cavity of CD. Thus, the hydrophobic groups of the guest that would be in contact with the solvent in the free-state interact with the atoms of the cavity of the CD instead. Thus, CDs can change the physical properties of guests, such as increasing water solubility or decreasing volatility (Table 2.4). Imparting these properties to the guest by forming inclusion complex with CDs has been ubiquitously found applications in the drug, textile and home products industries. Some examples of compounds whose physicochemical properties have been altered by complexation with CDs were given in Table 2.4 [25].

Table 2.4. Examples of CD applications [25]

Guest compound	**Guest found in, used in or used for the treatment of**	**Effect of complex formation with CD**
Limonin and Naringin	Citrus-based juice	Removes bitterness associated with the guest
Menthol	Chewing gum	Increases duration of flavor
Hexa- to Octadecanones	Food-can coatings	Removes stale flavor imparted by guest
Nicardipine hydrochloride	Angina/High blood pressure	Prolongs shelf-life of drug
Tolnafate	Antifungal agent	Increases solubility of drug
Urushiols	Topical creams used to treat poison ivy rashes	Reduces rashes
Peroxyacetic acid	Bleaching products	Increases lifetime and thermal stability of products

When the guest molecule is encompassed by a cyclodextrin derivative, the molecule becomes micro-encapsulated from a microscopical point of view. According to circumstances, chemical and physical properties of the guest molecule can attend to change advantageously.

2.3.1. Use in Cosmetics, Personal Care and Toiletry

Cyclodextrin is also used in cosmetic industry, generally in room fresheners, volatility suppression of perfumes and detergents generating controlled release of fragrances. Besides, the stabilization, process improvement upon conversion of a liquid ingredient to a solid form and odour control are significant advantages of cyclodextrin. These applications can be seen in the toothpaste, liquid-solid fabric softeners, skin cream, tissues and paper towels. The

interaction of the guest with cyclodextrins establishes a higher barrier and has an important role in long lasting aroma [26].

The fragrance is surrounded with CD and this process is caused stabilization of the aroma in the bathing preparations. In addition, CDs are used in cosmetic industry to help reducing of body smell. In addition, when the CD complexes are used in lipsticks, the effect is flavor protection and water solubility in oil. The combination of hydroxypropyl-β-cyclodextrin surfactant with other ingredients improves the antimicrobial activity and when the detergent components are mixed with CDs, undesirable odours vanish in washed items [27].

In addition, some silica based toothpastes contain CDs, which increase the antimicrobial activity. Furthermore, if CD is used in self-tanning emulsions, the performance of shelf life is affected [27].

2.3.2. Use in Foods and Flavors

In food industry, CDs are used to conserve flavor protection and they are introduced by encapsulation method. The other artificial and natural additives are volatile liquids or oils. In addition CDs have an important target that is to remove cholesterol from butter, milk and eggs. The CD-treated material indicates 80% removal of cholesterol and free fatty acids [28].

In Japan, cyclodextrins have been permitted as ‘modified starch’ for food applications and are used to prevent odours in fresh food. One or two European countries, for instance Hungary, have approved γ-cyclodextrin for applications due to its low toxicity. When cyclodextrin is used as food additive, it reduces bitterness, affects smell, shelf life, taste and stabilizes flavours [28]. Regularity of natural cyclodextrins is used in Food approval and Pharmacopoeia Monographs showed in Table 2.5.

The formation of CDs with artificial sweeteners such as aspartame can improve the taste and reduce the bitter after taste of glycyrrhizin, stevioside, and rubusoside [28].

Table 2.5. Regularity of natural cyclodextrins [29]

	Food Approval			**Pharmacopoeia Monographs**		
	US	**Europe**	**Japan**	**US/NF**	**Ph.Eur**	**JP**
α-CD	In preparation	Planned	Yes	No	Yes	Yes
β-CD	GRAS	Food Additive	Yes	Yes	Yes	Yes
γ-CD	GRAS	Pending	Yes	No	In Progress	Yes

The regularity of CD's are developing which means β-cyclodextrin and α-cyclodextrin are registered in pharmacopoeia sources, Japanese Pharmacopoeia and European Pharmacopoeia but γ-Cyclodextrin has not been registered yet in the US Pharmacopoeia. Besides, γ-cyclodextrin and β-Cyclodextrin are listed as food additives by FDA [29].

Table 2.6. Examples of marketed products containing cyclodextrin [29]

Active ingredient	**Drug name**	**Administration route**	**Trade name**	**Market**
α-Cyclodextrin	Alprostadil (PGE_1)	IV	Prostavastin	Europe, Japan, USA
	Cefotiam hexetil HCl	Oral	Pansporin T	Japan
β-Cyclodextrin	Benexeate HCl	Oral	Ulgut, Lonmiel	Japan
	Dexamethasone	Dermal	Glymessason	Japan
	Iodine	Topical	Mena-Gargle	Europe
	Nicotine	Sublingual	Nicorette	Europe
	Nimesulide	Oral	Nimedax, Mesulid	Japan
	Nitroglycerin	Sublingual	Nitropen	Europe
	Omeprazol	Oral	Omebeta	Japan
	PGE_2	Sublingual	Prostarmon E	Europe
	Piroxicam	Oral	Brexin	Europe

2.3.3. Use in Drug Delivery System

In drug delivery, cyclodextrin does not disperse through the membranes because of its partition coefficient, high molecular weight and chemical structure but the free form of drug that is equilibrium with drug/cyclodextrin (D/CD) complexes can be permeated through liquid membranes. In most cases, the composition of drug that is non-aqueous or aqueous, physicochemical properties of drug, physiological composition of membrane barrier will specify the cyclodextrins' effects on biological membranes [30].

In addition, the cyclodextrins will advance or will hamper drug delivery through a biological membrane. The cyclodextrins will advance drug delivery through aqueous diffusion-controlled barriers, but can hinder drug delivery through lipophilic membrane-controlled barriers. On the other hand, the drug bioavailability will be increased by using cyclodextrins [30].

Nonetheless, when the cyclodextrin increases or prevents drug delivery in membranes, it affects the formulation of drug with cyclodextrin. The quantity of cyclodextrin can affect the drug bioavailability [30].

2.3.3.1. Effect on Drug Solubility and Dissolution

In water soluble drugs, cyclodextrins have significant effect applicable to increase the different drug solubility and dissolution through the involvement or solid dispersion. Cyclodextrins have been used as hydrophilic carriers for drugs and increased the dissolution with maximum dose. The agents containing cyclodextrin are summarized in Table 2.7. For example, methylated cyclodextrin which is commercially available, are known as most powerful stabilizer despite of low molar substitution. The researchers display that β-cyclodextrin increases the water solubility of drugs such as antibiotics [31].

Table 2.7. Examples of CD enhanced solubility of drugs [31]

Cyclodextrins	**Drugs**
β-Cyclodextrin	Nimesulide, Sulfomethiazole, Lorazepam
α-Cyclodextrin	Praziquantel
γ-Cyclodextrin	Praziquantel, Omeprazole, Digoxin
HP-β-Cyclodextrin	Sulfomethiazole, Ketoprofen, Griseofulvin
DM-β-Cyclodextrin	Naproxen, Camptothesin
SBE-β-Cyclodextrin	Danazol, Fluasterone, Spiranolactone
RM-β-Cyclodextrin	Tacrolimus
Randomly acetylated amorphous β-Cyclodextrin	Naproxen

2.3.3.2. Effect on Drug Bioavailability

The drug solubility, permeability, bioavailability of insoluble drugs and dissolution can be increased with the use of cyclodextrins. These are useable at the surface of the barrier such as mucosa, skin, and eye cornea. Because of these, solubility of cyclodextrin is very significant in the aqueous medium. The studies show the addition of polymers increase the permeability of drug from cyclodextrin solutions. By the direct action of the membranes, cyclodextrin increases the permeability and bioavailability of the drugs in aqueous medium. α-Cyclodextrin increases the rectal bioavailability of morphine by inhibiting the drug's upward movement from areas impacted by first pass metabolism. In Table 2.8, some examples of cyclodextrins in oral, sublingual and buccal formulations and its clinical and bioavailability studies are given [32].

Table 2.8 Examples of cyclodextrins in oral, sublingual and buccal formulations and its clinical and bioavailability studies [33]

Class	**Drug**	**CD**	**Formulation**	**Species**	**Relative bioavalibity**
Class I	Piroxicam	βCD	Tablet, capsule and oral suspension	Human, rat, rabbit	≤1.4
Class II	Carbamazepine	DMβCD	Oral powder and solution, tablet	Rabbit, dog, rat	≤5.6
	Digoxin	γCD	Tablet	Dog	5.4
	Glibenclamide	βCD, SBEβCD	Capsule containing powder	Dog, rat	≤6.2
	Miconazole	HPβCD	Aqueous suspension	Rat	2.3
	Phenytoin	E-βCD, GluβCD, MalβCD, SEBβCD, HPβCD	Suspension, capsule containing powder	Rat, dog	≤5
	Spironolactone	βCD, γCD, DMβCD, SBEβCD, HPβCD	Oral solution and powder	Rat, dog	≤3.6
	Tolbutamide	βCD, HPβCD	Suspension, oral powder	Rabbit, dog	≤1.5
	α-Tocophenyl nicotinate	DMβCD	Capsule containing powder	Dog	App. 70
Class III	Acyclovir	βCD	Oral suspension	Rat	1.1
	Diphenhydramine, HCI	DMβCD, HPβCD	Solution	Rat	≤0.9
Class IV	Cyclosporin A	DMβCD	Oral suspension	Rat	4.7

2.3.3.3. Effect on Drug Safety and Stability

In drug safety applications, cyclodextrins are used to prohibit the irritation. The researches support that β-cyclodextrin increases the efficiency of preventation of cytomegalovirus (CMV) infections. The toxicity of parenteral drugs is decreased by the addition of cyclodextrin complexes. Moreover, addition of cyclodextrins into drugs can prohibit the side effect, direct contact of biological membrane and irritation [33].

According to studies, cyclodextrin can increase the shelf life, stability and oxidation of drugs. Table 2.9 shows the effect of cyclodextrin on the stability of different drugs. In addition cyclodextrin complexations can prohibit the decline of drugs and conserve many degradation processes. The stabilizing effect of cyclodextrins depends on the nature of the drug. The cyclodextrins are reported to have developed photostability of trimeprazine and promethazine [33].

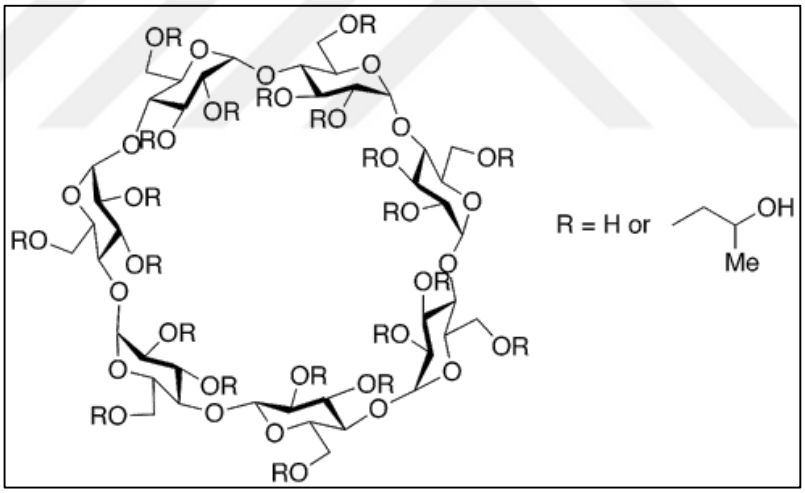


Figure 2.14.2-Hydroxypropyl-β-CD

Table 2.9. Effects of cyclodextrin [33]

Drug	**CD**	**Effect**
Promethazine	HP-β-CD, DM-β-CD	Photostability
2-ethylhexyl p-(dimethylamino) benzoate	HP-β-CD	Photostability
Glibenclmaide	β-CD	Shelf life with unaffected dissolution rates for four years
Diclofenac sodium	β-CD	Thermal stability in solid-state
Quinaril	β-CD, HP-β-CD	Stability against intramolecular cyclizaton in solid state
Doxorubicin	HP-β-CD, HP-γ-CD	Stability to acid hydrolysis and photodecomposition
Acyl ester prodrugs of Ganciclovir	HP-β-CD	Stability against hydrolysis
Digoxin	γ-CD	Stability against hydrolysis
Rutin	HP-β-CD	Stability against hydrolysis
Camptothesin	RDM-β-CD	Stability against hydrolysis
Melphalan and Carmustine	SBE-β-CD, HP-β-CD	Stability against hydrolysis
Paclitaxel	γ-CD, HP-γ-CD, HP-β-CD	Stability against hyrolysis
Spiranolactone	CD, HP-β-CD, γ-CD, β-CD	Deacylation or degradation
Flutamide	β-CD	Photoreactivity

2.3.4. Use in Textiles

Beta-CD can be incorporated onto textile by means of spraying, printing, padding, grafting, surface coating, impregnation, ink jet printing or via sol gel. Table 2.10 shows the various feasible interactions between beta-CD and some textile fibers.

Table 2.10. Feasible interactions between beta-CD and some textile fibers

Parameter	Cotton	Wool	PES	PA	PAN	PP
Ionic Interactions	-	+	-	+	+	-
Covalent bonds	+	+	-	+	-	-
Van der Waal forces	-	-	+	+	+	-
Cross linking agents	+	+	+	-	-	-
Graft polymerisation	+	+	+	+	+	+
PES : Polyamide, PAN : Polyacrylonitrile, PP : Polypropylene						

Various mechanisms are listed in the literature to fix beta-CD to fibers, a large volume of them are about grafting with the use of cross linking agents such as polycarboxylic acids onto cotton, wool, polyester, polyamide and polyacrylonitrile fibers, etc. [23].

There is a huge amount of literature on the influence of beta-CDs on dyeing. It has been reported that beta-CDs can absorb dyes and can therefore be used to reduce loss of dye in waste water, in addition they can improve dye uniformity and prevent the running of dyes during washing. For instance, dyeing of cotton-polyester blends with disperses dyes and beta- CDs led to improved dye strength and deeper dye shades [23].

2.4. LITERATURE SURVEY OF COMPLEXATION OF CYCLODEXTRIN WITH DRUG MOLECULES

Several studies is done on the complexation of cyclodextrin with drug molecules. Some of them were chosen to make comparison with the result of this study.

Wang et al. studied the effects of the inclusion complex of orange G and β-cyclodextrin (β-CD) by using both spectrophotometry and infrared spectroscopy. Effects of the pH, concentration of β-CD and ionic strength on the inclusion complex of β-CD and orange G were examined. The thermodynamic parameters of inclusion complex, ΔG^0, ΔH^0 and ΔS^0 were obtained [27].

Filipa et al. studied the complexation of methyl salicylate (MS) and ethyl salicylate (ES), which are non-steroidal analgesic, anti-inflammatory and antirrheumatic drugs with β-CD from thermodynamic and structural points view. The complexation of MS and ES with β-CD has been investigated using reversed phase liquid chromatography. HPLC and UV-vis measurements and quantum mechanics calculations led to the result that MS and ES form 1:1 inclusion complex with β-CD [25].

Bonilla et al. developed a reversed phase high performance liquid chromatography (RP-HPLC) method for the determination of pterostilbene in food samples. The method is based on the addition of CDs to the mobile phase where the complexation of pterostilbene by CDs takes place. In order to select the most suitable conditions for the RP-HPLC method, the effect of several physicochemical parameters, such as the free energy change (ΔG^o), the enthalpy change (ΔH^o), and the entropy change (ΔS^o), on the complexation of pterostilbene by CDs was studied [26].

Domanska et al. developed a Guest-host complex formation of three drug derivatives of anthranilic acid, mefenamic acid, niflumic acid, and flufenamic acid with 2-hydroxypropyl-β-cyclodextrin in aqueous solutions by using "Phase solubility study" with UV-spectrophotometry. Solubility of sparingly soluble drugs has been improved by addition of 2HP-β-CD at two temperatures, which are 298.15 K and 310.15 K, and 2 pH values that are 2 and 7. The 2HP-β-CD-drug complex stability constants (K_s) and dissociations contants (K_d) as well as the thermodynamic parameters of reaction, which were the free energy change (ΔG^o), the enthalpy change (ΔH^o), and the entropy change (ΔS^o), were determined [34].

Yuvaraja et al. studied to enhance aqueous solubility of carvedilol by solid dispersion technique using wide variety of carriers such as β-cyclodextrin, hydroxypropyl-β-cyclodextrin, tartaric acid, polyvinyl pyrrolidone K-30 and poloxamer-407. Various products of carvedilol-solid dispersion had been studied extensively invarious pH conditions

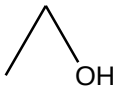
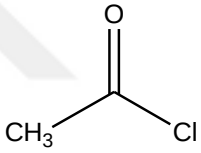
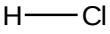
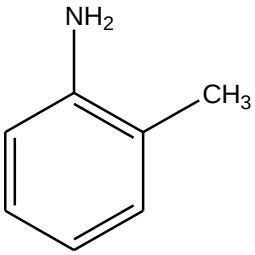
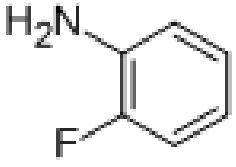
to check enhancement of solubility and dissolution characteristics of carvedilol. Negative change of Gibb's free energy and complexation constants were the evidence of stable nature of the binding between carvedilol and carriers [35].

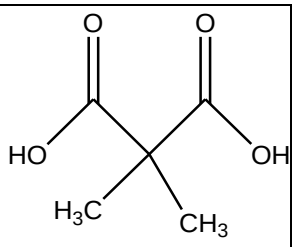
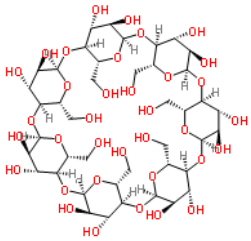
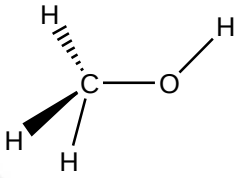
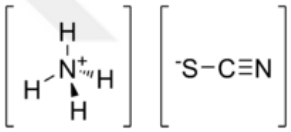
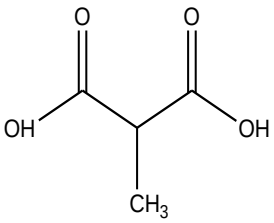
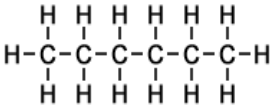
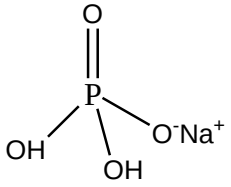
3. MATERIALS AND METHODS

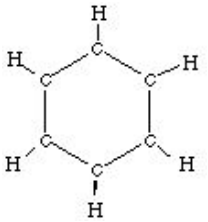
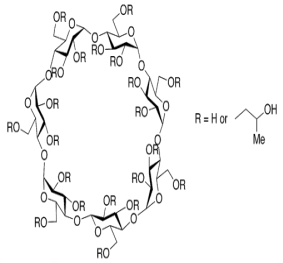
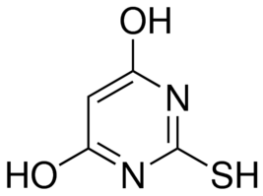
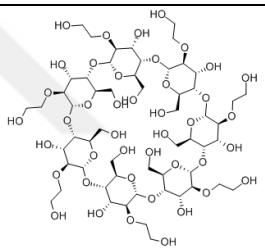
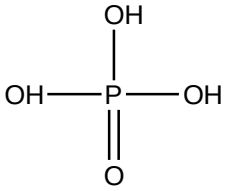
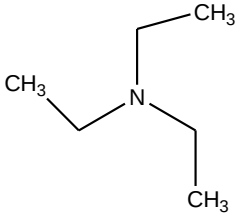
A list of chemicals used in this work, together with the names of suppliers and the apparatus used in the studies are briefly described in this part.

3.1. CHEMICALS

Table 3.1. Reagents

Chemical name	Formula	Supplier	Purity (per cent)	Chemical Structure
Ethanol (Absolute)	C_2H_5OH	Sigma Aldrich	37	
Acetyl chloride	C_2H_3ClO	Acros Organics	99	
Hydrochloric acid	HCl	Sigma Aldrich	37	
o-Toluidine	C_7H_9N	Acros Organics	99	
2-Fluoroaniline	C_6H_6FN	Merck	98	

Dimethylmalonic acid	$(CH_3)_2(COOH)_2$	Sigma Aldrich	98	
Beta-Cyclodextrin	$C_{42}H_{70}O_{35}$	Sigma Aldrich	97	
Methanol (HPLC)	CH_4O	Sigma Aldrich	99.9	
Ammonium thiocyanate	CH_4N_2S	Sigma Aldrich	98	
Methylmalonic acid	$C_4H_6O_4$	Sigma Aldrich	99	
n-Hexane	$CH_3(CH_2)_4CH_3$	Merck	98	
Sodium dihydrogen phosphate	$NaH_2PO_4{*}2H_2O$	Merck	98	

Benzene	C_6H_6	Merck	99.5	
2-(Hydroxypropyl)-βCD	$C_6H_{112}O_{42}$	Abcr	99	
2-Thiobarbituric acid	$C_4H_4N_2O_2S$	Sigma Aldrich	99	
2-(Hydroxyethyl)-βCD	$C_{56}H_{98}O_{42}$	Sigma Aldrich	90	
Phosphoric acid	H_3PO_4	Sigma Aldrich	99	
Triethylamine (TEA)	$C_6H_{15}N$	Sigma Aldrich	99	

3.2. METHODS

3.2.1. HPLC (HIGH PERFORMANCE LIQUID CHROMATOGRAPHY)

High performance liquid chromatography (or high pressure liquid chromatography, HPLC) is basically a highly improved form of column chromatography. HPLC is used in biochemistry and chemical analysis to separate, identify, and quantify the active compounds. Instead of a solvent being allowed to drip through a column under gravity, it is forced through under high pressures of up to 400 atmospheres, which makes the flow of the solvent much faster. It also allows using a very much smaller particle size for the column packing material which gives a much greater surface area for interactions between the stationary phase and the molecule passes through it. This allows a much better separation of the components of the mixture [36].

HPLC mainly utilize a column that holds packing material (stationary phase), a pump that let the mobile phase(s) move through the column, and a detector that identifies the compounds coming out of the column and a recorder (mostly computer) that shows the chromatogram with the retention times of the molecules (Figure 3.1). Retention time varies depending on the interactions between the stationary phases, the molecules being analyzed, and the solvent(s) used [37].

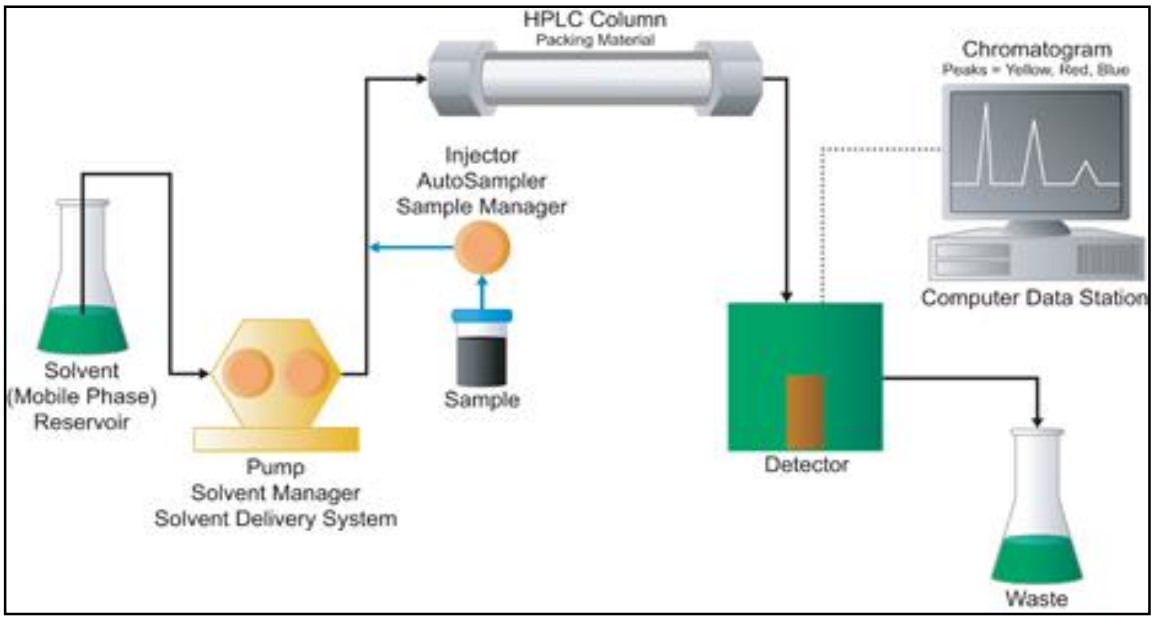


Figure 3.1. Components of HPLC [38]

The sample to be analyzed is given in small volume to the stream of mobile phase and retards by specific chemical or physical interactions with the stationary phase. The amount of the retardation depends on the nature of the analyte and the composition of both the stationary and the mobile phase. The time at which the specific analyte elutes (comes out of the end of the column) is called the retention time. Common solvents used include any miscible combinations of water and organic liquids (the most common are methanol and acetonitrile). When the separation has been done with the help of varying degrees of the mobile phase composition during the analysis; this is known as isocratic. The gradient separates the analyte mixtures as a function of the affinity of the analyte for the current mobile phase. The choice of solvents, additives and gradient depends on the nature of the stationary phase and the analyte [37].

Properties of HPLC columns:

- made up of stainless steel,
- 10-30 cm long,
- 4-10 mm internal diameter,
- 1-10 mm particle size,
- speed range: 40,000-60,000 plates/meter.

High speed isocratic separation:

- Speed: 100,000 plates/meter.

Gradient elution:

- Solvent polarity [composition] continuously varied or stepped.

HPLC is used for pharmaceutical, clinical, forensic, food, environmental and industrial research and development analyses for purifying chemical compounds, developing processes for synthesizing chemical compounds, isolating natural products, or predicting physical properties, analyzing air and water pollutants, monitoring pesticide levels in the environment and also in quality control to ensure the purity of raw materials. Additionally, it is used to control and improve process yields, quantify assays of final products, and to evaluate product stability and monitor degradation [39].

In a very non-polar environment, hydrophilic molecules will tend to associate with each other. The hydrophilic molecules in the mobile phase will tend to adsorb to the solid support if the solid support on a chromatographic resin is also hydrophilic. Increasing the mobile phase polarity will subsequently decrease the adsorption and cause the elution of the molecules into the mobile phase. This mechanism is called Normal Phase Chromatography. It is a very powerful technique but often requires non-polar solvents. Due to safety and environmental concerns this mode is used mostly as an analytical technique and not for process applications [40].

The opposite of normal phase, or Reversed Phase Chromatography, results from the adsorption of hydrophobic molecules onto a hydrophobic solid support in a polar mobile phase. Decreasing the mobile phase polarity by using organic solvents reduces the hydrophobic interaction between the solute and the solid support resulting in desorption. The more hydrophobic the molecule, the more strongly it will adsorb onto the solid support. This requires a higher concentration of organic solvent to promote desorption. Reversed phase chromatography is another very powerful technique and is effective for the separation of a very wide range of molecules. However, at process scale it is not typically used for proteins, due to presence of the organic solvent which denatures many proteins and destroys their biological activity. Reversed phase chromatography is used very frequently as an analytical technique and there are many different stationary phases available for method optimization [40].

3.2.2. UV-Visible Spectroscopy

A spectrum is a graphical representation of the amount of light absorbed or transmitted by matter as a function of the wavelength. A UV-visible spectrophotometer is measured absorbance or transmittance from the UV range to which the human eye is not sensitive to the visible wavelength range to which the human eye is been sensitive.

UV-vis spectrophotometry can deliver the following qualitative information [41]:

- Identification of pure substances
- Identification of substances following HPLC separation (preferably with diode array systems)

- Purity testing (for example of proteins or DNA/RNA)
- Melting point curves of proteins and nucleic acids
- Differentiation of saturated and unsaturated compounds
- Differentiation of keto and enol forms
- Identification of carbonyl bands
- Clarification of bonding relationships and substituent effects
- Enzyme activities.

Figure 3.2. UV-Visible spectrophotometer [42]

The minimum requirements needed for an instrument to study absorption spectra [43]:

i. Source of radiation of appropriate wavelengths,
ii. Means of isolating light of a single wavelength and getting it to the sample compartment as monochromator and optical geometry,
iii. Means of introducing the test sample into the light beam as sample handling,
iv. Means of detecting and measuring the light intensity.

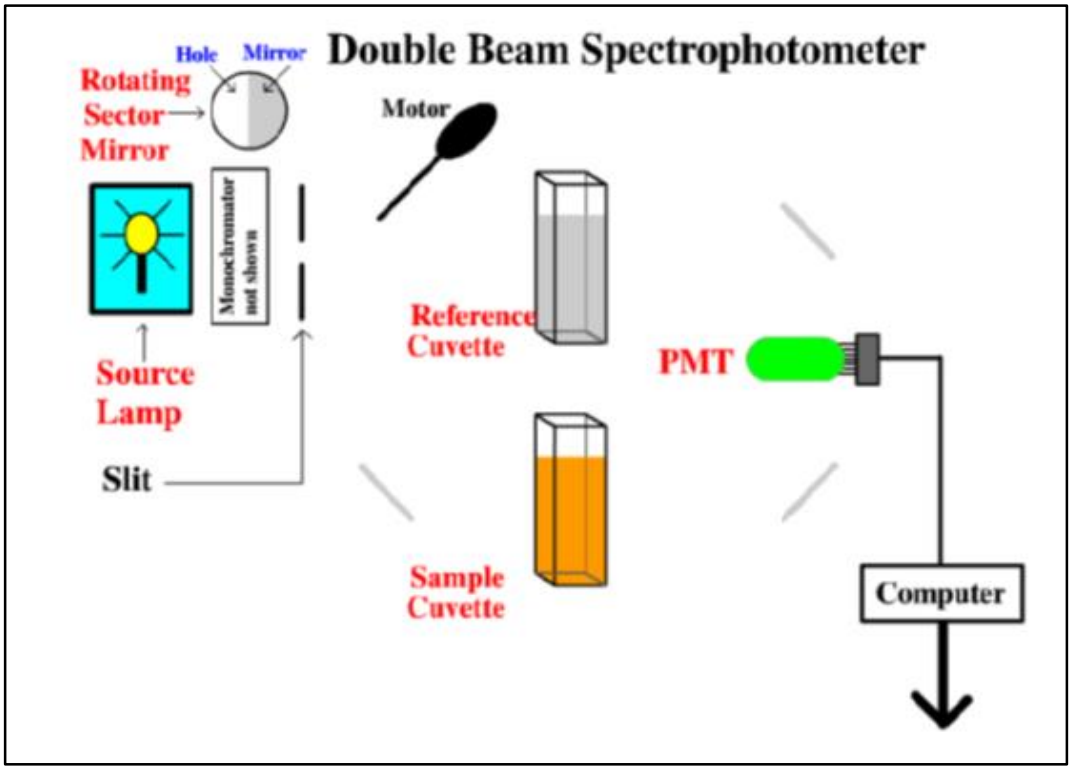


Figure 3.3. Basic construction of a spectrophotometer [42]

UV/VIS spectroscopy is the study of how a sample responds to light. When a beam of light passes through a substance or a solution, some of the light may be absorbed and the remainder is transmitted through the sample. The ratio of the intensity of the light entering the sample (I_0) to that exiting the sample (I_t) at a particular wavelength is defined as the transmittance (T). This is often expressed as the percentage transmittance (%T), which is the transmittance multiplied by 100 is given in Equation 3.1:

$$T = \frac{I}{I_0} \qquad or \quad \%T = \left(\frac{I}{I_0}\right) \times 100 \tag{3.1}$$

The absorbance (A) of sample is the negative logarithm of the transmittance:

$$A = -\log T \tag{3.2}$$

The UV/VIS range of the electromagnetic spectrum covers the range 190-700 nm (most instruments are capable of measuring at longer wavelengths than this, depending on their detector type). For clinical analysis, this is useful as water (most assays are in aqueous solution) is almost completely transparent in this region.

The most important principle in absorption analysis is the Beer-Lambert law. This law states that, for a given ideal solution, there is a linear relationship between concentration and absorbance provided that the path length is kept constant; the absorptivity (ε) is a constant for each molecule for each wavelength is given in Equation 3.3:

$$A = \varepsilon \times c \times l \tag{3.3}$$

Provided that ε and l are kept constant for a given set of experiments, a plot of the sample absorbance against the concentration of the absorbing substance should give a straight line. In practice, a calibration curve is prepared by plotting the absorbance of a series of standard samples as a function of their concentration. If the absorbance of an unknown sample is then measured, the concentration of the absorbing component can be assessed from this graph. Another consequence of the Beer-Lambert law is that it is possible to change the path length to affect the absorbance. This can be useful where lower detection limits are required as the path length can be increased (longer path length cuvettes are available) or, where the absorbance is too high to be measured on the instrument, the path length can be reduced. Alternatively, it is possible to reduce the absorbance by diluting the sample, but one has to take care when dealing with biologically active samples, particularly enzyme-based solutions, as this may have a profound effect on the activity.

Most samples studied using visible and ultraviolet spectroscopy is liquid. The sample must therefore be placed in a transparent container to allow measurement. These containers are called cuvettes. It is important that the absorbance properties of the cuvette are appropriate for the experiment. So, glass cuvettes are used for wavelengths in the visible range from 380 nm to 780 nm and quartz cuvettes are used for wavelengths below 380 nm [44].

Figure 3.4. Quartz cuvette

Cuvettes are generally made from transparent plastic, glass, or quartz. Different cuvettes have different optical properties. Plastic cuvettes are increasingly popular because they do not shatter when dropped, and because their low price makes them disposable. However, plastic cuvettes tend to have considerable absorbance in the ultraviolet. Performing measurements in the far ultraviolet (below ~250 nm) requires relatively expensive (and relatively fragile) quartz cuvettes [41].

In this project, UV-Vis Spectroscopy is used to quantify the complexation of thiobarbituric acids with different types of β-cyclodextrins. UV-Vis spectroscopy analysis of the thiobarbituric acid solutions with and without β-cyclodextrins is performed using a Perkin Elmer UV/Vis Spectrophotometer. It is known that typical maximum absorbance value of barbituric acid is 190 nm. In this measurement, an absorbance range of 190-300 nm is used [41].

4. ORGANIC SYNTHESIS AND ANALYSIS METHODS

4.1. SYNTHESIS OF THIOBARBITURIC ACID DERIVATIVES

1-(*o*-aryl)-2-thiobarbituric acid synthesis was performed by the reaction of *ortho*-substituted phenylthioureas with dimethyl- or methylmalonic acids in acetyl chloride. First of all the corresponding thioureas were synthesized. Then they were used in the synthesis of thiobarbituric acid derivatives.

4.1.1. Procedure for the Preparation of *ortho*-Substituted Phenylthioureas

Ortho-substituted phenylthioureas were prepared from the reaction of *ortho*-substituted aniline hydrochloride with ammonium thiocyanate in water. The chemical equation of the reaction is shown in Figure 4.1.

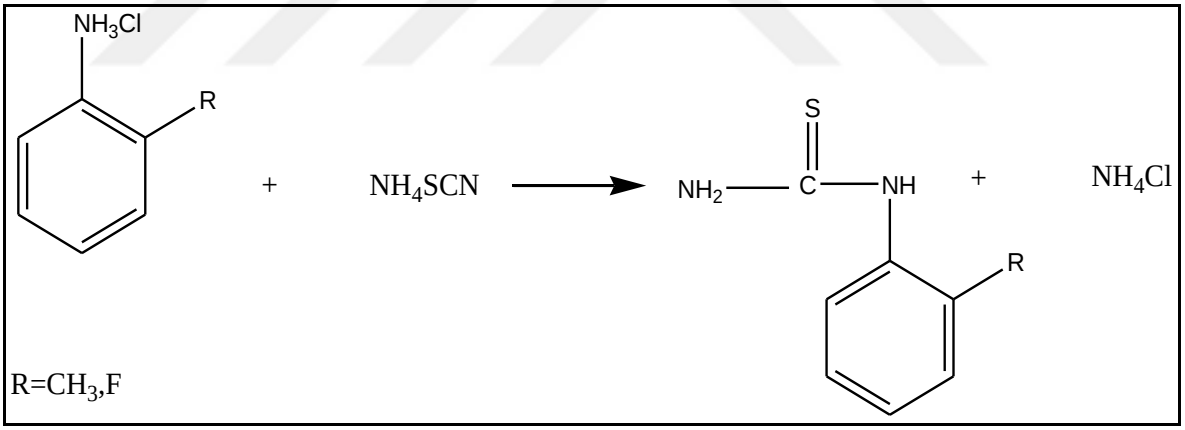


Figure 4.1. Synthesis of ortho-substituted phenylthioureas

0.30 moles of *ortho*-substituted aniline was put in a 300 mL of warm water. Then, 27.5 mL (0.33 moles) of hydrochloric acid (HCI) was added in the water containing *ortho*-substituted aniline mixture. After heating this mixture, the obtained homogenous solution was put in a 500 mL porcelain bowl, and 25 g of ammonium thiocyanate was added into the prepared homogenous solution. The obtained homogenous solution was heated on the steam bath until the water in the solution was evaporated and dry residual crystal powders were obtained. The resulting crystalline residue consists of *ortho*-substituted phenylthiourea and

ammonium chloride. This crystalline residue was powdered finely. 300 mL of water at the room temperature was added onto the crystals and again the mixture was evaporated. Then, 300 mL of water was put onto the resulting mixture in a beaker and was heated until the temperature of the mixture reached to 70˚C. After reaching to 70**°**C, the beaker was put on the bench to cool the mixture to 35**°**C. Then, the vacuum filtration of the resulting mixture was done. The filtrated mixture was dissolved in 60 mL of absolute ethanol by the reflux apparatus and was boiled for a few minutes. Then, the solution was put in a beaker and was diluted by adding 100 mL hot benzene and 20 mL of light petroleum ether. In order to obtain crystalline of *ortho*-substituted phenylthiourea, the vacuum filtration was performed [41].

4.1.1.1. o-Tolylthiourea

o- Tolylthiourea was synthesized according to the general procedure. Starting materials are listed as the below:

- *o*-toluidine: 32.1 g (0.300 moles),
- hydrochloric acid: 37.5 mL (1.21 moles),
- ammonium thiocyanate: 25 g (0.328 moles), and
- water: 300 mL.

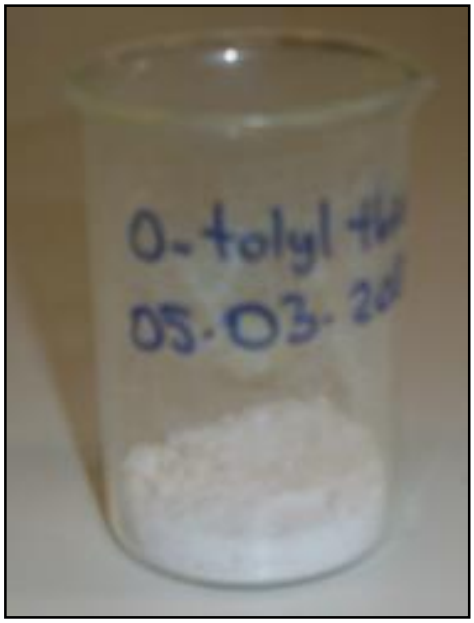


Figure 4.2. *o*-tolylthiourea

4.1.1.2. o-Fluorophenylthiourea

o-Fluorophenylthiourea was synthesized according to the general procedure. Starting materials are listed at the following:

- *o*-fluoroaniline: 33.34 g (0.30 moles),
- hydrochloric acid: 41 mL (1.325 moles),
- ammonium thiocyanate: 25 g (0.328 moles), and
- water: 300 mL.

Figure 4.3. *o*-fluorophenylthiourea

4.2. SYNTHESIS OF 5-METHYL- AND 5,5-DIMETHYL-1-(*O*-ARYL)-2-THIOBARBITURIC ACID DERIVATIVES

In the synthesis of 5-methyl-1-(*o*-aryl)-2-thiobarbituric acid and 5,5-dimethyl -1-(*o*-aryl)-2-thiobarbituric acid, appropriate malonic acid and *o*-arylthiourea were used in 1:1 ratio.

Same amount (0.011 moles) of appropriate malonic acid and *o*-arylthiourea was put into the flask. Acetyl chloride was used as solvent. The prepared mixture was heated by the help of

a reflux condenser. The reaction has been completed in approximately twenty four hours. The type of malonic acids that are dimethylmalonic acid and methylmalonic acid, determines the R' and R'' substituents on the fifth position of the heterocyclic ring (Figure 4.4). After the approximately 24 hours heating, the reaction solution was put into the beaker containing ice cubes with water. The solvent of the prepared solution was evaporated by using vacuum rotary evaporator. In order to take the residual crystalline solids more easily, approximately 10 mL of absolute ethanol was added to the flask. After removing the crystalline from the flask, residual crystalline-absolute ethanol solution was cooled down and the cold solution was filtered by using vacuum filtration to obtain the crystals of 5,5 dimethyl-1-(*o*-aryl)-2-thiobarbituric acid and 5-methyl-1-(*o*-aryl)-2-thiobarbituric acids. The obtained crystals from vacuum filtration were recrystallized to obtain purer products. For the recrystallization method, absolute ethanol was used as the solvent. The color of the formed products is white.

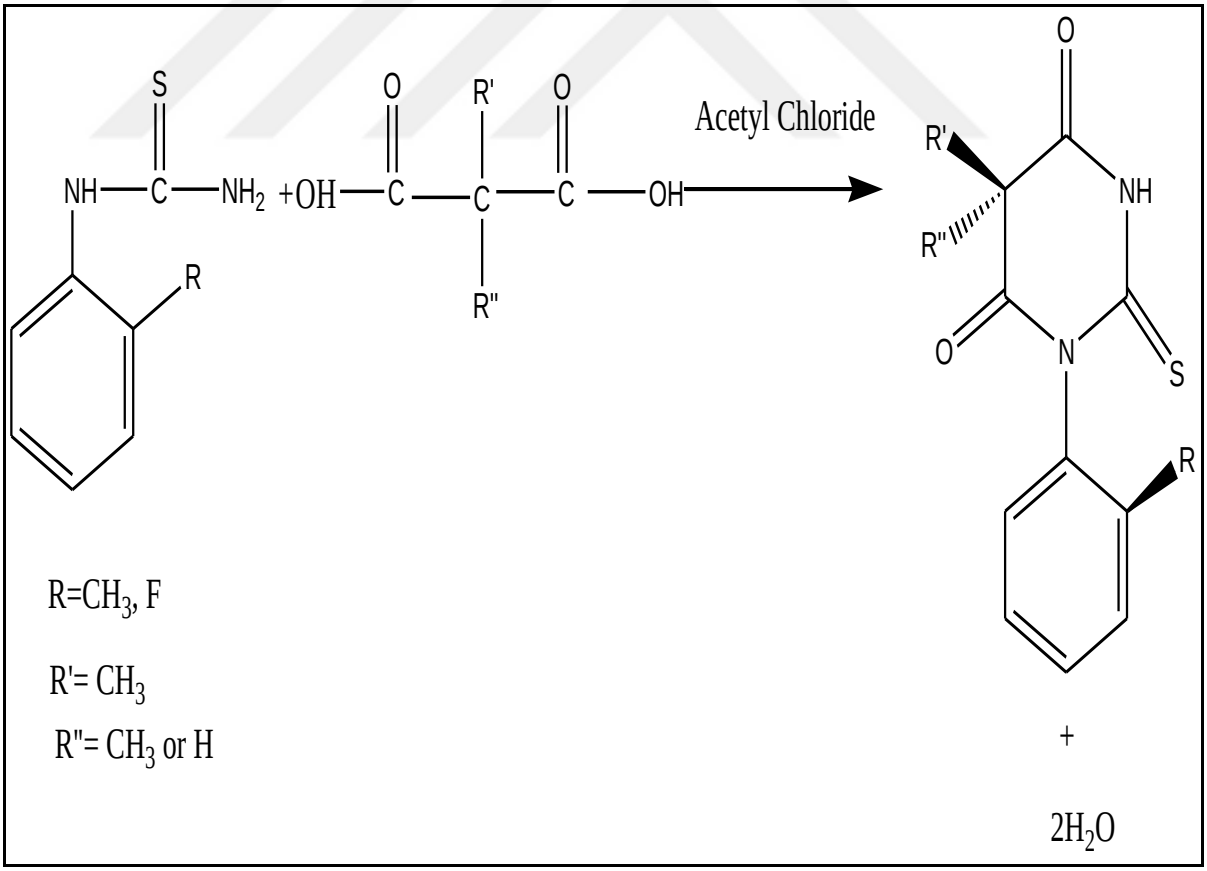


Figure 4.4. Synthesis reaction of 5-5 dimetyl-1-(*o*-aryl)-2-thiobarbituric acid and 5-methyl-1-(*o*-aryl)-2-thiobarbituric acids

4.2.1. 5-Methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid

Starting materials are listed as the following:

- *o*-fluorophenylthiourea: 1.87 g (0.011 moles),
- methylmalonic acid: 1.29 g (0.011 moles), and
- acetyl chloride: 60 mL.

4.2.2. 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric Acid

Starting materials are listed at the below:

- *o*-tolylthiourea: 1.829 g (0.011 moles),
- dimethylmalonic acid: 1.45 g (0.011 moles), and
- acetyl chloride: 60 mL.

Figure 4.5. 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid

4.3. ANALYTICAL METHODS

4.3.1. Uv-Spectroscopy Analysis Methods

Complex formation between thiobarbiturates and cyclodextrin was followed by UV spectroscopy analysis.

First saturated solutions of 1-(*o*-aryl)-2-thiobarbituric acid derivatives in different solvents were prepared in 25 mL volumetric flasks. The solvents used were 0.1 M HCl solution, distilled water and buffer solutions at different pH values.

The pHs of the buffer solutions were 1, 2.4, 3, and 4.2. First of all, the sock solution was put in the thiobarbiuric acid. Then, the solutions were shaken at 200 rpm for 30 minutes. Then, 200 μL of stock solutions were taken and were put in the 10 mL volumetric flask. Later, 10 mL was completed with buffer solutions. Dilution was made in each measurement at UV-spectroscopy. Absorbance values were measured. The absorbance values were determined in the wavelength range from 190 to 300 nm. After that, these stock solutions were put in the β-CD. The solutions were shaken then again at 200 rpm for 30 minutes. Next, 200 μL of stock solutions were taken and were put in the 10 mL volumetric flask. Then, 10 mL was completed with buffer solutions. As necessary, stock solutions were diluted with the appropriate solvent in the ratio of 9.8:0.2, v/v (solvent: stock solution), prior to analysis. This process was repeated for each measurement. Different types of cyclodextrins were added to the solutions to observe the effect of the substituents on the cyclodextrin in the complexation process. Additionally the effects of the following variables on the complexation were determined:

- the ratio between thiobarbiturates and cyclodextrins,
- time of mixing,
- concentration of thiobarbiturates, and
- pH value.

The chemicals used in this part were: sodium dihydrogen phosphate, *ortho* phosphoric acid, triethylamine, acetic acid, hydrochloric acid, derivatives of beta cyclodextrin and derivatives of the thiobarbituric acids.

4.3.1.1. Concentrations & Thermodynamic Calculations Using UV-Spectroscopy

4.3.1.1.1. Concentration Calculations Using UV-Spectroscopy

In the UV-spectroscopy analysis, Beer Lambert law was used to calculate and compare concentration of thiobarbituric acids in the solution. Molar absorptivity was calculated by measuring absorbances of saturated solution with different concentrations. These solutions were solubilized at maximum thiobarbituric acid. For these reasons, 100 µL, 300 µL, 500 µL, 700 µL, 900 µL, 1000 µL of stock solutions were taken and were put in a 10 mL volumetric flask. Then, 10 mL was completed with buffer solutions. The concentrations of the diluted solutions were measured by UV-spectroscopy. 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid and 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid were tried to be complexed with β-cyclodextrin.

The concentration of the solution in the original (stock) solution can be calculated by the Equation 4.1.

$$M = {}^{n}/_{V} \tag{4.1}$$

Sample for the calculation of Equation 4.1 is 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid.

$$m = 0.0065\ g\ of\ the\ sample$$

$$M = \frac{2.48 \times 10^{-5}\ mole}{25 \times 10^{-3}\ L}$$

$$M = 9.92 \times 10^{-4}\ mole/L$$

Determination of the concentration after the dilution is shown at the following equations. The concentration of the diluted solution M_2 can be found from the concentration of the original solution M_1 by applying the Equation 4.2.

$$M_1 \times V_1 = M_2 \times V_2 \quad (4.2)$$

$$1 \times 10^{-2}\, L \times M_2 = (9.92 \times 10^{-4}\, mole/L) \times (1 \times 10^{-4}\, L)$$

$$M_2 = 9.92 \times 10^{-6}\, mole/L$$

Determination of the concentration of thiobarbituric acid derivative in the solution containing β-cyclodextrin is displayed at the following equations. This calculation was done by applying Beer-Lambert Law (Equation 4.3).

$$A = \varepsilon \times c \times l \quad (4.3)$$

A = absorbance of dilution of 100 µL of stock solution

c = concentration of thiobarbituric acid

l = quartz cuvette dimension

ε = absorptivity

For example, the absorbance 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid (9.9:0.1, v/v) was measured as 0.005 by UV-spectroscopy. The concentration was plotted against absorbance and the concentration was calculated. This graph can be seen at Results and Discussion part (Figure 5.7, 5.8, 5.49, and 5.50).

4.3.1.1.2. Thermodynamic Calculations Using UV-Spectroscopy

The phase solubility diagram was made up according to Higuchi and Connor's method [28]. The Experiment was conducted with different aqueous media such as phosphate buffer pH 2.4 and constant temperature at 25°C and 37°C. The phase solubility curve was made up by plotting solubility of TBA (mol/L) against concentration of the β-CD (mol/L). Slope and intercept attained at each profile were used to calculate the apparent complexation constant (K_c) of the complex system from Equation 4.4. Intercept was calculated by instrinsic solubility of TBA in the absence of carrier at each temperature. In addition, the change in enthalpy (ΔH°) upon complexation between TBA and carrier was specified using Van't Hoff Equation 4.4.

$$K_{1:1} = \frac{Slope}{Intercept\ (1 - Slope)} \tag{4.4}$$

$$\ln\left(\frac{K_{37}}{K_{25}}\right) = \Delta H^{\circ} \frac{T_{37} - T_{25}}{R \times T_{37} \times T_{25}} \tag{4.5}$$

where K_{37} and K_{25} were stability constants at 37°C and 25°C respectively. T_2 and T_1 were the corresponding absolute temperatures in Kelvin. The formula of the change in Gibbs-Free energy is shown at Equation 4.6:

$$\Delta G^{\circ} = -RT \ln k \tag{4.6}$$

The formula of the entropy can be displayed at Equation 4.7:

$$\Delta S^{\circ} = \frac{\left(\Delta H^{\circ} - \Delta G^{\circ}\right)}{T} \tag{4.7}$$

Universal gas constant is represented by R and R equals to 8.314 J/mol/K.

4.3.2. HPLC Analysis

The HPLC analysis was used to check the purity of the compounds, to determine the complexation between thiobarbiturates and cyclodextrin and to control the formation of diastereomeric complexes.

4.3.2.1. Conditions

Column : Ace Column, X-Bridge column
Mobile phase : 60:40, 70:30 and 80:20 buffer solution/methanol
Mobile phase (with cyclodextrin) : methanol-buffer solutions containing Beta-CD derivatives in the concentration of 10 mmol/L.
Sample : 1.5 mg sample is dissolved in 3 mL methanol
Flow rate : 0.8 mL/min
Wavelength (λ) : 254 nm
Buffer solutions :

- Triethylamine-acetic acid buffer solution (pH = 4.2)
- Sodium dihydrogen phosphate-*ortho* phosphoric acid buffer solution (pH = 2.4)

4.3.2.2. Sample Introduction to the HPLC Column

0.0015 g of thiobarbiturate sample was weighed and dissolved in 1 mL HPLC grade methanol. Then, it is poured into vial with the help of a syringe. In this step, filtration was most significant. Syringe filter with 0.45 μm pores was used.

4.3.2.3. Preparation of Buffer Solutions

4.3.2.3.1. Triethylamine and Acetic Acid Buffer

Firstly, 8 mL of TEA was poured into a one liter volumetric flask. Then, the flask was completed to one liter with double-distilled water. In addition, ultrasonic bath was used to speed up the dissolution of the sample. After that, the pH level was adjusted to 4.2 by the addition of acetic acid with the help of a pH-meter. Then 350 mL of this mixture was poured into a 500 mL volumetric flask and 150 mL methanol was added onto it to obtain 70:30 buffer solution/methanol.

4.3.2.3.2. Sodium Dihydrogen Phosphate and Orthophosphoric Acid Buffer

Firstly, 1.7687 g of sodium dihydrogen phosphate was weighed and then were dissolved in 1 L of distilled water. In addition, ultrasonic bath was used to speed up the dissolution of the sample. After that, the pH level was adjusted to 2.4 by the addition of phosphoric acid with the help of a pH-meter. The 350 mL of this mixture was poured into a 500 mL volumetric flask and 150 mL methanol was added onto it to obtain 70:30 buffer solution/methanol.

5. RESULTS AND DISCUSSIONS

The aim of this study was to increase transport abilities of 5-substitued-1-(*o*-aryl)-2-thiobarbituric acids, which are supposed to be biologically active, in aqueous media by forming a complex with cyclodextrin hence to increase their biovailability.

In this study, two thiobarbituric acid derivatives were studied, one of them has one 5-methyl substitutent and the other has 5,5-dimethyl substitutents. Firstly the thioureas to be used in the synthesis of thiobarbiturates were synthesized: *o*-fluorophenylthiourea and *o*-tolylthiourea. Then, 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid and 5,5-dimethyl-1-(-*o*-tolyl)-2-thiobarbituric acid were synthesized from the corresponding thioureas. The occurrence of the reactions was first controlled by HPLC analysis. Then the products, thiobarbituric acid derivatives were characterized by NMR anaylsis. The purity of the reactants and products were determined by HPLC analysis.

To study the complexation of thiobarbiturates and cyclodextrin, the thiobarbituric acids and cyclodextrin derivatives were mixed at specific temperature for a specified period of time and the complexation process of the thiobarbituric acid and cyclodextrin derivatives were followed by HPLC and UV-absorption analyses.

In HPLC anaylsis, samples were taken from the mixture solution after a specified time and were given to a reversed phase column.

In the UV-spectroscopy analysis, firstly, the absorption spectra of thio-barbituric acid derivatives and β-CD were recorded, separately. Then UV-absorption of the samples from the mixture solution was taken at specified time to observe the increase in the concentration of thiobarbiturate in the aqueous solution.

5.1. HPLC ANALYSES RESULTS

HPLC anaylsis was used to control the purity of the reactants, thiourea derivatives, and the products. The synthesized thiourea derivatives, *o*-tolylthiourea and *o*-fluorophenylthiourea were analyzed by HPLC for their purity. The results can be seen in Figures 5.1 and 5.3. The products were analyzed by HPLC for their purity and also for the determination of the

complex formation. Thiobarbituric acid derivatives are chiral and have enantiomeric isomers, when they form complexes with cyclodextrin, they form diastereomeric complexes, therefore it is expected that complexation will give rise to the separation of diastereomers in the reversed phase column.

In the chromatogram of *o*-tolylthiourea (Figure 5.1) only one peak was obtained at 6 minutes during 15 minutes running time. This result showed that the synthesized compound, *o*-tolylthiourea is pure.

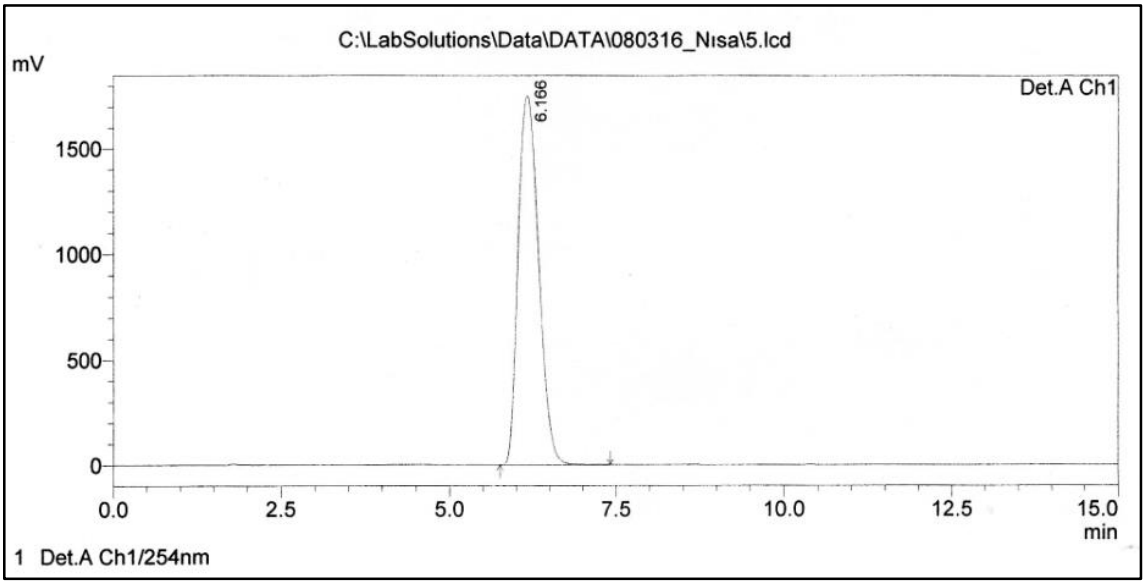


Figure 5.1. HPLC analysis of *o*-tolylthiourea (mobile phase: methanol: water, 50:50)

In the chromatogram of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid, two peaks were obtained in 30 minutes running time. However, in order to have a pure product, only one peak must be formed. However, if the two peaks were compared, the second peak at 7 minutes compared to the first peak at 4 minutes was too small. From this comparison, it was concluded that the smaller peak was negligible with respect to the first peak and the reason of the appearance of the smaller peak might be to the presence of some impurity or unreacted thiourea.

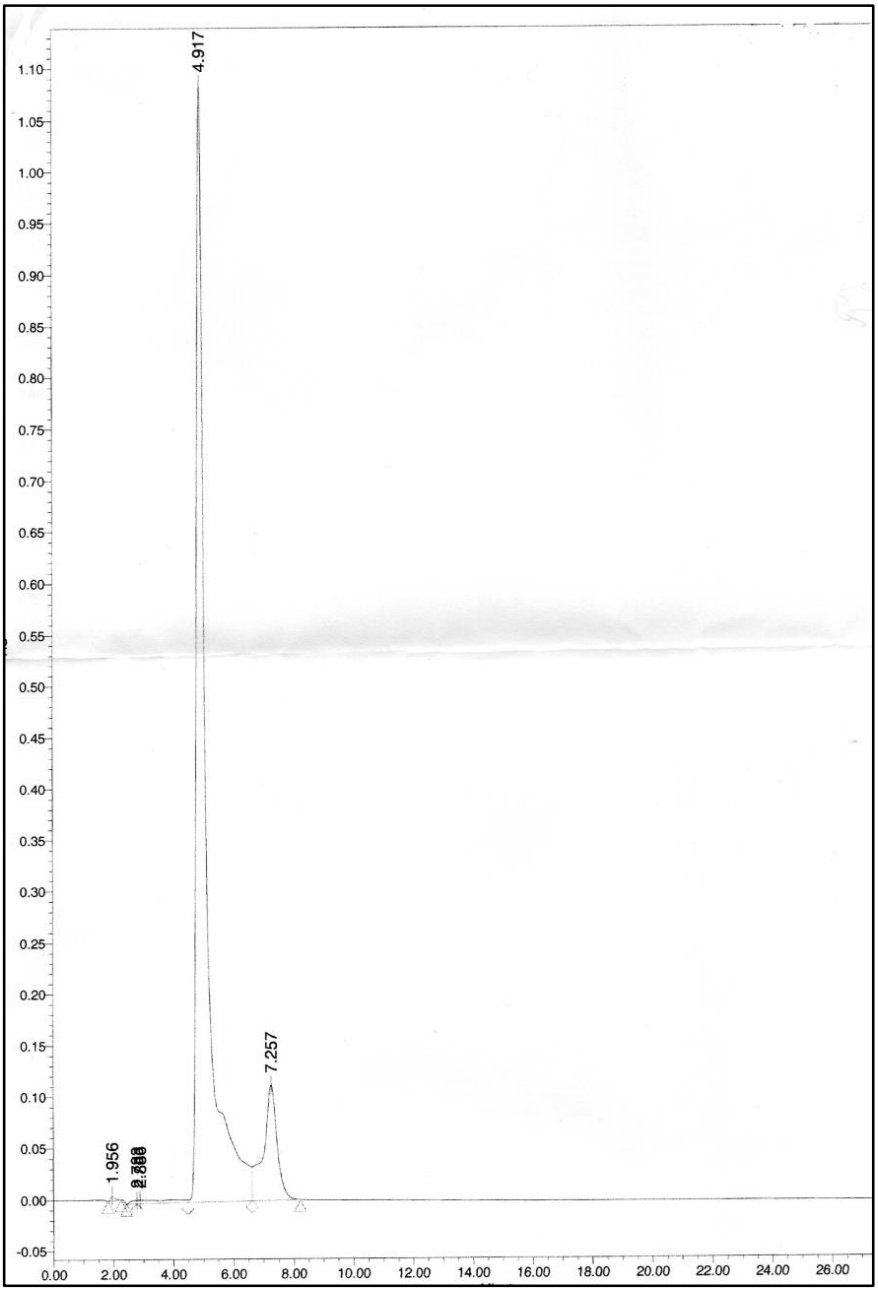


Figure 5.2. HPLC analysis of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid (mobile phase: methanol: water, 50:50)

In the chromatogram of *o*-fluorophenylthiourea (Figure 5.3), only one peak was obtained at 6 minutes during 15 minutes running time. This result showed that the synthesized compound, *o*-fluorophenylthiourea is pure.

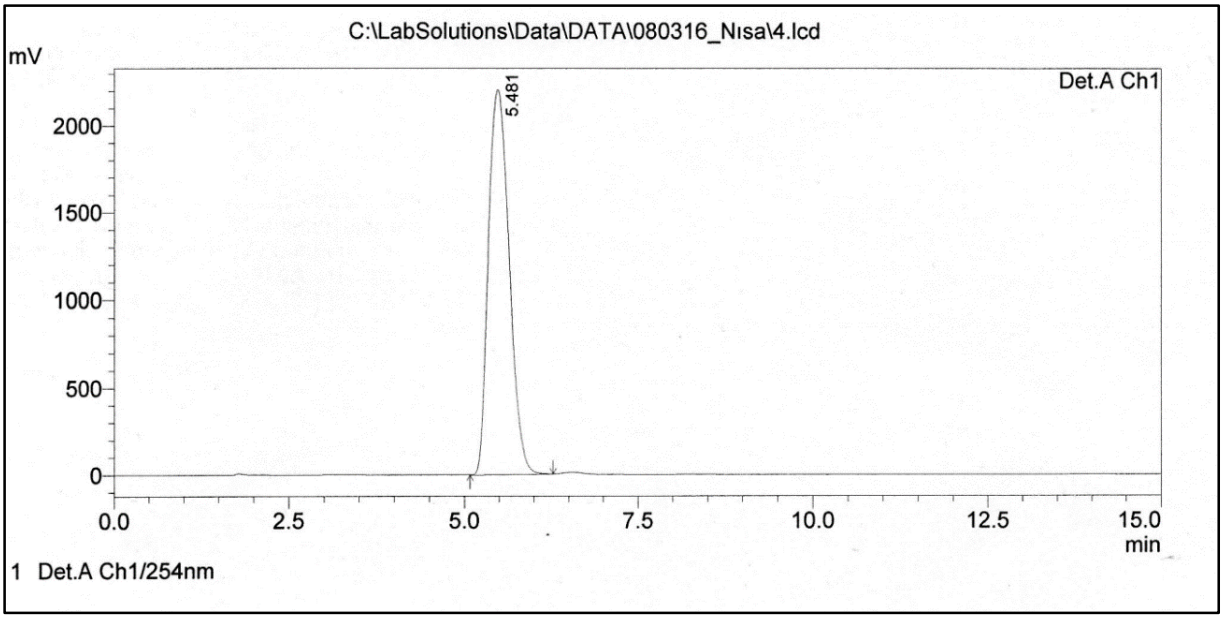


Figure 5.3. HPLC analysis of *o*-fluorophenylthiourea (mobile phase: methanol: water, 50:50)

In the chromatogram of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid (Figure 5.4), two peaks were obtained in 20 minutes running time. The first peak came in 3 minutes. The second peak came in the range of 5 and 7.5 minutes and this peak could be due to a small amount of impurity in the product. According to this result, the synthesized product, 5-methyl-1-(o-fluorophenyl)-2-thiobarbituric acids could be accepted as pure and could be used in the UV-analysis.

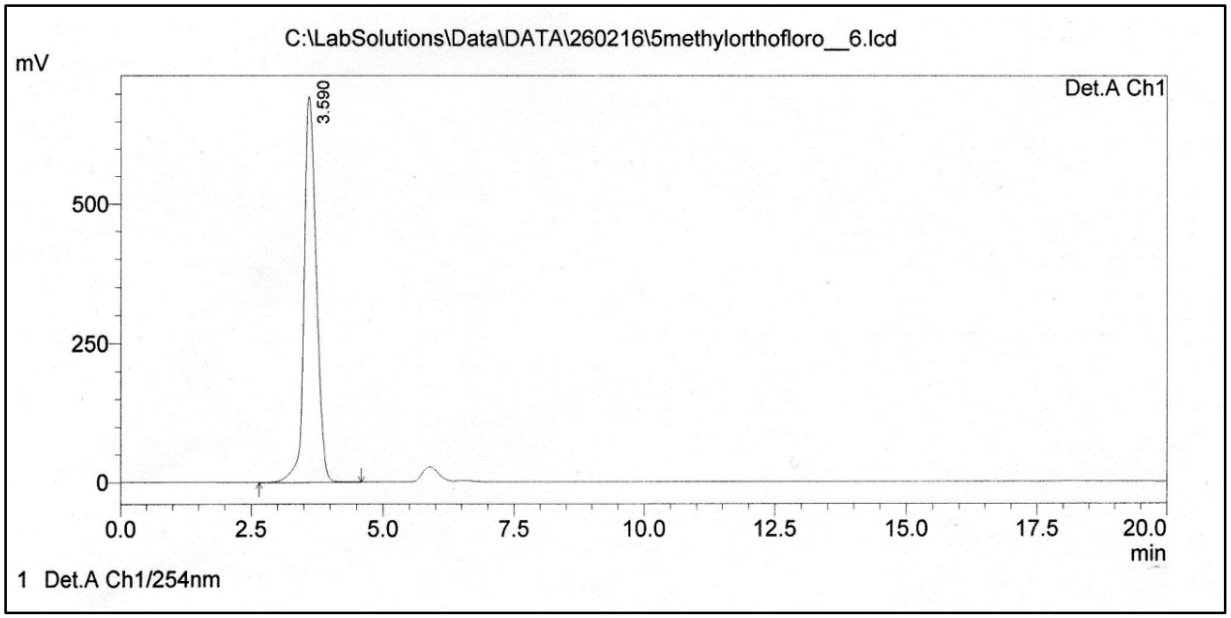
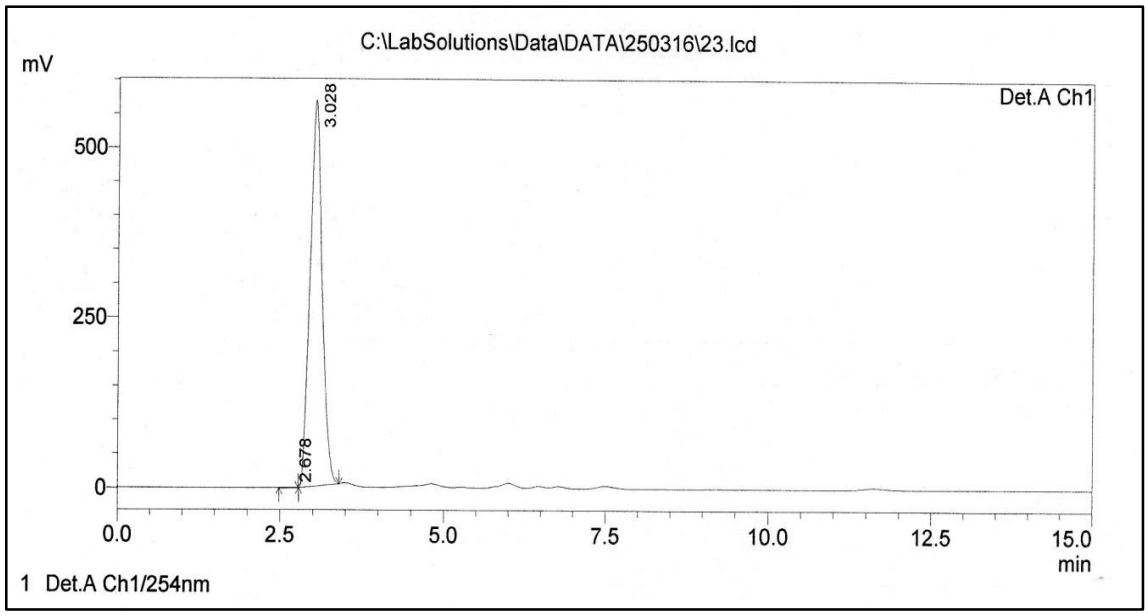


Figure 5.4. HPLC analysis of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid (mobile phase: methanol: water, 50:50)

To observe the formation of diastereomeric complexes of thiobarbituric acid derivative with β-CD, the samples from the solution in which complexation process was carried out were taken and given to the reversed phase column. At least two peaks were expected to be seen, however only one peak was seen as in Figure 5.5 and Figure 5.6. The complexation process was carried in phosphate buffer and in distilled water. Thiobarbituric acid derivative and cyclodextrin derivative were mixed (at least 24 hours) in aqueous solution, and then the samples were injected to the column. The mole ratio of thiobarbituric acid: cyclodextrin was changed and all the trials (thiobarbituric acid: cyclodextrin (by mole): 1:0.25 ratio; 1:0.5 ratio; 1:0.75 ratio; 1:1 ratio; 1:2 ratio; 1:4 ratio) were analyzed by HPLC. The chromatograms of the samples from the complexation process carried out in distilled water were given in Figure 5.5, and the chromatograms of the samples from the complexation process carried out in phosphate buffer were given in Figure 5.6.

(a)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250
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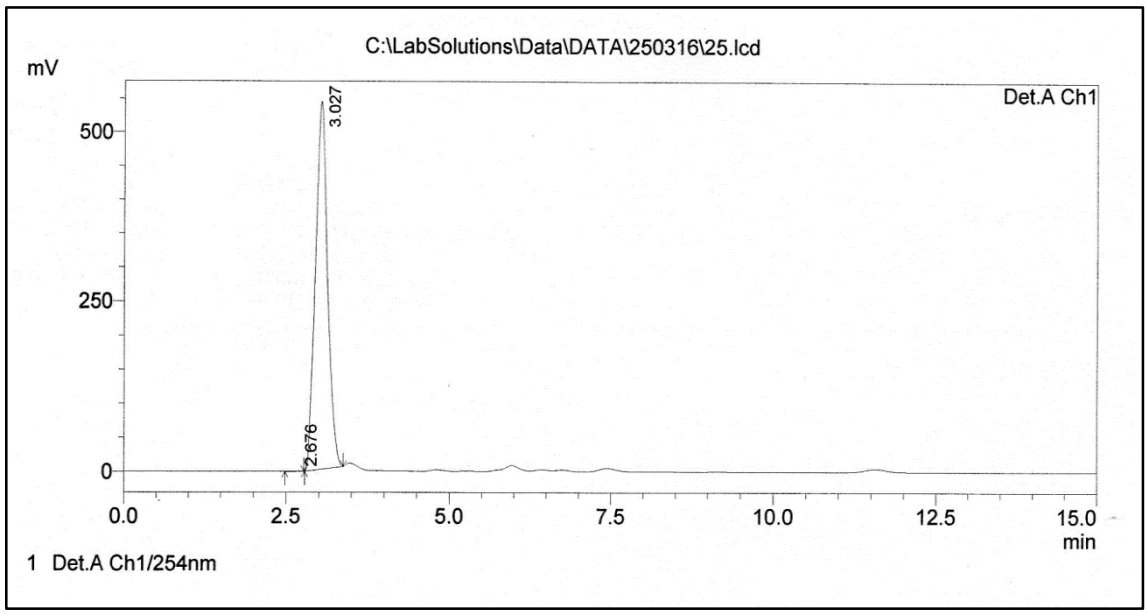
2.5
5.0
7.5
10.0
12.5
15.0
min
1 Det.A Ch1/254nm

(b)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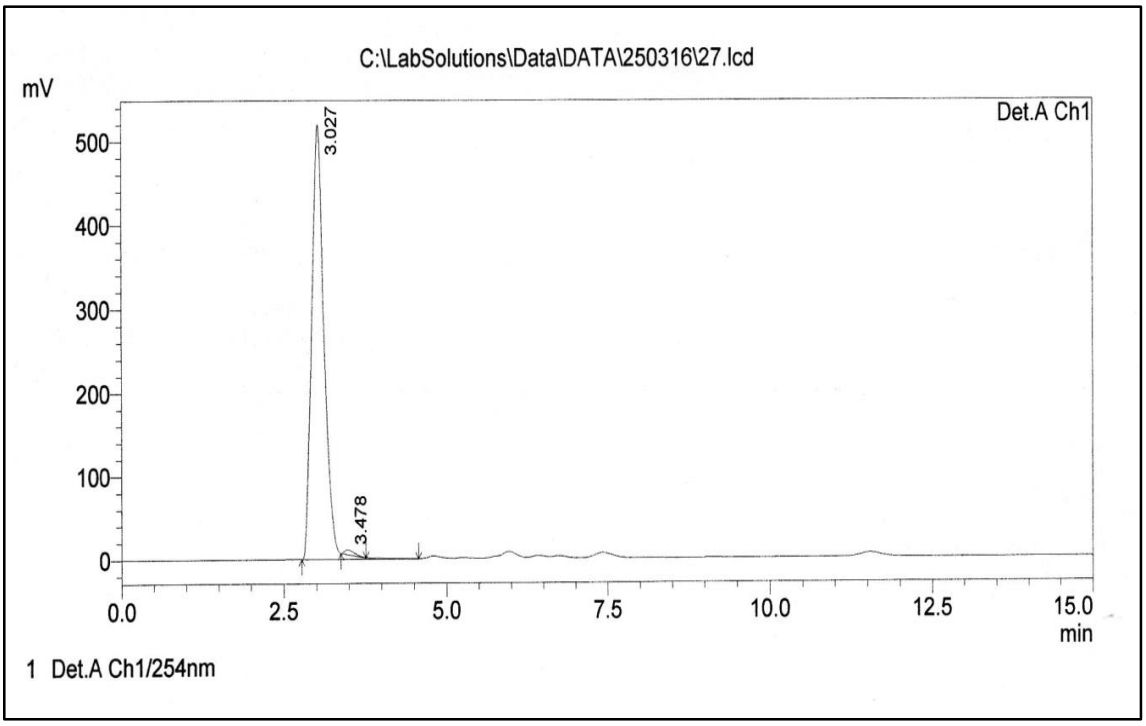
min
1 Det.A Ch1/254nm

(c)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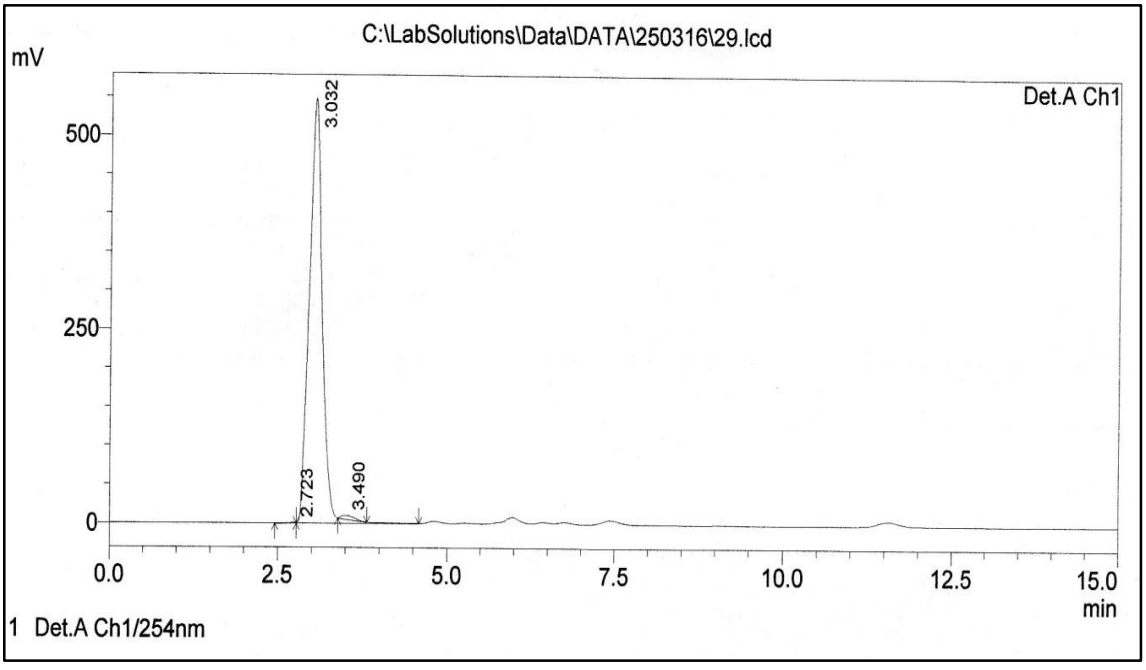
2.5
5.0
7.5
10.0
12.5
15.0
min
1 Det.A Ch1/254nm

(d)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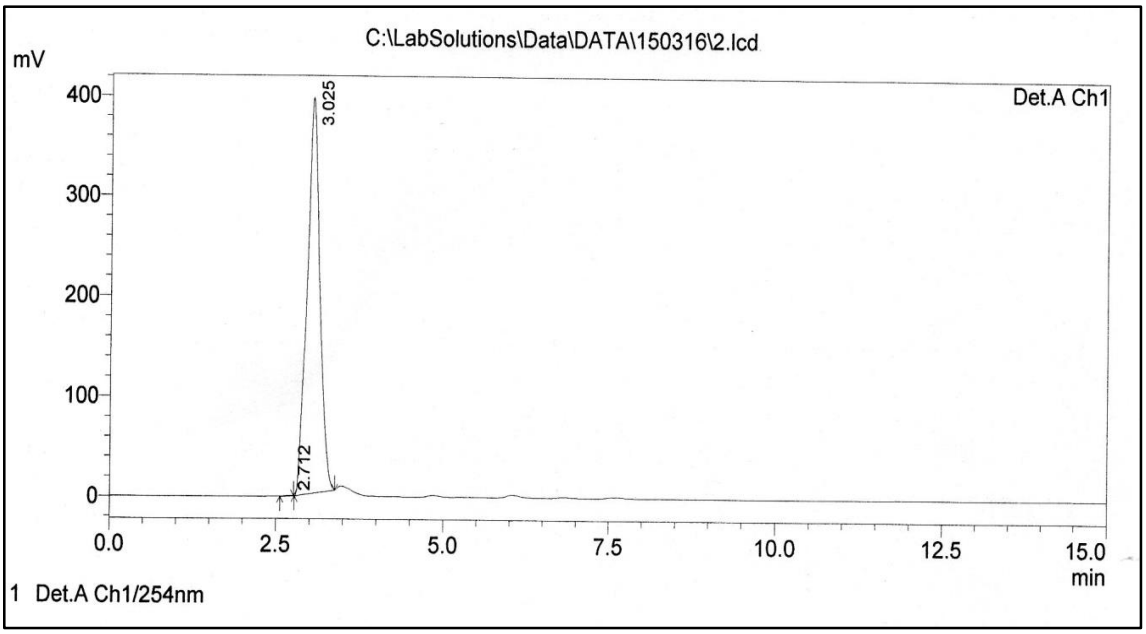
5.0
7.5
10.0
12.5
15.0
min
1 Det.A Ch1/254nm

(e)



(f)

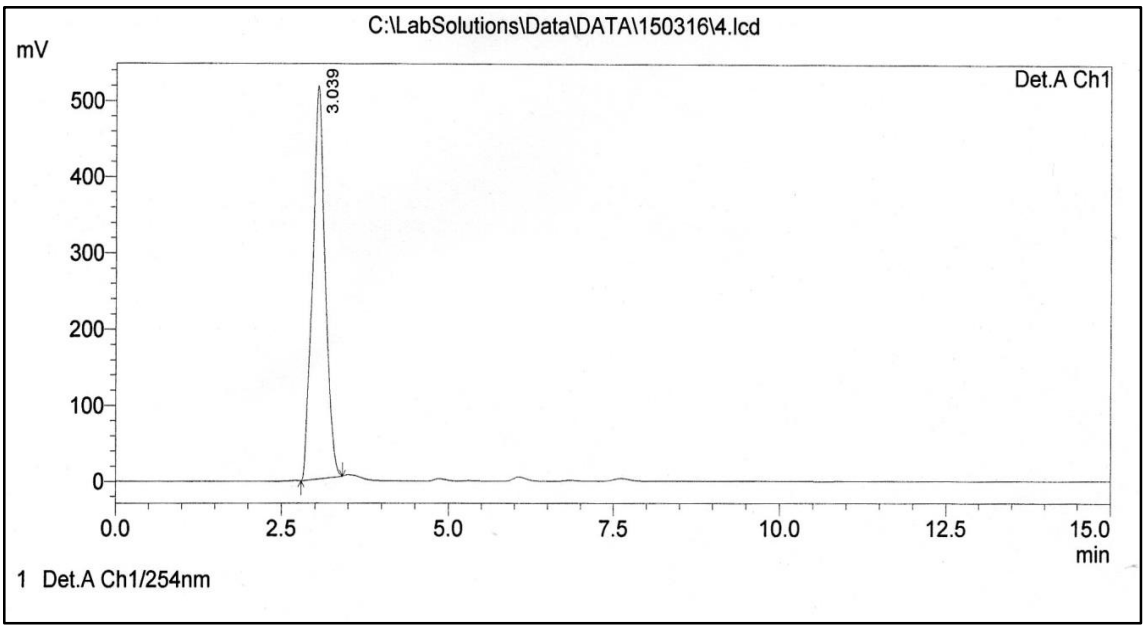
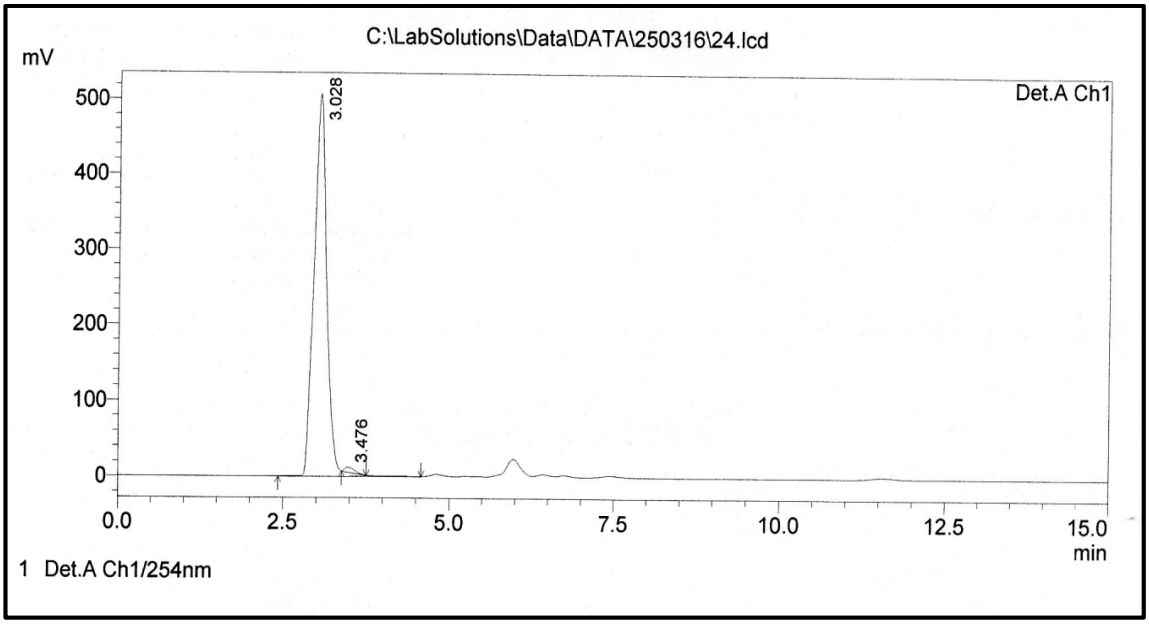


Figure 5.5. HPLC chromatograms of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex in distilled water (mobile phase: (70 per cent phosphate buffer: 30 per cent methanol); thiobarbituric acid: cyclodextrin by mole (a) 1:0.25 ratio, (b) 1:0.5 ratio, (c) 1:0.75 ratio, (d) 1:1 ratio, (e) 1:2 ratio, (f) 1:4 ratio

(a)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Det.A Ch1
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400
300
200
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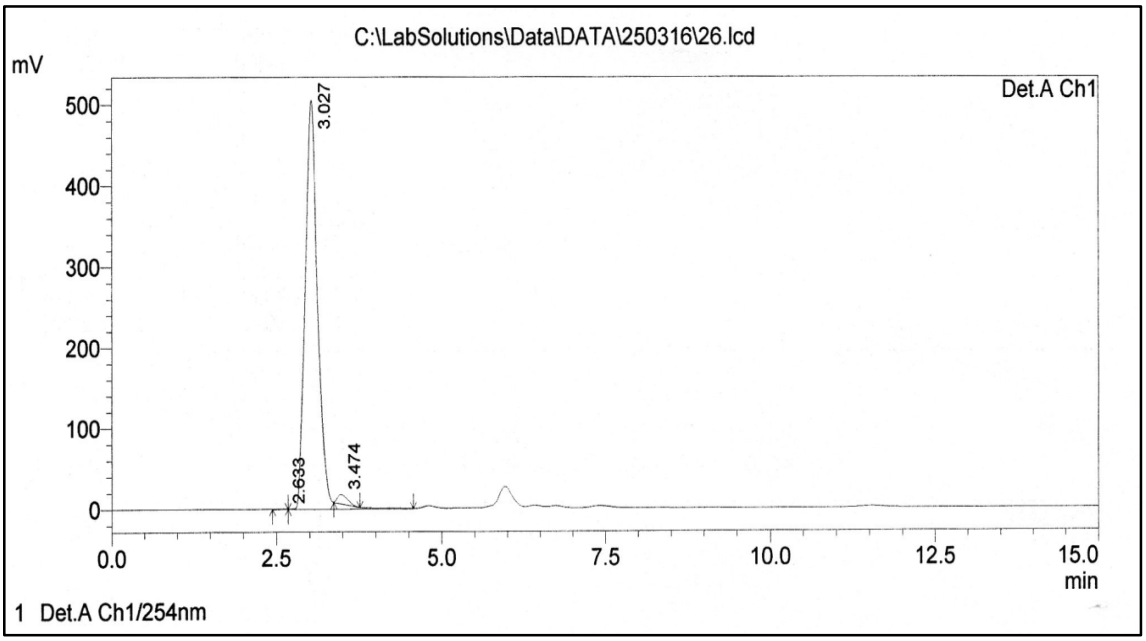
5.0
7.5
10.0
12.5
15.0
min
1 Det.A Ch1/254nm

(b)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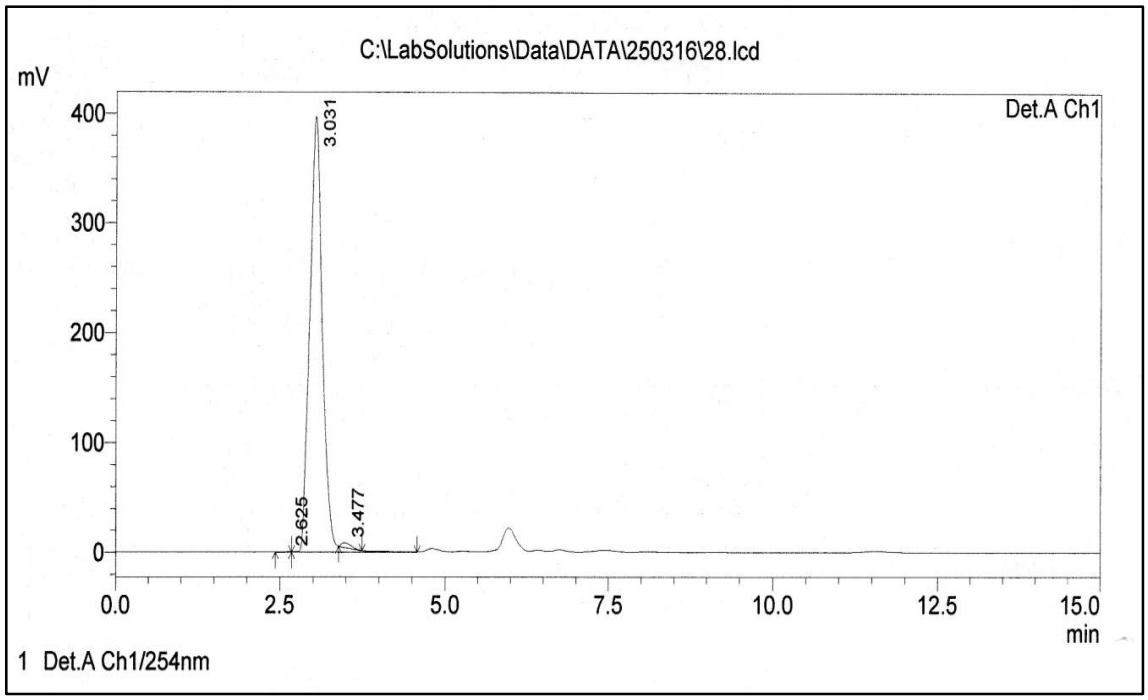
200
100
0
0.0
2.5
5.0
7.5
10.0
12.5
15.0
min
1 Det.A Ch1/254nm

(c)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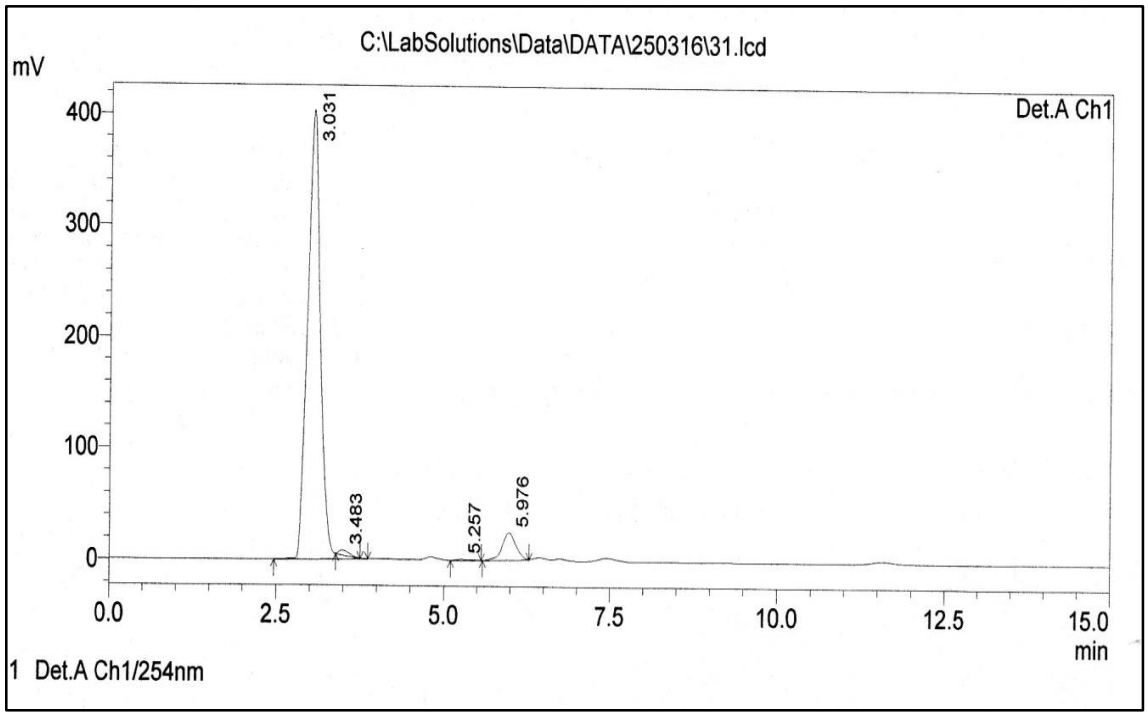
5.0
7.5
10.0
12.5
15.0
min
1 Det.A Ch1/254nm

(d)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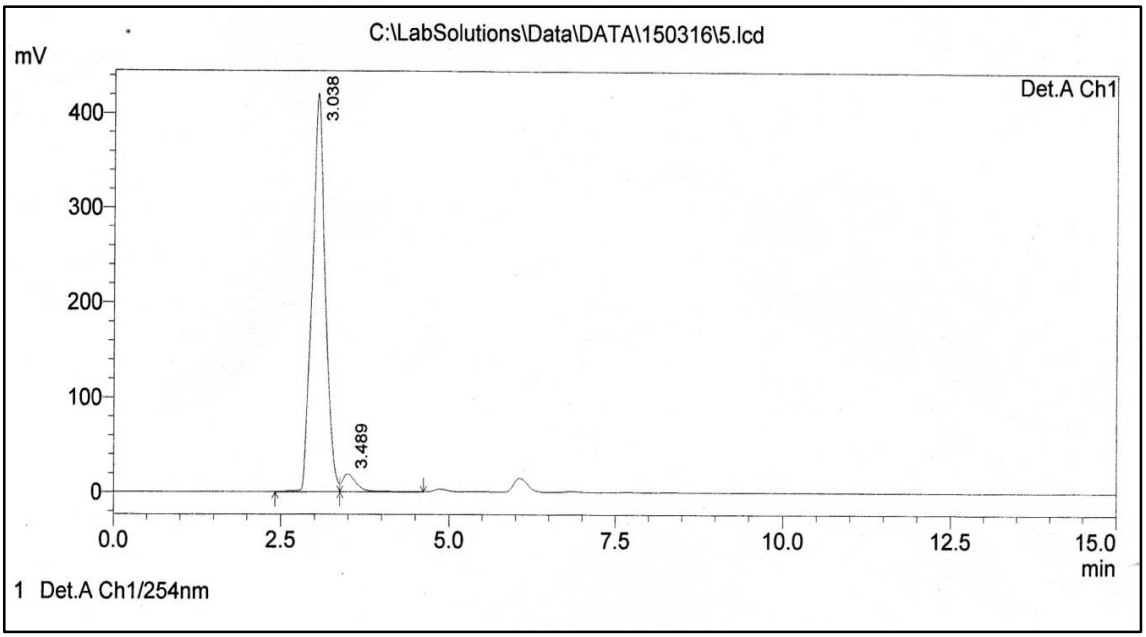
15.0
min
1 Det.A Ch1/254nm

(e)



(f)

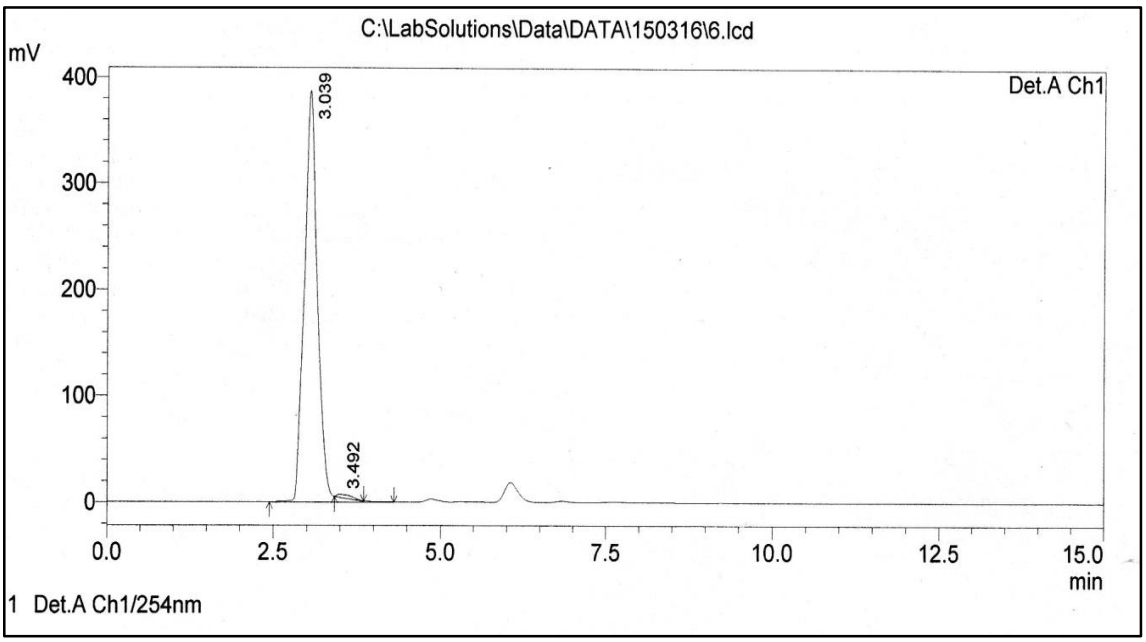


Figure 5.6. HPLC chromatograms of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex in phosphate buffer (mobile phase:(70 per cent phosphate buffer: 30 per cent methanol); thiobarbituric acid: cyclodextrin, by mole (a) 1:0.25 ratio, (b) 1:0.5 ratio, (c) 1:0.75 ratio, (d) 1:1 ratio, (e) 1:2 ratio, (f) 1:4 ratio

5.2. CHARACTERIZATION OF THIBARBITURIC ACID DERIVATIVES/NMR RESULTS

In the ^{1}H NMR spectrum of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid (Figure 5.7), two quartets for the proton at C-5, two doublets peaks for the methyl protons at C-5 and one singlet for the of NH proton were observed. The assignments of the peaks were given in Table 5.95. Plus, the water peak of acetone solvent was observed at 2.97 ppm [45].

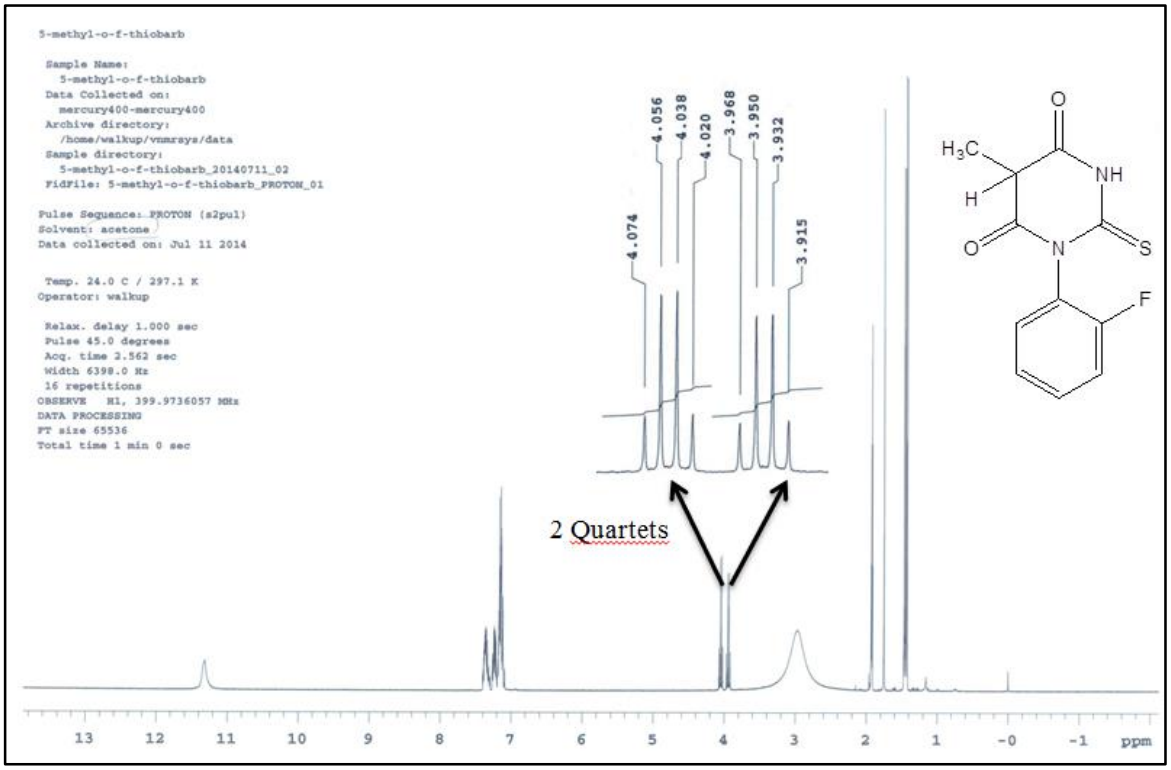


Figure 5.7. ^{1}H NMR spectrum of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid ($C_{11}H_9FN_2O_2S$): NMR solvent: acetone-d_6

Table 5.1. ^{1}H NMR (400 MHz) data of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid, solvent: acetone-d_6

Multiplicity, Number of Protons	**δ (ppm)**
(s, 1 H)	11.32
(m, 4 H)	7.396-7.087
(q, J=7.2 Hz and J=7.2Hz, 1 H)	4.047 & 3.942
(d, J=7.2 Hz and J=7.2 Hz, 3 H)	1.4571.431

Table 5.2. ^{1}H NMR (400 MHz) data of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid, ($CDCl_3$) [41]

Multiplicity, Number of Protons	**δ (ppm)**
(b, 1 H)	9.08
(m, 4 H)	7.04-7.39
(s, 3H)	2.16
(s, 3H)	1.70
(s, 3H)	1.69

5.3. UV-ABSORPTION ANALYSES

In the UV-absorption analyses, first the UV-spectra of thiobarbituric acid derivatives and cyclodextrin derivative were taken. As seen from Figure 5.7, β-CD had no absorption in the range of 190-300 nm. Therefore it was concluded, the absorption curve belongs only to thiobarbituric acid derivative. As explained in Materials and Methods section (4.3.1), thiobarbituric acid and cyclodextrin were mixed for a specific period of time, then the increase in absorption was measured, which is due to increase in the concentration of

thiobarbituric acid. Thiobarbituric acid-cyclodextrin complex is more soluble in water, than thiobarbituric itself, thus increase in absorption of thiobarbituric acid was observed.

The effect of different variables on the concentration, consequently on the solubility of thiobarbituric acid in aqueous medium was determined by UV-spectroscopy. The effect of ratio of thiobarbituric acid: cyclodextrin, mixing time, temperature structure of cyclodextrin and pH of the aqueous solution were studied.

First saturated solutions of 1-(*o*-aryl)-2-thiobarbituric acid derivatives in different solvents (distilled water, HCl solution, phosphate buffer and TEA buffer) were prepared in 25 mL volumetric flasks. (The pH values of the HCl, phosphate buffer distilled water and TEA buffer solutions were 1.0, 2.4, 3.0 and 4.2 respectively). First of all, the stock solutions (1.0mM) of the thiobarbituric acid were prepared. Then, the solutions were shaken at 200 rpm for 30 minutes. Then, 200 μL of stock solutions were taken and were put in the 10 mL volumetric flask. Later, 10 mL volumetric flasks were completed with buffer solutions, so (1.0mM) solutions were obtained. (Dilution was made for each measurement at UV-spectroscopy). Then the absorbance values of these solutions were determined in the wavelength range from 190nm to 300 nm. After that, the stock solutions (1.0 mM) were mixed with appropriate amount of β-CD. The solutions were shaken then at 200 rpm for 30 minutes. Next, 200 μL of stock solutions were taken and were put in the 10 mL volumetric flask. Again, 10 mL was completed with buffer solutions, so dilution was done in the the ratio of 9.8:0.2, v/v (solvent: stock solution), prior to analysis to obtain 1.0mM solutions. This process was repeated for each measurement.

In Table 5.3-5.6 calculated concentrations of 5-5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid and 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid without β-CD in d.water and phosphate buffer, 0.1M HCl and TEA buffer were shown. The graphs of the absorbance vs. concentration of these thiobarbituric acid derivatives in these solutions were plotted (Figure 5.8 - 5.13) and from the data of these graphs, molar absorptivity values of thiobarbituric acids in these solutions were found as 26557 M^{-1} $cm^{-1}$and 14767 M^{-1} cm^{-1} for 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid, in distilled water and phosphate buffer, respectively, and as, 13747 M^{-1} cm^{-1}, 10364 M^{-1} cm^{-1}, 488.01 M^{-1} cm^{-1} and 360.28 M^{-1} cm^{-1} for 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid in distilled water, phosphate buffer, 0.1M HCl and TEA buffer, respectively (calculation methods were described in Section 4.4.1.1).

Table 5.3. Absorbance & concentration results of control study 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid in distilled water

C (mol\L)	A
$9.92x10^{-6}$	0.005
$2.98x10^{-5}$	0.2112
$4.96x10^{-5}$	0.7724
$6.94x10^{-5}$	1.4557
$8.93x10^{-5}$	1.9344

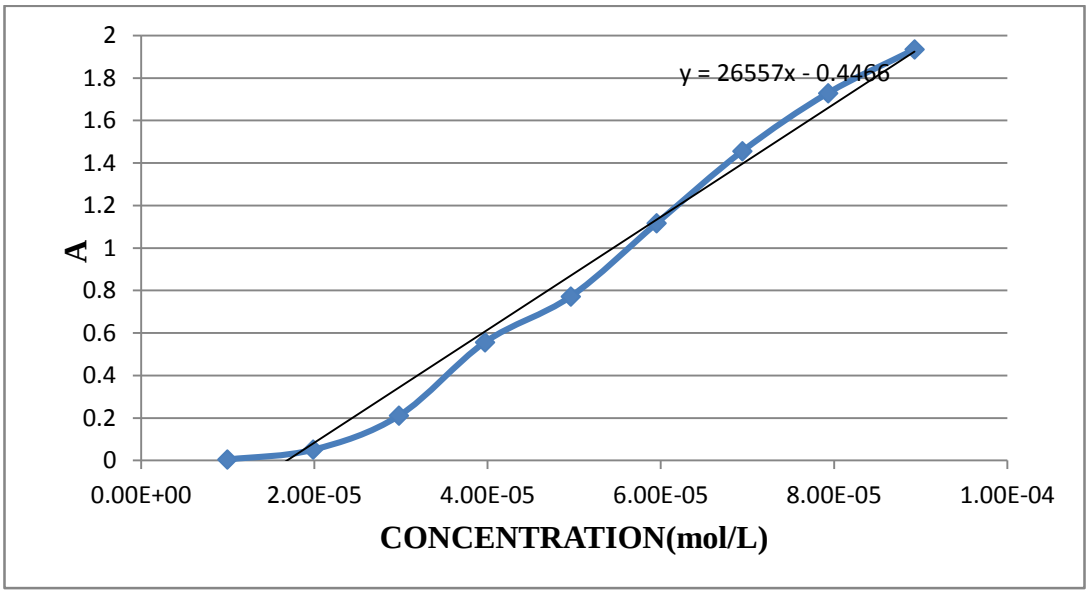


Figure 5.8. Absorbance vs. concentration graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid used for the calculation of molar absorptivity in distilled water

Table 5.4. Absorbance & concentration results of control study 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid in phosphate buffer

C (mol\L)	A
$9.92x10^{-6}$	0.4435
$2.98x10^{-5}$	0.5022
$4.96x10^{-5}$	0.7203
$6.94x10^{-5}$	1.2005
$8.93x10^{-5}$	1.5175
$9.92x10^{-5}$	1.6354

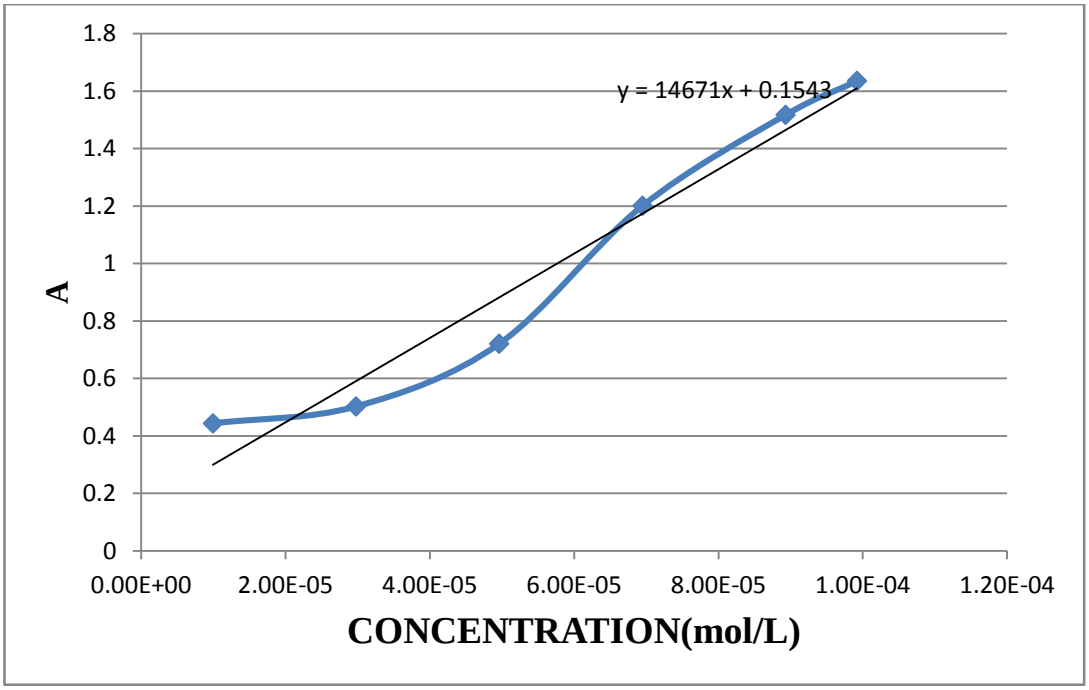


Figure 5.9. Absorbance vs. concentration graph of 5-5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid used for calculation of molar absorptivity in phosphate buffer

Table 5.5. Absorbance & concentration results of control study 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid in distilled water

C (mol\L)	A
$9.92x10^{-6}$	0.4014
$2.98x10^{-5}$	0.6562
$4.96x10^{-5}$	1.0175
$6.94x10^{-5}$	1.3243
$8.93x10^{-5}$	1.5308
$9.92x10^{-5}$	1.5722

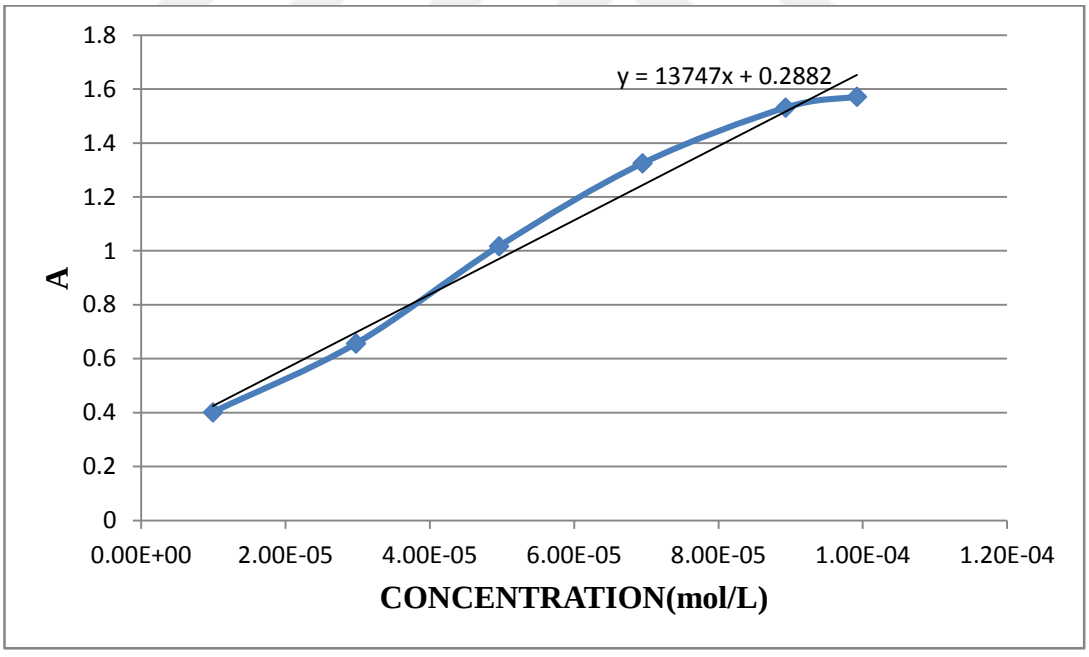


Figure 5.10. Absorbance vs. concentration graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid used for calculation of molar absorptivity in distilled water

Table 5.6. Absorbance & concentration results of control study 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid in phosphate buffer

C (mol\L)	A
$9.92x10^{-6}$	0.6406
$2.98x10^{-5}$	0.7349
$4.96x10^{-5}$	0.9688
$6.94x10^{-5}$	1.23
$8.93x10^{-5}$	1.4341
$9.92x10^{-5}$	1.5033

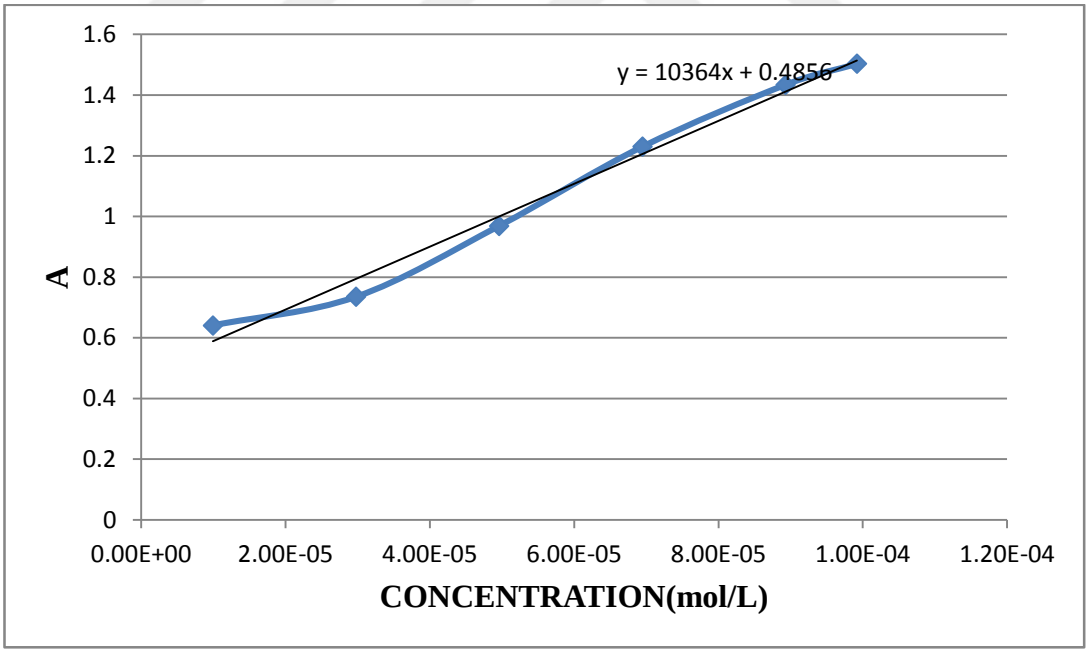


Figure 5.11. Absorbance vs. concentration graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid used for calculation of molar absorptivity in phosphate buffer

Table 5.7. Absorbance & concentration results of control study 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid in 0.1 M HCl

C (mol/L)	A
$9.92x10^{-6}$	0.4559
$2.98x10^{-5}$	0.4671
$4.96x10^{-5}$	0.4757
$6.94x10^{-5}$	0.4781
$8.93x10^{-5}$	0.4974
$9.92x10^{-5}$	0.5004

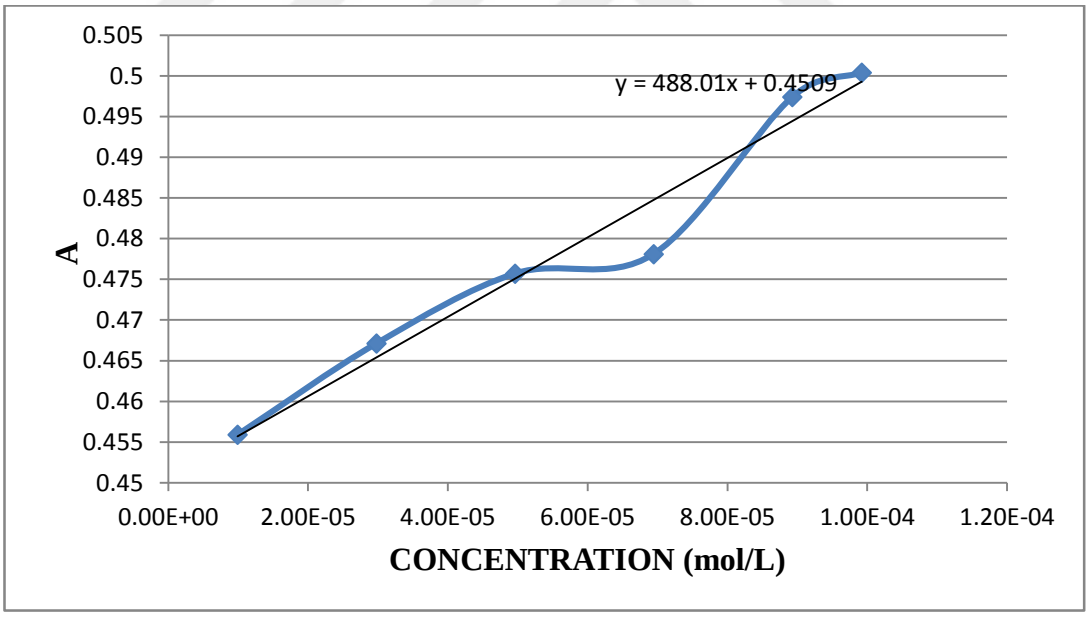


Figure 5.12. Absorbance vs. concentration graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid used for calculation of molar absorptivity in 0.1 M HCl

Table 5.8. Absorbance & concentration results of control study 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid TEA buffer

C (mol/L)	A
$9.92x10^{-6}$	0.3904
$2.98x10^{-5}$	0.4033
$4.96x10^{-5}$	0.4054
$6.94x10^{-5}$	0.4083
$8.93x10^{-5}$	0.4219
$9.92x10^{-5}$	0.4254

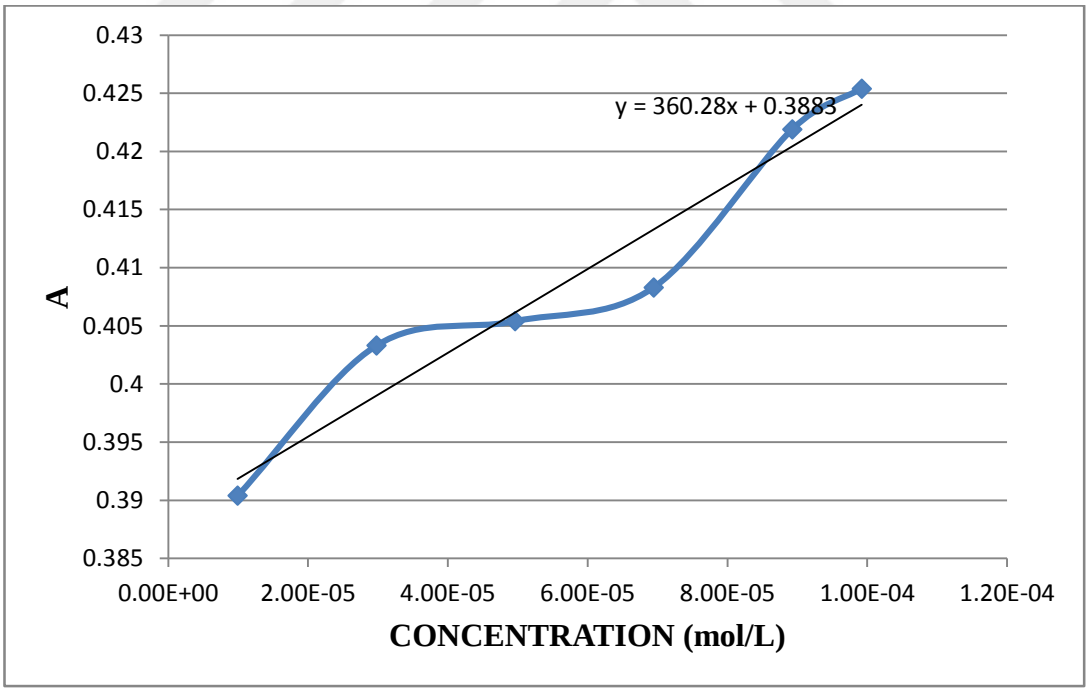


Figure 5.13. Absorbance vs. concentration graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid used for calculation of molar absorptivity in TEA buffer

5.3.1. Proof of Thiobarbituric acid-Cyclodextrin Compex Formation

5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid solution without β-CD and with β-CD were studied at 24 hours mixing time as explained in Section 4.4.4.1. Absorbance values at 190 nm where characteristic peak of thiobarbituric acid can be seen, were measured to determine the maximum concentration of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid in distilled water and phosphate buffer. The measurements were done for two trials. In each measurement, the same solution was measured three times, and the average absorbance was calculated as described in Section (4.3.1.1.1). The results from the measurement in distilled water are given in Table 5.9 and Table 5.10.

Table 5.9.Concentration of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid without and with β-CD at 24 hours in distilled water (37ºC) (1st trial)

Time (h)	**Type of solution**	**Concentration of TBA (mole/L)**	
		Without β-CD	**With β-CD**
0	D. water + TBA	1.4081×10^{-5}	1.9554×10^{-5}
0.5	D. water + TBA	1.6576×10^{-5}	2.1030×10^{-5}
1	D. water + TBA	1.8189×10^{-5}	2.5758×10^{-5}
2	D. water + TBA	2.2535×10^{-5}	3.3176×10^{-5}
3	D. water + TBA	2.8559×10^{-5}	3.3466×10^{-5}
23	D. water + TBA	3.2150×10^{-5}	3.4061×10^{-5}
24	D. water + TBA	3.1704×10^{-5}	3.4959×10^{-5}

Table 5.10. Concentration of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid without and with β-CD at 24 hours in distilled water (37ºC) (2nd trial)

Time (h)	Type of solution	Concentration of TBA (mole/L)	
		Without β-CD	With β-CD
0	D. water + TBA	1.4102×10^{-5}	1.9338×10^{-5}
0.5	D. water + TBA	1.6414×10^{-5}	2.1040×10^{-5}
1	D. water + TBA	1.8204×10^{-5}	2.5699×10^{-5}
2	D. water + TBA	2.2600×10^{-5}	3.3127×10^{-5}
3	D. water + TBA	2.9085×10^{-5}	3.3381×10^{-5}
23	D. water + TBA	3.2282×10^{-5}	3.4074×10^{-5}
24	D. water + TBA	3.1655×10^{-5}	3.4981×10^{-5}

The results form the measurements in phosphate buffer are given in Table 5.11 and Table 5.12.

Table 5.11. Concentration of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid without and with β-CD at 24 hours in phosphate buffer (37ºC) (1st trial)

Time (h)	Type of solution	Concentration of TBA (mole/L)	
		Without β-CD	With β-CD
0	Phosphate Bf + TBA	2.0571×10^{-5}	2.7142×10^{-5}
0.5	Phosphate Bf + TBA	2.7864×10^{-5}	3.1191×10^{-5}
1	Phosphate Bf + TBA	$3.4197 \times 10^{-5}5$	3.8777×10^{-5}
2	Phosphate Bf + TBA	4.5062×10^{-5}	5.2457×10^{-5}
3	Phosphate Bf + TBA	4.9744×10^{-5}	6.0507×10^{-5}
23	Phosphate Bf + TBA	5.2573×10^{-5}	5.9689×10^{-5}
24	Phosphate Bf + TBA	5.5286×10^{-5}	6.2307×10^{-5}

Table 5.12. Concentration of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid without and with β-CD at 24 hours in phosphate buffer (37ºC) (2nd trial)

Time (h)	**Type of solution**	**Concentration of TBA (mole/L)**	
		Without β-CD	**With β-CD**
0	Phosphate Bf + TBA	2.1655×10^{-5}	2.7012×10^{-5}
0.5	Phosphate Bf + TBA	2.7667×10^{-5}	3.1082×10^{-5}
1	Phosphate Bf + TBA	3.543×10^{-5}	3.9084×10^{-5}
2	Phosphate Bf + TBA	4.4925×10^{-5}	5.2594×10^{-5}
3	Phosphate Bf + TBA	4.9165×10^{-5}	6.0453×10^{-5}
23	Phosphate Bf + TBA	5.2471×10^{-5}	5.9826×10^{-5}
24	Phosphate Bf + TBA	5.4645×10^{-5}	6.2293×10^{-5}

When cyclodextrin and thiobarbituric acid derivative were mixed in the distilled water and phosphate buffer, TBA concentration increased in appreciable amount in comparison with the concentration of TBA in solution without cyclodextrin. This was accepted as a proof of cyclodextrin and TBA complex formation.

5.3.2. Factor Affecting Complexation Ratio of CD

The effects of the following variables on the complexation were determined:

- solvent effect,
- time factor,
- temperature
- TBA: cyclodextrin ratio,
- structure of β-CD

5.3.2.1. Solvent Effect

First thiobarbituric acid derivative was left for a specific time period in distilled water, phosphate buffer TEA, and 0.1 M HCl solutions to examine the solvent effect o n the complex formation. The absorbance of thiobarbituric acid derivative was measured in all solutions to conclude in which solution the complexation occurs at highest rate. The absorbance vs. time graphs are shown in Figure 5.14-5.21.

All complexation process in this section was studied for 24 hours mixing time as explained in Section 4.4.1.1. Absorbance values at 190 nm were measured to follow the increase in the concentration of the thiobarbituric acid in specified solvent. The measurements were done for two trials. In each measurement, the same solution was measured three times, and the average absorbance was calculated as described in Section (4.3.1.1).

First 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complexation was studied as described in distilled water (pH=3.0). The results are given in Table 5.13, Table 5.14 and Figure 5.14.

Table 5.13. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:1 ratio) in distilled water (37ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	D. water + TBA	0.45385	$3.3014x10^{-5}$
0.5	D. water+TBA+βCD	0.56935	$4.1416x10^{-5}$
1	D. water+TBA+βCD	0.5927	$4.3115x10^{-5}$
2	D. water+TBA+βCD	0.60245	$4.3824x10^{-5}$
3	D. water+TBA+βCD	0.55025	$4.0027x10^{-5}$
23	D. water+TBA+βCD	0.5434	$3.9529x10^{-5}$
24	D. water+TBA+βCD	0.5577	$4.0569x10^{-5}$

Table 5.14. . Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:1 ratio) in distilled water (37ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.44835	3.2614×10^{-5}
0.5	D. water+TBA+βCD	0.5672	4.1260×10^{-5}
1	D. water+TBA+βCD	0.5918	4.3049×10^{-5}
2	D. water+TBA+βCD	0.60185	4.3780×10^{-5}
3	D. water+TBA+βCD	0.5461	3.9725×10^{-5}
23	D. water+TBA+βCD	0.5419	3.9420×10^{-5}
24	D. water+TBA+βCD	0.5572	4.0532×10^{-5}

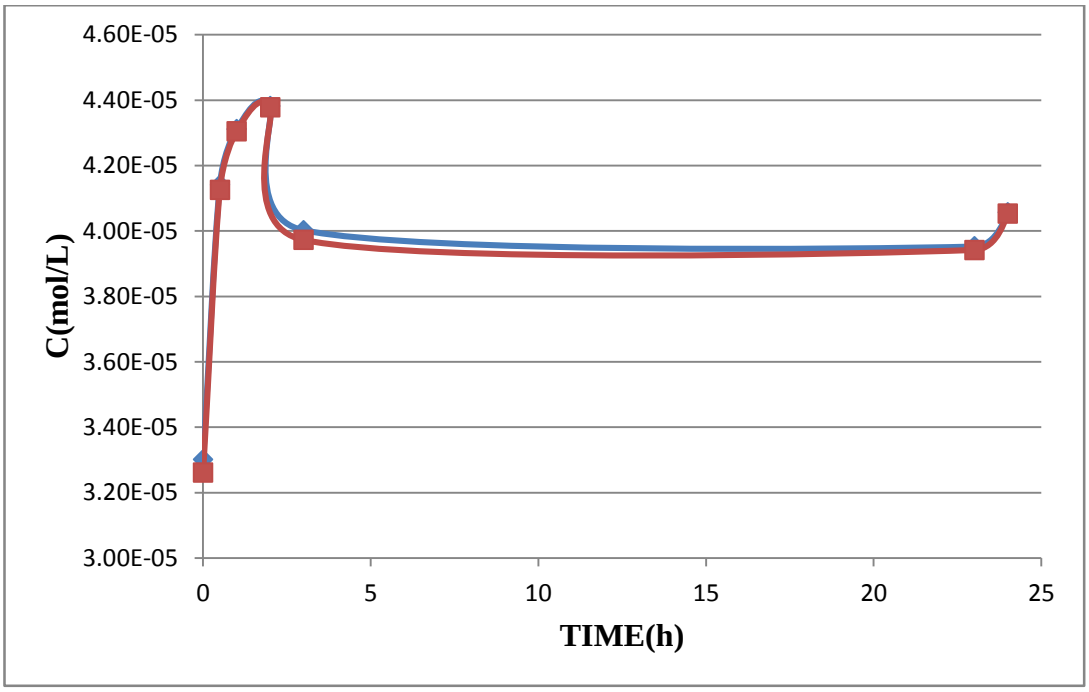


Figure 5.14. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:1 ratio) in distilled water (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complexation was also studided in phosphate buffer (pH=2.4). The results are given in Table 5.15, Table 5.16 and Figure 5.15.

Table 5.15. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:1 ratio) in phosphate buffer (37ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.53665	$5.1780x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.6182	$5.9649x10^{-5}$
1	Phosphate Bf+TBA+βCD	0.69025	$6.6601x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.66795	$6.4449x10^{-5}$
3	Phosphate Bf+TBA+βCD	0.6304	$6.0826x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.56325	$5.4347x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.59755	$5.7656x10^{-5}$

Table 5.16. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:1 ratio) in phosphate buffer (37ºC) (2nd trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.53475	$5.1597x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.61555	$5.9393x10^{-5}$
1	Phosphate Bf+TBA+βCD	0.69385	$6.6948x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.6628	$6.3952x10^{-5}$
3	Phosphate Bf+TBA+βCD	0.6296	$6.0749x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.56865	$5.4868x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.59065	$5.6991x10^{-5}$

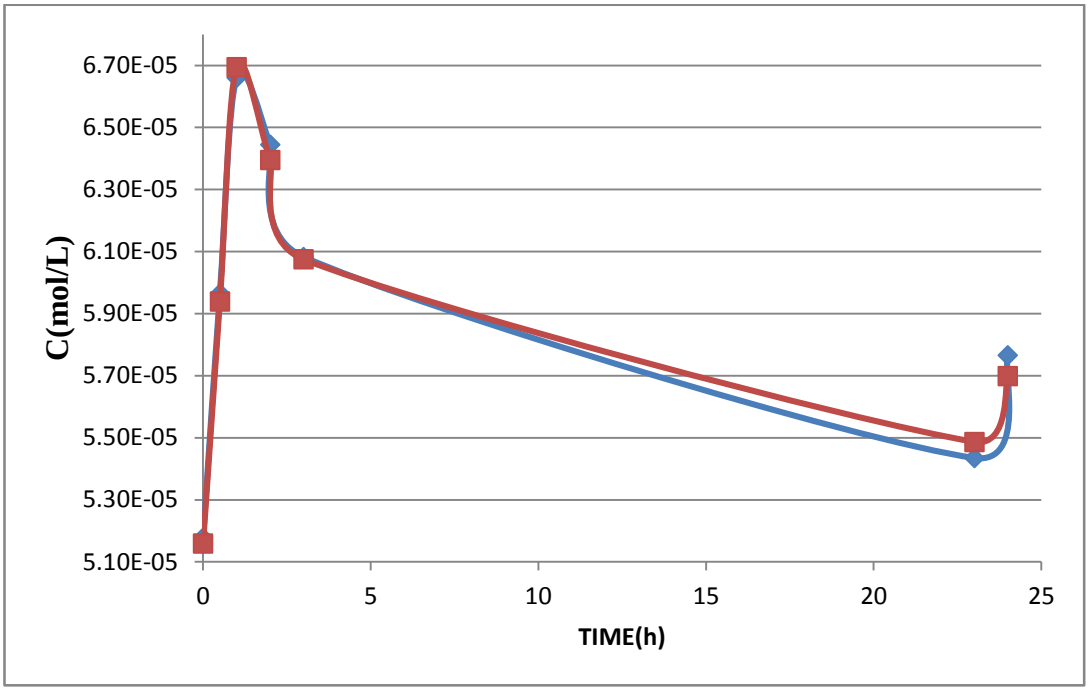


Figure 5.15. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:1 ratio) in phosphate buffer (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complexation was also studied as described in 0.1M HCl (pH=1.0).The results are given in Table 5.17, Table 5.18 and Figure 5.16.

Table 5.17. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid complex (1:1 ratio) in 0.1 M HCL solution (37ºC) (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	HCl + TBA	0.4896	$1.0033x10^{-3}$
0.5	HCl + TBA + βCD	0.4991	$1.0227x10^{-3}$
2	HCl + TBA + βCD	0.5126	$1.0504x10^{-3}$
4	HCl + TBA + βCD	0.4981	$1.0207x10^{-3}$
23	HCl + TBA + βCD	0.5037	$1.0322x10^{-3}$
24	HCl + TBA + βCD	0.5159	$1.0572x10^{-3}$

Table 5.18. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid complex (1:1 ratio) in 0.1 M HCL solution (37ºC) (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	HCl + TBA	0.4881	1.0002×10^{-3}
0.5	HCl + TBA + βCD	0.497	1.0184×10^{-3}
2	HCl + TBA + βCD	0.5144	1.0541×10^{-3}
4	HCl + TBA + βCD	0.4979	1.0203×10^{-3}
23	HCl + TBA + βCD	0.5034	1.0315×10^{-3}
24	HCl + TBA + βCD	0.5159	1.0572×10^{-3}

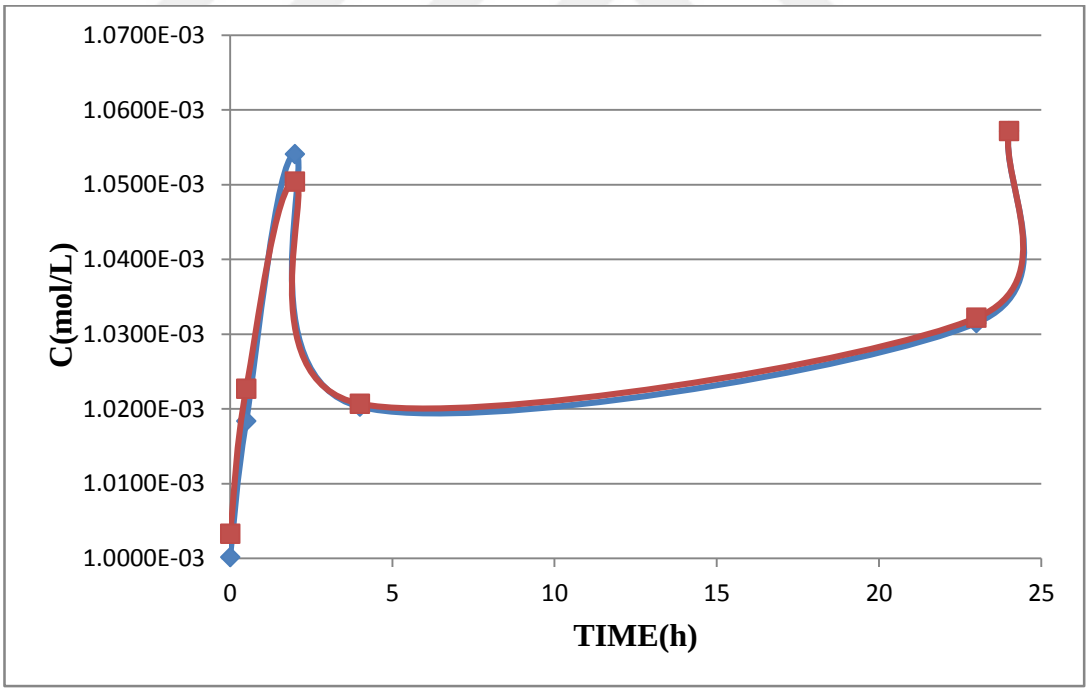


Figure 5.16. Absorbance vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid- β-CD complex (1:1 ratio) in 0.1 M HCl (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complexation was studied in TEA buffer (pH=2.4), too. The results are given in Table 5.19, Table 5.20 and Figure 5.17.

Table 5.19. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:1 ratio) in TEA buffer (37ºC) (1st trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	TEA + TBA	0.4051	$1.1244x10^{-3}$
0.5	TEA + TBA + βCD	0.4117	$1.1427x10^{-3}$
2	TEA + TBA + βCD	0.3942	$1.0942x10^{-3}$
4	TEA + TBA + βCD	0.3933	$1.0917x10^{-3}3$
23	TEA + TBA + βCD	0.3998	$1.1097x10^{-3}$
24	TEA + TBA + βCD	0.4121	$1.1438x10^{-3}$

Table 5.20. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:1 ratio) in TEA buffer (37ºC) (2nd trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	TEA + TBA	0.4044	$1.1225x10^{-3}$
0.5	TEA + TBA + βCD	0.4092	$1.1358x10^{-3}$
2	TEA + TBA + βCD	0.3955	$1.0978x10^{-3}$
4	TEA + TBA + βCD	0.3939	$1.0933x10^{-3}$
23	TEA + TBA + βCD	0.4010	$1.1130x10^{-3}$
24	TEA + TBA + βCD	0.4104	$1.1391x10^{-3}$

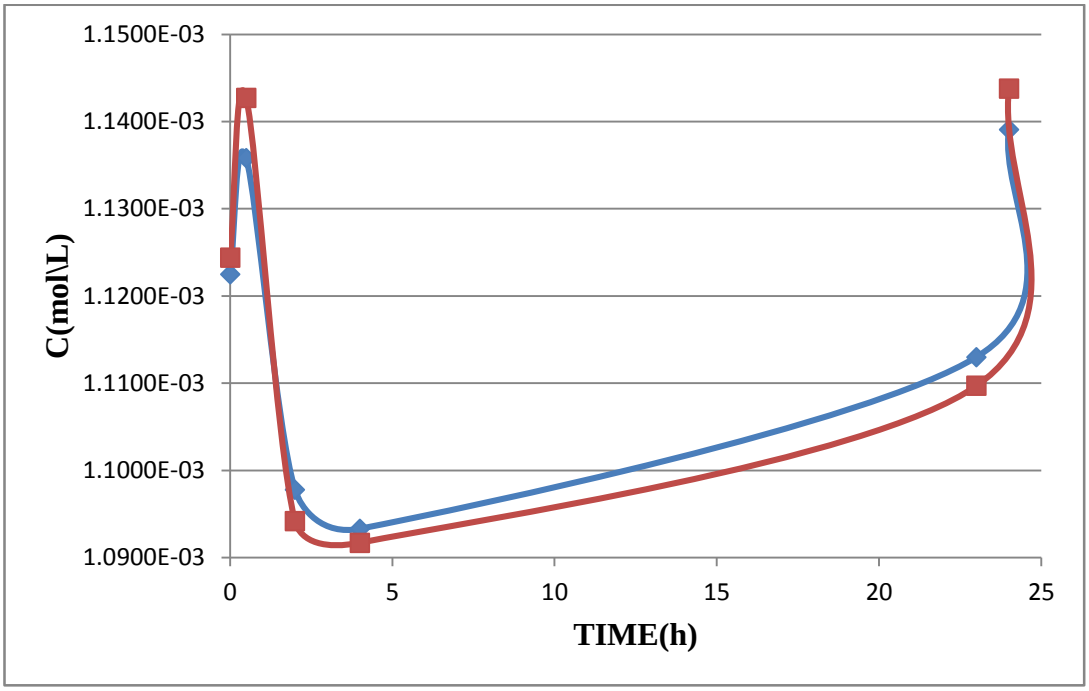


Figure 5.17. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid β-CD complex (1:1 ratio) in TEA buffer (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

According to above Figure 5.14-5.17, the concentrations of TBA in the solvents were compared to which solvent the complexation ratio is the highest. The concentrations were approximately between $5x10^{-5}$ M and $7x10^{-5}$ M in distilled water and phosphate buffer, whereas in other solutions the highest concentrations of TBA were found as $1x10^{-3}$ M. But HCl and TEA buffer solutions were not clear and measurements were done with difficulty. In this study, distilled water and phosphate buffer were used as solvents in other complexation studies.

5.3.2.2. Time Factor

In this section, effect of mixing time on the concentration was studied. For this reason, the absorbance of thiobarbituric acid at 190 nm was followed at specific time intervals. Samples from the mixing solution were taken at specific hours and their UV-analyses were done. The aim is to find time, at which maximum concentration was achieved and also to determine if the complex is stable with time or not.

5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex was studied at 96 hours mixing time (in distilled water and phosphate buffer) and different ratios (1:2 and 1:4) as explained in Section 4.4.4.1. Absorbance values at 190 nm where characteristic peak of thiobarbituric acid can be seen, were measured to determine the concentration of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid. The measurements were done for two trials. In each measurement, the same solution was measured three times, and the average absorbance was calculated as described in Section (4.3.1.1.1). The results are given in Table 5.21 and Table 5.22.

The results for the complexation process in distilled water (TBA:CD=1:2) are given in Table 5.21, Table 5.22 and Figure 5.18.

Table 5.21. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:2 ratio) in distilled water (37ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	D. water + TBA	0.4927	3.5841×10^{-5}
0.5	D. water+TBA+βCD	0.5652	4.1114×10^{-5}
1	D. water+TBA+βCD	0.6095	4.4337×10^{-5}
2	D. water+TBA+βCD	0.5747	4.1805×10^{-5}
3	D. water+TBA+βCD	0.5617	4.0860×10^{-5}
4	D. water+TBA+βCD	0.5881	4.2780×10^{-5}
5	D. water+TBA+βCD	0.5994	4.3602×10^{-5}
23	D. water+TBA+βCD	0.6208	4.5159×10^{-5}
24	D. water+TBA+βCD	0.6413	4.6650×10^{-5}
25	D. water+TBA+βCD	0.6388	4.6468×10^{-5}
26	D. water+TBA+βCD	0.6294	4.5785×10^{-5}
28	D. water+TBA+βCD	0.6102	4.4388×10^{-5}
47	D. water+TBA+βCD	0.5994	4.3602×10^{-5}
48	D. water+TBA+βCD	0.576	4.1900×10^{-5}
72	D. water+TBA+βCD	0.5892	4.2860×10^{-5}
96	D. water+TBA+βCD	0.5411	3.9361×10^{-5}

Table 5.22. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:2 ratio) in distilled water (37ºC) (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D. water + TBA	0.4816	$3.5033x10^{-5}$
0.5	D. water+TBA+βCD	0.5537	$4.0278x10^{-5}$
1	D. water+TBA+βCD	0.6125	$4.4555x10^{-5}$
2	D. water+TBA+βCD	0.5767	$4.1951x10^{-5}$
3	D. water+TBA+βCD	0.5688	$4.1376x10^{-5}$
4	D. water+TBA+βCD	0.5889	$4.2838x10^{-5}$
5	D. water+TBA+βCD	0.5994	$4.3602x10^{-5}$
23	D. water+TBA+βCD	0.6209	$4.5166x10^{-5}$
24	D. water+TBA+βCD	0.6415	$4.6665x10^{-5}$
25	D. water+TBA+βCD	0.6389	$4.6476x10^{-5}$
26	D. water+TBA+βCD	0.6295	$4.5792x10^{-5}$
28	D. water+TBA+βCD	0.6101	$4.4381x10^{-5}$
47	D. water+TBA+βCD	0.5993	$4.3595x10^{-5}$
48	D. water+TBA+βCD	0.5763	$4.1922x10^{-5}$
72	D. water+TBA+βCD	0.5889	$4.2838x10^{-5}$
96	D. water+TBA+βCD	0.5414	$3.9383x10^{-5}$

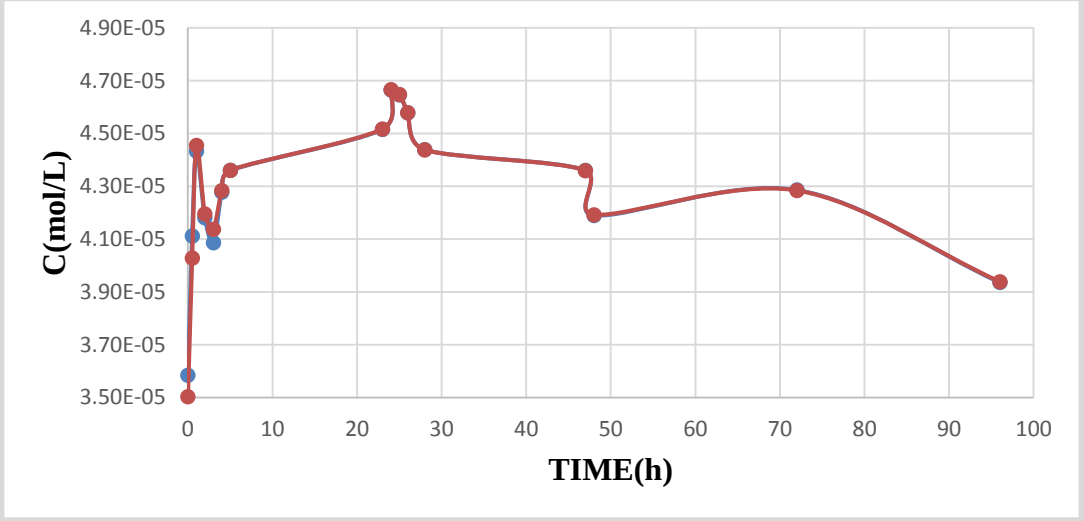


Figure 5.18. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:2 ratio) in distilled water (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The results for the complexation process (TBA:CD=1:2) in phosphate buffer are given in Table 5.23, 5.24 and Figure 5.19.

Table 5.23. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:2 ratio) in phosphate buffer (37ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.5341	5.1534x10-5
0.5	Phosphate Bf+TBA+βCD	0.6336	6.1135x10-5
1	Phosphate Bf+TBA+βCD	0.6796	6.5573x10-5
2	Phosphate Bf+TBA+βCD	0.6398	6.1733x10-5
3	Phosphate Bf+TBA+βCD	0.6213	5.9948x10-5
4	Phosphate Bf+TBA+βCD	0.6692	6.4570x10-5
5	Phosphate Bf+TBA+βCD	0.685	6.6094x10-5
23	Phosphate Buffer+TBA	0.7013	6.7667x10-5
24	Phosphate Bf+TBA+βCD	0.7208	6.9548x10-5
25	Phosphate Bf+TBA+βCD	0.7165	6.9134x10-5
26	Phosphate Buffer+TBA	0.7068	6.8198x10-5
28	Phosphate Bf+TBA+βCD	0.6935	6.6914x10-5
47	Phosphate Bf+TBA+βCD	0.6736	6.4994x10-5
48	Phosphate Buffer+TBA	0.6522	6.2929x10-5
72	Phosphate Bf+TBA+βCD	0.5996	5.7854x10-5
96	Phosphate Bf+TBA+βCD	0.5715	5.5143x10-5

Table 5.24. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:2 ratio) in phosphate buffer (37ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.5292	5.1061×10^{-5}
0.5	Phosphate Bf+TBA+βCD	0.6288	6.0672×10^{-5}
1	Phosphate Bf+TBA+βCD	0.6808	6.5689×10^{-5}
2	Phosphate Bf+TBA+βCD	0.6469	6.2418×10^{-5}
3	Phosphate Bf+TBA+βCD	0.6212	5.9938×10^{-5}
4	Phosphate Bf+TBA+βCD	0.6654	6.4203×10^{-5}
5	Phosphate Bf+TBA+βCD	0.6847	6.6065×10^{-5}
23	Phosphate Buffer+TBA	0.7016	6.7696×10^{-5}
24	Phosphate Bf+TBA+βCD	0.7209	6.9558×10^{-5}
25	Phosphate Bf+TBA+βCD	0.7141	6.8902×10^{-5}
26	Phosphate Buffer+TBA	0.7086	6.8371×10^{-5}
28	Phosphate Bf+TBA+βCD	0.6951	6.7069×10^{-5}
47	Phosphate Bf+TBA+βCD	0.6738	6.5014×10^{-5}
48	Phosphate Buffer+TBA	0.6522	6.2929×10^{-5}
72	Phosphate Bf+TBA+βCD	0.5994	5.7835×10^{-5}
96	Phosphate Bf+TBA+βCD	0.5716	5.5152×10^{-5}

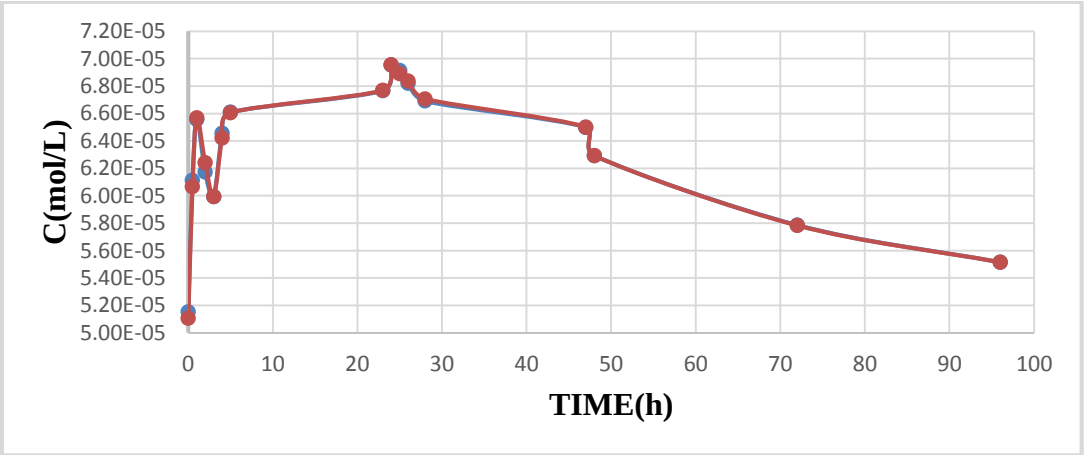


Figure 5.19. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:2 ratio) in phosphate buffer (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The results for the complexation process (TBA:CD=1:4) in distilled water are given in Table 5.25, Table 5.26 and Figure 5.20.

Table 5.25. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:4 ratio) in distilled water (37ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	D. water + TBA	0.4899	$3.5637x10^{-5}$
0.5	D. water+TBA+βCD	0.5621	$4.0889x10^{-5}$
1	D. water+TBA+βCD	0.6249	$4.5457x10^{-5}$
2	D. water+TBA+βCD	0.5847	$4.2533x10^{-5}$
3	D. water+TBA+βCD	0.5768	$4.1958x10^{-5}$
4	D. water+TBA+βCD	0.5907	$4.2969x10^{-5}$
5	D. water+TBA+βCD	0.6074	$4.4184x10^{-5}$
23	D. water+TBA+βCD	0.6488	$4.7196x10^{-5}$
24	D. water+TBA+βCD	0.6699	$4.8731x10^{-5}$
25	D. water+TBA+βCD	0.6574	$4.7821x10^{-5}$
26	D. water+TBA+βCD	0.6593	$4.7960x10^{-5}$
28	D. water+TBA+βCD	0.6318	$4.5959x10^{-5}$
47	D. water+TBA+βCD	0.6011	$4.3726x10^{-5}$
48	D. water+TBA+βCD	0.5815	$4.2300x10^{-5}$
72	D. water+TBA+βCD	0.6005	$4.3682x10^{-5}$
96	D. water+TBA+βCD	0.5433	$3.9521x10^{-5}$

Table 5.26. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:4 ratio) in distilled water (37ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.4866	$3.5397x10^{-5}$
0.5	D. water+TBA+βCD	0.5779	$4.2038x10^{-5}$
1	D. water+TBA+βCD	0.6278	$4.5668x10^{-5}$
2	D. water+TBA+βCD	0.5809	$4.2256x10^{-5}$
3	D. water+TBA+βCD	0.5773	$4.1995x10^{-5}$
4	D. water+TBA+βCD	0.5907	$4.2969x10^{-5}$
5	D. water+TBA+βCD	0.6078	$4.4213x10^{-5}$
23	D. water+TBA+βCD	0.6483	$4.7159x10^{-5}$
24	D. water+TBA+βCD	0.6695	$4.8702x10^{-5}$
25	D. water+TBA+βCD	0.6574	$4.7821x10^{-5}$
26	D. water+TBA+βCD	0.6592	$4.7952x10^{-5}$
28	D. water+TBA+βCD	0.6319	$4.5966x10^{-5}$
47	D. water+TBA+βCD	0.6012	$4.3733x10^{-5}$
48	D. water+TBA+βCD	0.5815	$4.2300x10^{-5}$
72	D. water+TBA+βCD	0.6010	$4.3719x10^{-5}$
96	D. water+TBA+βCD	0.5431	$3.9507x10^{-5}$

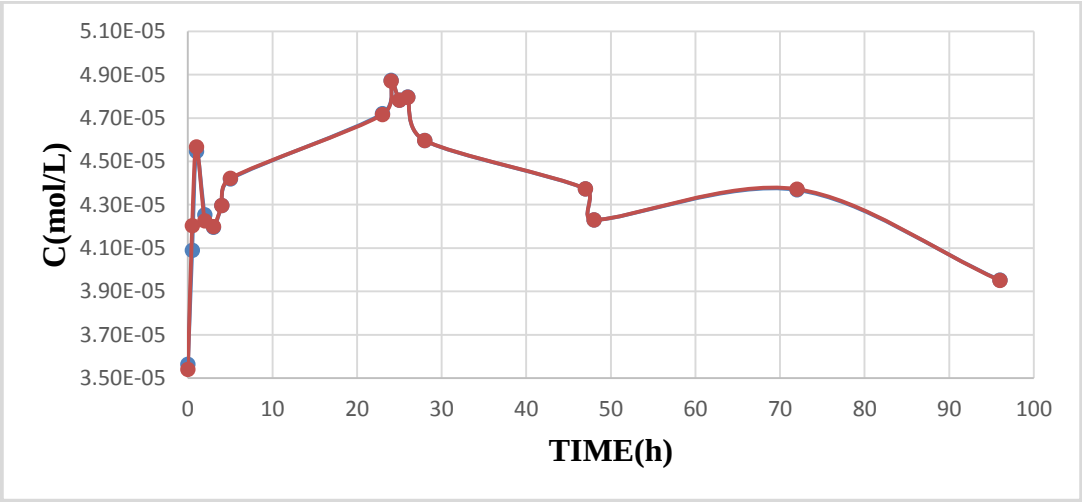


Figure 5.20. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD in (1:4 ratio) complex distilled water (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The results for the complexation process (TBA:CD=1:4) in phosphate buffer are given in Table 5.27, Table 5.28 and Figure 5.21.

Table 5.27. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:4 ratio) in phosphate buffer (37ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.5298	$5.1119x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	1.1672	$1.1262x10^{-4}$
1	Phosphate Bf+TBA+βCD	1.2155	$1.1728x10^{-4}$
2	Phosphate Bf+TBA+βCD	1.1868	$1.1451x10^{-4}$
3	Phosphate Bf+TBA+βCD	1.1757	$1.1344x10^{-4}$
4	Phosphate Bf+TBA+βCD	1.1996	$1.1575x10^{-4}$
5	Phosphate Bf+TBA+βCD	1.2019	$1.1597x10^{-4}$
23	Phosphate Buffer+TBA	1.2410	$1.1974x10^{-4}$
24	Phosphate Bf+TBA+βCD	1.2749	$1.2301x10^{-4}$
25	Phosphate Bf+TBA+βCD	1.2538	$1.2098x10^{-4}$
26	Phosphate Buffer+TBA	1.2432	$1.1995x10^{-4}$
28	Phosphate Bf+TBA+βCD	1.2216	$1.1787x10^{-4}$
47	Phosphate Bf+TBA+βCD	1.2054	$1.1631x10^{-4}$
48	Phosphate Buffer+TBA	1.1875	$1.1458x10^{-4}$
72	Phosphate Bf+TBA+βCD	1.2009	$1.1587x10^{-4}$
96	Phosphate Bf+TBA+βCD	1.1270	$1.0874x10^{-4}$

Table 5.28. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:4 ratio) in phosphate buffer (37ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.5258	$5.0733x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	1.1673	$1.1263x10^{-4}$
1	Phosphate Bf+TBA+βCD	1.2201	$1.1772x10^{-4}$
2	Phosphate Bf+TBA+βCD	1.1838	$1.1422x10^{-4}$
3	Phosphate Bf+TBA+βCD	1.1788	$1.1374x10^{-4}$
4	Phosphate Bf+TBA+βCD	1.1992	$1.1571x10^{-4}$
5	Phosphate Bf+TBA+βCD	1.2045	$1.1622x10^{-4}$
23	Phosphate Buffer+TBA	1.2411	$1.1975x10^{-4}$
24	Phosphate Bf+TBA+βCD	1.2752	$1.2304x10^{-4}$
25	Phosphate Bf+TBA+βCD	1.2538	$1.2098x10^{-4}$
26	Phosphate Buffer+TBA	1.2473	$1.2035x10^{-4}$
28	Phosphate Bf+TBA+βCD	1.2226	$1.1797x10^{-4}$
47	Phosphate Bf+TBA+βCD	1.2051	$1.1628x10^{-4}$
48	Phosphate Buffer+TBA	1.1876	$1.1459x10^{-4}$
72	Phosphate Bf+TBA+βCD	1.2004	$1.1582x10^{-4}$
96	Phosphate Bf+TBA+βCD	1.1574	$1.1168x10^{-4}$

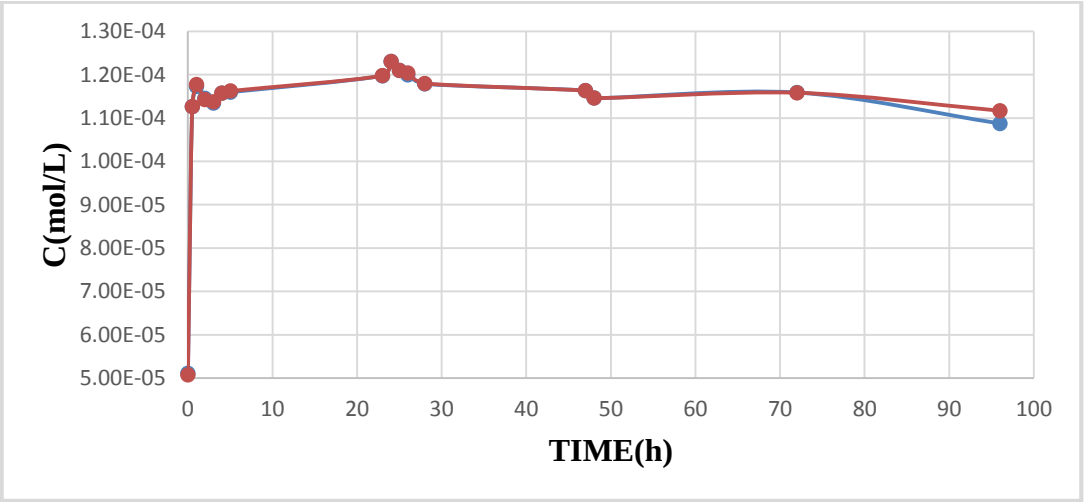


Figure 5.21. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex (1:4 ratio) in phosphate buffer (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

As seen from all graphs, in the first three hours there is a sharp increase in the concentration of TBA, and the maximum concentration was achieved after 24 hours. After 24 hours, a decrease in the concentration of TBA was observed, so the complexation process seems not to be stable after that time. Therefore it was concluded to perform other process to determine the effect on the complexation process in 24 hours period.

For conforming the result, same procedure was applied to 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex for 48 hours mixing time in the concentration of 0.8mM and in the ratio (TBA=CD:1:1) as explained in Section 4.4.1.1. The results are given in Table 5.29, Table 5.30 and Figure 5.22.

Table 5.29. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex (0.8 mM) in distilled water (37ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	D. water + TBA	0.3282	$1.2358x10^{-5}$
0.5	D. water+TBA+βCD	0.3796	$1.4294x10^{-5}$
1	D. water+TBA+βCD	0.4743	$1.7860x10^{-5}$
2	D. water+TBA+βCD	0.5262	$1.9814x10^{-5}$
3	D. water+TBA+βCD	0.6688	$2.5184x10^{-5}$
23	D. water+TBA+βCD	0.7729	$2.9102x10^{-5}$
24	D. water+TBA+βCD	0.7848	$2.9550x10^{-5}$
25	D. water+TBA+βCD	0.8285	$3.1195x10^{-5}$
26	D. water+TBA+βCD	0.9082	$3.4196x10^{-5}$
27	D. water+TBA+βCD	0.9296	$3.5004x10^{-5}$
28	D. water+TBA+βCD	0.8278	$3.1169x10^{-5}$
47	D. water+TBA+βCD	0.8110	$3.0536x10^{-5}$
48	D. water+TBA+βCD	0.8326	$3.1351x10^{-5}$

Table 5.30. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex (0.8 mM) in distilled water (37ºC) (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D. water + TBA	0.3254	$1.2251x10^{-5}$
0.5	D. water+TBA+βCD	0.3774	$1.4211x10^{-5}$
1	D. water+TBA+βCD	0.4769	$1.7958x10^{-5}$
2	D. water+TBA+βCD	0.5239	$1.9725x10^{-5}$
3	D. water+TBA+βCD	0.6683	$2.5163x10^{-5}$
23	D. water+TBA+βCD	0.7738	$2.9135x10^{-5}$
24	D. water+TBA+βCD	0.7794	$2.9346x10^{-5}$
25	D. water+TBA+βCD	0.8258	$3.1093x10^{-5}$
26	D. water+TBA+βCD	0.9054	$3.4093x10^{-5}$
27	D. water+TBA+βCD	0.9306	$3.5042x10^{-5}$
28	D. water+TBA+βCD	0.8373	$3.1528x10^{-5}$
47	D. water+TBA+βCD	0.8109	$3.0534x10^{-5}$
48	D. water+TBA+βCD	0.8285	$3.1195x10^{-5}$

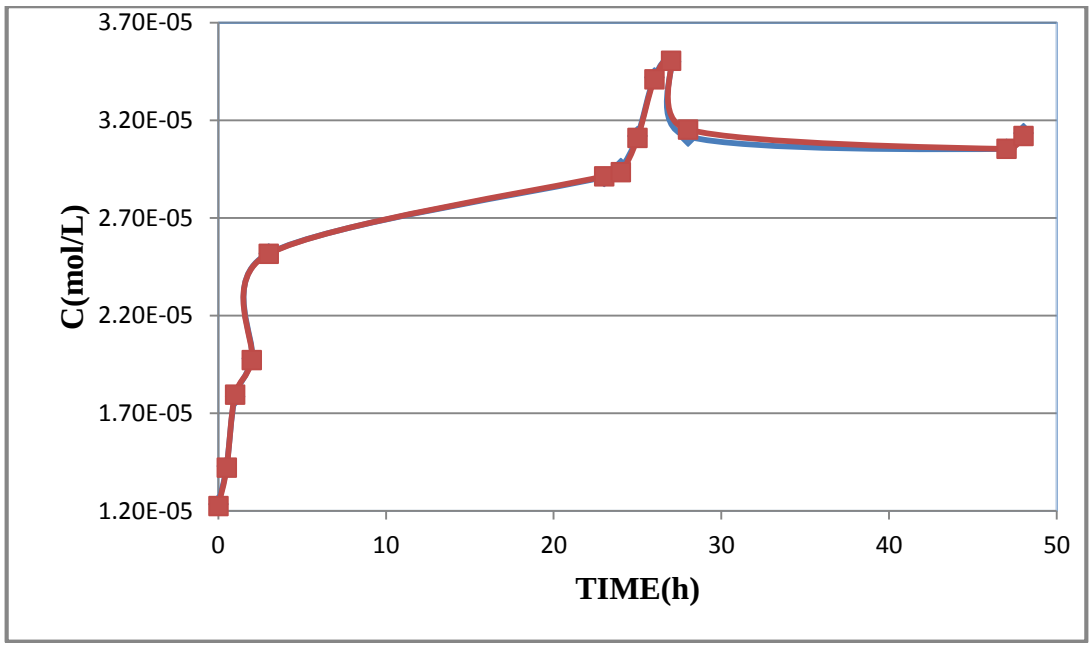


Figure 5.22. Concnetration vs. time graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD in (0.8 mM) complex distilled water (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

As seen from Figure 5.22 and Figure 5.23, the concentration of TBA in distilled water increases in the first 24-26 hours, then there is no sharp decrease, but also no increase.

The same procedure was applied for the mixing process in phosphate buffer. The results are given in Table 5.31, Table 5.32 and Figure 5.23.

Table 5.31. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex (0.8 mM) in phosphate buffer (37ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.4188	$2.8546x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.4836	$3.2963x10^{-5}$
1	Phosphate Bf+TBA+βCD	0.5649	$3.8505x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.6157	$4.1967x10^{-5}$
3	Phosphate Bf+TBA+βCD	0.6837	$4.6602x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.7874	$5.3671x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.8041	$5.4809x10^{-5}$
25	Phosphate Bf+TBA+βCD	0.7590	$5.1735x10^{-5}$
26	Phosphate Bf+TBA+βCD	0.8145	$5.5518x10^{-5}$
27	Phosphate Bf+TBA+βCD	0.7886	$5.3752x10^{-5}$
28	Phosphate Bf+TBA+βCD	0.8061	$5.4945x10^{-5}$
47	Phosphate Bf+TBA+βCD	0.7791	$5.3105x10^{-5}$
48	Phosphate Bf+TBA+βCD	0.8259	$5.6295x10^{-5}$

Table 5.32. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex (0.8 mM) in phosphate buffer (37ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.4203	2.8648×10^{-5}
0.5	Phosphate Bf+TBA+βCD	0.4821	3.2861×10^{-5}
1	Phosphate Bf+TBA+βCD	0.5622	3.8320×10^{-5}
2	Phosphate Bf+TBA+βCD	0.6153	4.1940×10^{-5}
3	Phosphate Bf+TBA+βCD	0.6878	4.6882×10^{-5}
23	Phosphate Bf+TBA+βCD	0.7867	5.3623×10^{-5}
24	Phosphate Bf+TBA+βCD	0.8044	5.4829×10^{-5}
25	Phosphate Bf+TBA+βCD	0.7634	5.2035×10^{-5}
26	Phosphate Bf+TBA+βCD	0.8146	5.5525×10^{-5}
27	Phosphate Bf+TBA+βCD	0.7873	5.3664×10^{-5}
28	Phosphate Bf+TBA+βCD	0.8097	5.5191×10^{-5}
47	Phosphate Bf+TBA+βCD	0.7776	5.3003×10^{-5}
48	Phosphate Bf+TBA+βCD	0.8379	5.7113×10^{-5}

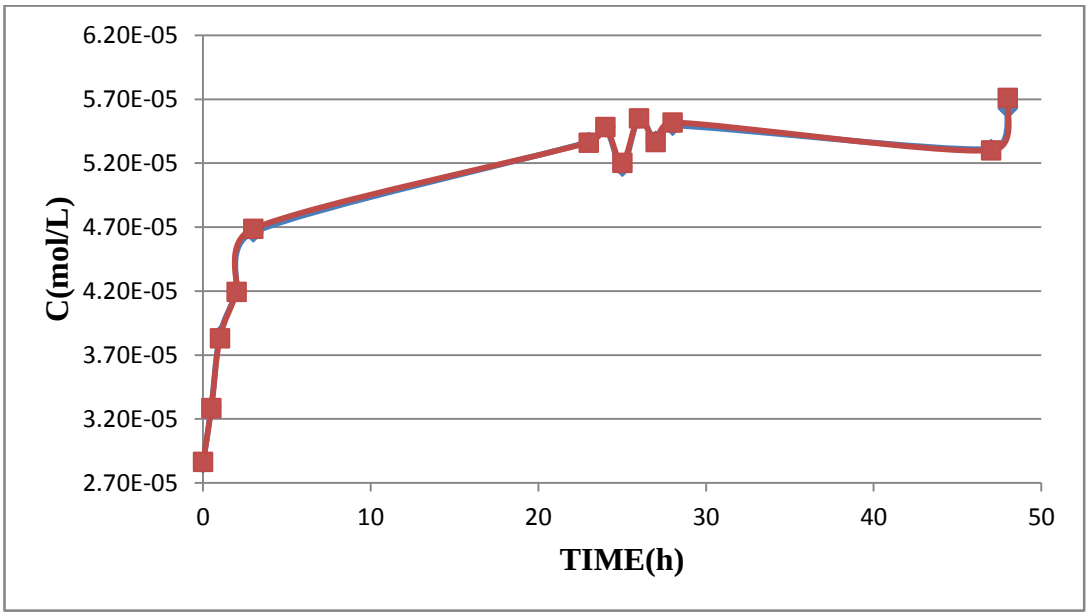


Figure 5.23. Concentration vs. time graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD in (0.8 mM) complex phosphate buffer (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The concentration of *o*-tolyl derivative increases in phosphate buffer sharply also in the first three hours as in the fluoro-derivative, then there is increase in the first 24 hours and the concentration stays approximately in the same range. Therefore all processes were performed in 24 hours.

5.3.2.3. Temperature Effect

In this section temperature effect on the complexation was investigated. All conditions were kept constant except temperature. UV-absorption values of the solutions at two different temperatures 25ºC and 37ºC were compared.

The thiobarbituric acid derivative-β-CD complex was studied at 24 hours mixing time at 37ºC and 25ºC in distilled water and phosphate buffer in 5 different ratios (thiobarbituric acid derivative:β-CD=4:1; 2:1; 1:1; 1:2; 1:4) as explained in Section 4.4.1.1. Absorbance values at 190 nm, where characteristic peak of thiobarbituric acid can be seen, were measured to determine the concentration of thiobarbituric acid derivative. The measurements were done for two trials. In each measurement, the same solution was measured three times, and the average absorbance was calculated as described in Section (4.3.1.1.1).

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (4:1 ratio) complex in distilled water at 37ºC are given in Table 5.33, Table 5.34 and Figure 5.24.

Table 5.33. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (4:1 ratio) complex in distilled water (37ºC) (1st trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.4563	3.3193×10^{-5}
0.5	D. water+TBA+βCD	0.5313	3.8648×10^{-5}
2	D. water+TBA+βCD	0.5418	3.9412×10^{-5}
4	D. water+TBA+βCD	0.5577	4.0569×10^{-5}
23	D. water+TBA+βCD	0.5707	4.1515×10^{-5}
24	D. water+TBA+βCD	0.6011	4.3726×10^{-5}

Table 5.34. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (4:1 ratio) complex in distilled water (37ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.4555	$3.3135x10^{-5}$
0.5	D. water+TBA+βCD	0.5248	$3.8176x10^{-5}$
2	D. water+TBA+βCD	0.5417	$3.9405x10^{-5}$
4	D. water+TBA+βCD	0.5581	$4.0598x10^{-5}$
23	D. water+TBA+βCD	0.5710	$4.1536x10^{-5}$
24	D. water+TBA+βCD	0.6011	$4.3726x10^{-5}$

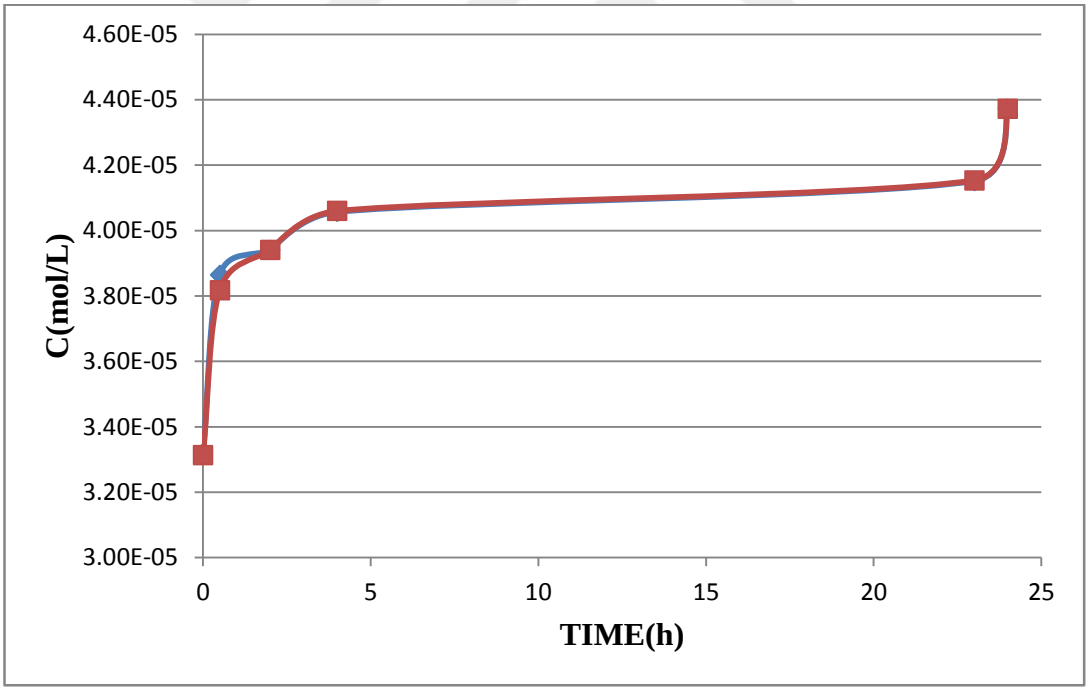


Figure 5.24. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2thiobarbituric acid-β-CD in (4:1 ratio) complex distilled water (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (4:1 ratio) complex in distilled water at 25ºC are given in Table 5.35, Table 5.36 and Figure 5.25.

Table 5.35. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (4:1 ratio) complex in distilled water (25ºC) (1st trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.6502	$4.7298x10^{-5}$
0.5	D. water+TBA+βCD	1.065	$7.7471x10^{-5}$
2	D. water+TBA+βCD	1.1291	$8.2134x10^{-5}$
4	D. water+TBA+βCD	1.1907	$8.6615x10^{-5}$
23	D. water+TBA+βCD	1.1749	$8.5466x10^{-5}$
24	D. water+TBA+βCD	1.2157	$8.8434x10^{-5}$

Table 5.36. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (4:1 ratio) complex in distilled water (25ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.6433	$4.6796x10^{-5}$
0.5	D. water+TBA+βCD	1.0878	$7.9130x10^{-5}$
Th	D. water+TBA+βCD	1.1339	$8.2483x10^{-5}$
4	D. water+TBA+βCD	1.1906	$8.6608x10^{-5}$
23	D. water+TBA+βCD	1.1747	$8.5451x10^{-5}$
24	D. water+TBA+βCD	1.2127	$8.8216x10^{-5}$

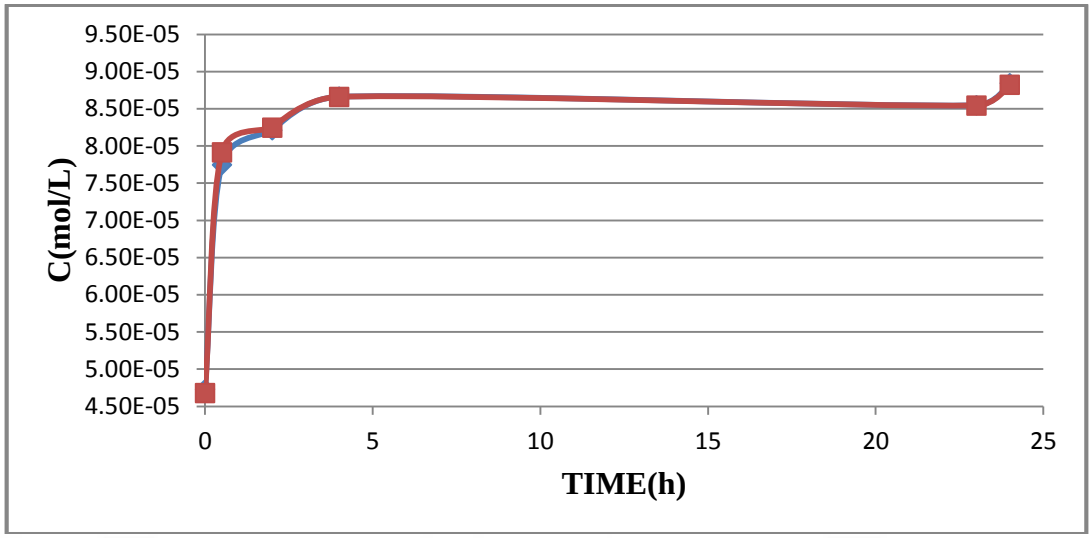


Figure 5.25. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD in (4:1 ratio) complex distilled water (25ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

As decrease in the concentration of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid with the increase in the temperature was observed when the Figure 5.24-5.25 are compared. As a result complexation ratio decreses with increasing temperature in distilled water. The complexation process can be thermodynamically more stable at lower temperature at these conditions.

The results for the measurements 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (4:1 ratio) complex in phosphate buffer at 37ºC are given in Table 5.37, Table 5.38 and Figure 5.26.

Table 5.37. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (4:1 ratio) complex in phosphate buffer (37ºC) (1st trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.5400	5.2103×10^{-5}
0.5	Phosphate Bf+TBA+βCD	0.5416	5.2258×10^{-5}
2	Phosphate Bf+TBA+βCD	0.6365	6.1415×10^{-5}
4	Phosphate Bf+TBA+βCD	0.6349	6.1260×10^{-5}
23	Phosphate Bf+TBA+βCD	0.6511	6.2823×10^{-5}
24	Phosphate Bf+TBA+βCD	0.6974	6.7291×10^{-5}

Table 5.38. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (4:1 ratio) complex in phosphate buffer (37ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.5406	5.2161×10^{-5}
0.5	Phosphate Bf+TBA+βCD	0.5564	5.3686×10^{-5}
2	Phosphate Bf+TBA+βCD	0.6356	6.1328×10^{-5}
4	Phosphate Bf+TBA+βCD	0.6353	6.1299×10^{-5}
23	Phosphate Bf+TBA+βCD	0.6514	6.2852×10^{-5}
24	Phosphate Bf+TBA+βCD	0.6934	6.6905×10^{-5}

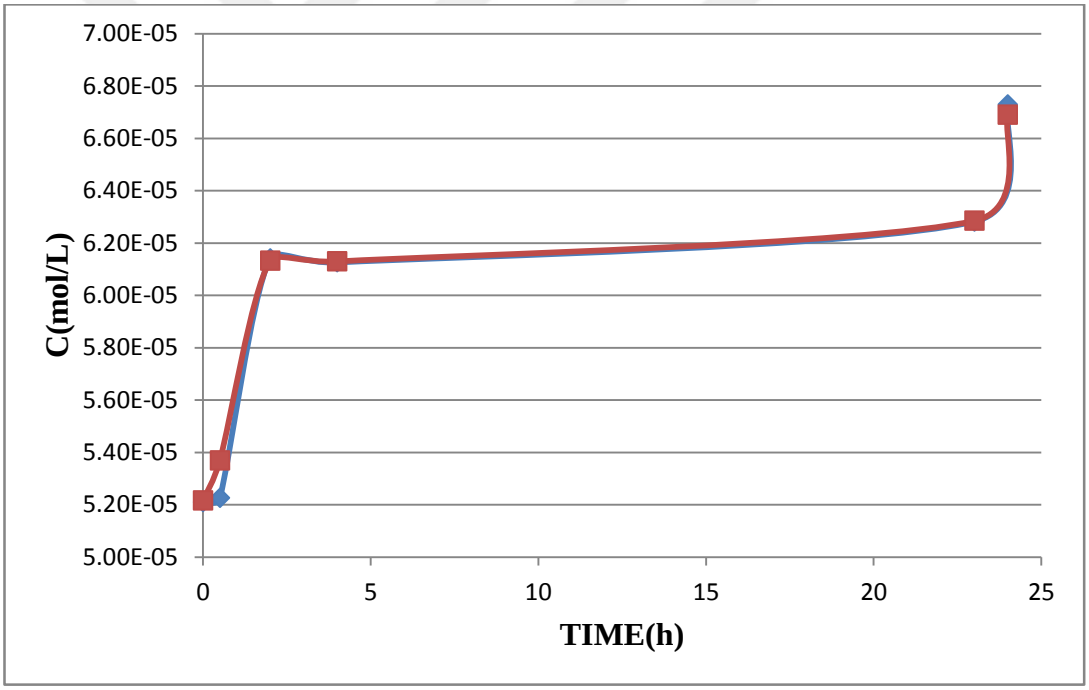


Figure 5.26. Absorbance vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD in (4:1 ratio) complex phosphate buffer (37ºC) (1st & 2nd trial)) (blue line: 1st trial, red line: 2nd trial)

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (4:1 ratio) complex in phosphate buffer at 25ºC are given in Table 5.39, Table 5.40 and Figure 5.27.

Table 5.39. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (4:1 ratio) complex in phosphate buffer (25ºC) (1st trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.5962	$5.7526x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.7405	$7.1449x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.7761	$7.4884x10^{-5}$
4	Phosphate Bf+TBA+βCD	0.8054	$7.7711x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.7575	$7.3090x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.8264	$7.9738x10^{-5}$

Table 5.40. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (4:1 ratio) complex in phosphate buffer (25ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.5996	$5.7854x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.7467	$7.2047x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.7769	$7.4961x10^{-5}$
4	Phosphate Bf+TBA+βCD	0.8058	$7.7750x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.7589	$7.3225x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.8231	$7.9419x10^{-5}$

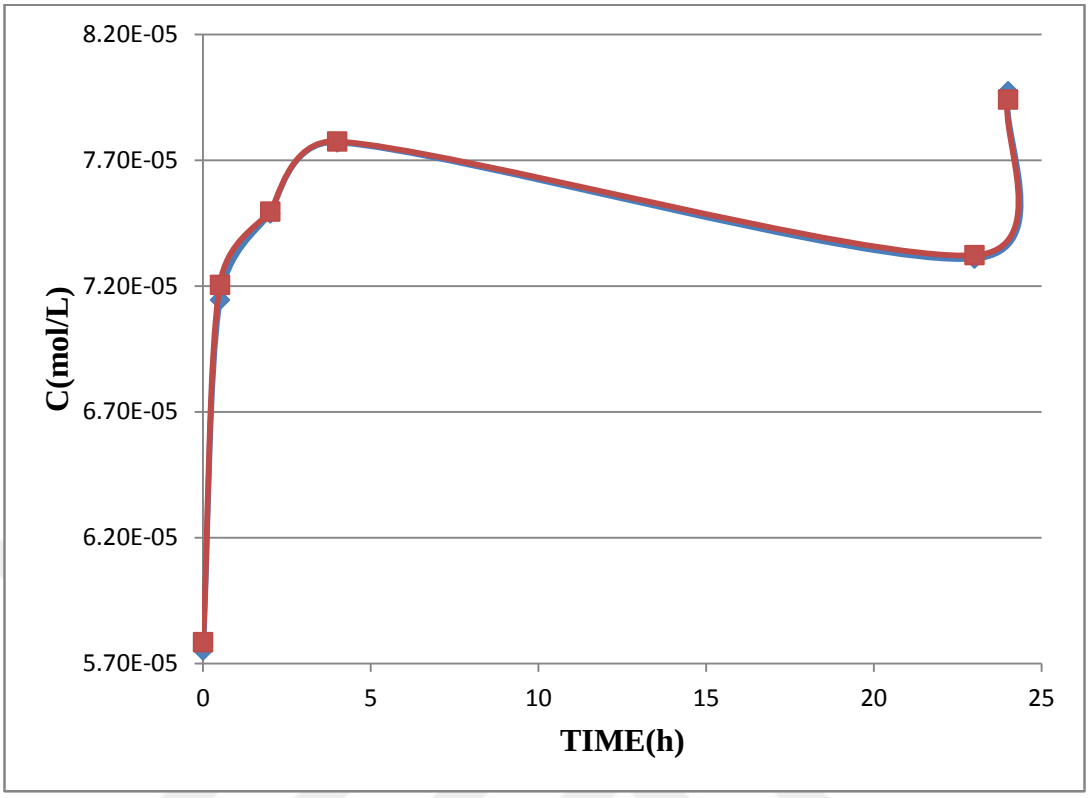


Figure 5.27. Absorbance vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD in (4:1 ratio) complex phosphate buffer (25ºC) (1^{st} & 2^{nd} trial) (blue line: 1^{st} trial, red line: 2^{nd} trial)

A decrease in the concentration of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid with the increase in the temperature was observed when the Figure 5.25 and Figure 5.26 are compared. As a result complexation ratio decreases with increasing temperature also in phosphate buffer. The complexation process can be thermodynamically more stable at lower temperature at these conditions.

To investigate if the temperature effect changes, when the ratio of TBA:CD changes, several experiments were done with different TBA:CD ratios. The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (2:1 ratio) complex in distilled water at 37ºC are given in Table 5.41, Table 5.42 and Figure 5.28.

Table 5.41. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (2:1 ratio) complex distilled water (37ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	D. water + TBA	0.4546	$3.3069x10^{-5}$
0.5	D. water+TBA+βCD	0.5525	$4.0191x10^{-5}$
2	D. water+TBA+βCD	0.5612	$4.0823x10^{-5}$
4	D. water+TBA+βCD	0.5706	$4.1507x10^{-5}$
23	D. water+TBA+βCD	0.5917	$4.3042x10^{-5}$
24	D. water+TBA+βCD	0.6253	$4.5486x10^{-5}$

Table 5.42. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (2:1 ratio) complex in distilled water (37ºC) (2nd trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	D. water + TBA	0.4546	$3.3069x10^{-5}$
0.5	D. water+TBA+βCD	0.5525	$4.0191x10^{-5}$
2	D. water+TBA+βCD	0.5612	$4.0823x10^{-5}$
4	D. water+TBA+βCD	0.5704	$4.1493x10^{-5}$
23	D. water+TBA+βCD	0.5920	$4.3064x10^{-5}$
24	D. water+TBA+βCD	0.6275	$4.5646x10^{-5}$

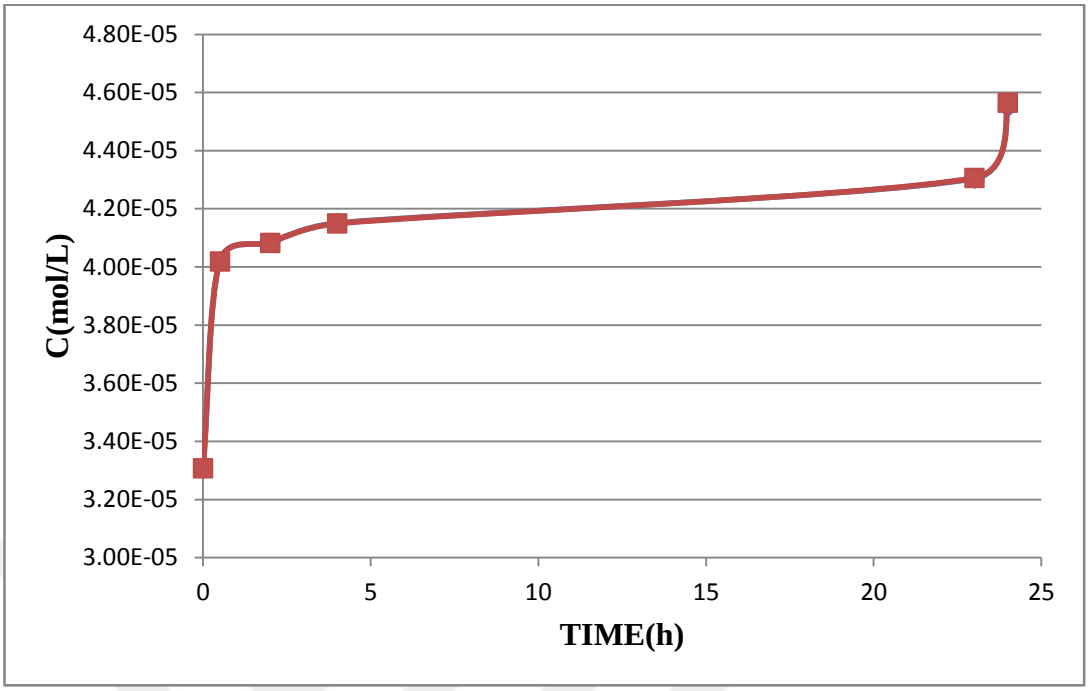


Figure 5.28. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD in (2:1 ratio) complex distilled water (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (2:1 ratio) complex in distilled water at 25ºC are given in Table 5.43, Table 5.44 and Figure 5.29.

Table 5.43. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (2:1 ratio) complex distilled water (25ºC) (1st trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.6446	$4.6890x10^{-5}$
0.5	D.water+TBA+βCD	1.1839	$8.6121x10^{-5}$
2	D.water+TBA+βCD	1.2519	$9.1067x10^{-5}$
4	D.water+TBA+βCD	1.2864	$9.3577x10^{-5}$
23	D.water+TBA+βCD	1.2652	$9.2035x10^{-5}$
24	D.water+TBA+βCD	1.3115	$9.5403x10^{-5}$

Table 5.44. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (2:1 ratio) complex in distilled water (25ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.6763	$4.9196x10^{-5}$
0.5	D.water+TBA+βCD	1.1755	$8.5510x10^{-5}$
2	D.water+TBA+βCD	1.1248	$9.0783x10^{-5}$
4	D.water+TBA+βCD	1.2866	$9.3591x10^{-5}$
23	D.water+TBA+βCD	1.2701	$9.2391x10^{-5}$
24	D.water+TBA+βCD	1.3023	$9.4733x10^{-5}$

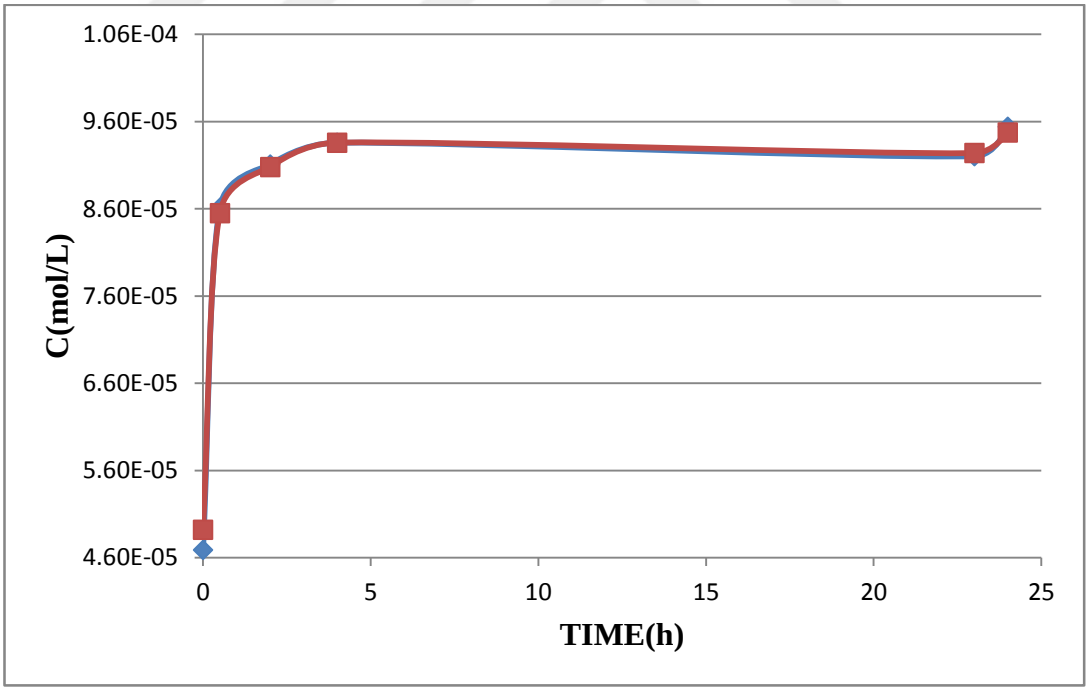


Figure 5.29. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD in (2:1 ratio) complex distilled water (25ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

A decrease in the concentration of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid with the increase in the temperature was also in distilled water observed, when the TBA:CD ratio is 2:1 (Figure 5.28 and Figure 5.29). As a result complexation ratio decrease with increasing temperature also in different ratio. The complexation process can be thermodynamically more stable at lower temeperature at these conditions.

The results for the measurement of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (2:1 ratio) complex in phosphate buffer at 37ºC are given in Table 5.45, Table 5.46 and Figure 5.30.

Table 5.45. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (2:1 ratio) complex in phosphate buffer (37ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.5345	$5.1573x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.6151	$5.9350x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.6527	$6.2978x10^{-5}$
4	Phosphate Bf+TBA+βCD	0.641	$6.1849x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.6633	$6.4000x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.7183	$6.9307x10^{-5}$

Table 5.46. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (2:1 ratio) complex in phosphate buffer (37ºC) (2nd trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.5409	$5.2190x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.6127	$5.9118x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.6591	$6.3595x10^{-5}$
4	Phosphate Bf+TBA+βCD	0.6427	$6.2013x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.6637	$6.4039x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.7159	$6.9076x10^{-5}$

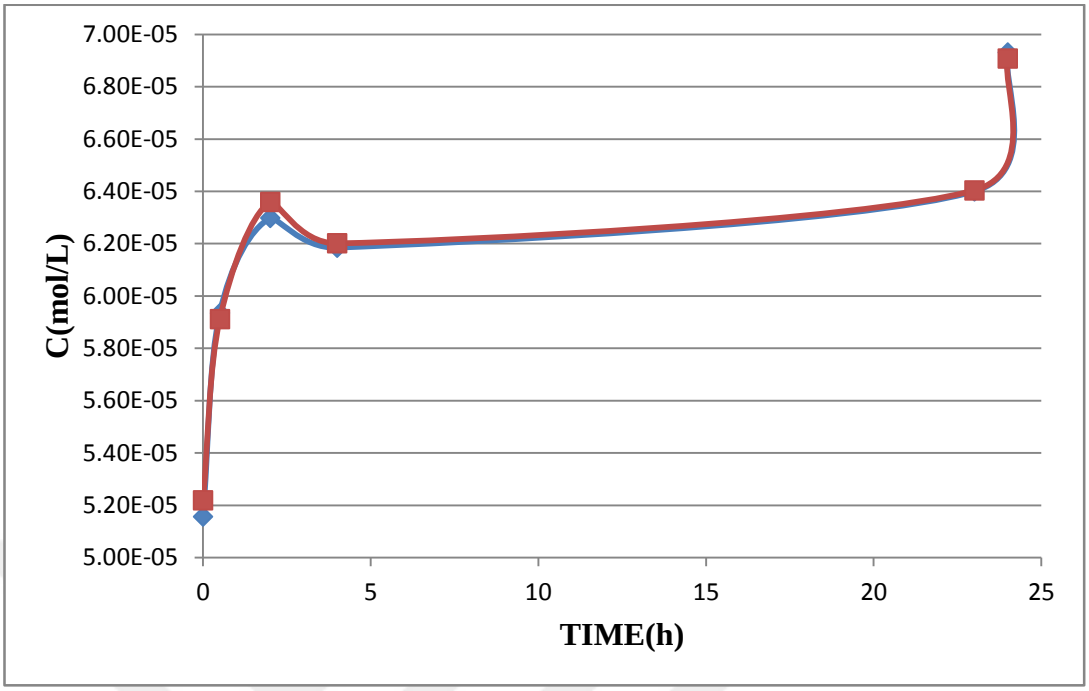


Figure 5.30. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD in (2:1 ratio) complex phosphate buffer (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (2:1 ratio) complex in phosphate buffer at 25ºC are given in Table 5.47, Table 5.48 and Figure 5.31.

Table 5.47. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (2:1 ratio) complex in phosphate buffer (25ºC) (1st trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.5848	5.6426×10^{-5}
0.5	Phosphate Bf+TBA+βCD	0.8561	8.2603×10^{-5}
2	Phosphate Bf+TBA+βCD	0.8604	8.3018×10^{-5}
4	Phosphate Bf+TBA+βCD	0.8827	8.5170×10^{-5}
23	Phosphate Bf+TBA+βCD	0.8582	8.2806×10^{-5}
24	Phosphate Bf+TBA+βCD	0.9062	8.7437×10^{-5}

Table 5.48. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (2:1 ratio) complex in phosphate buffer (25ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.5951	5.7420×10^{-5}
0.5	Phosphate Bf+TBA+βCD	0.8594	8.2922×10^{-5}
2	Phosphate Bf+TBA+βCD	0.8668	8.3636×10^{-5}
4	Phosphate Bf+TBA+βCD	0.8804	8.4948×10^{-5}
23	Phosphate Bf+TBA+βCD	0.8580	8.2787×10^{-5}
24	Phosphate Bf+TBA+βCD	0.9024	8.7071×10^{-5}

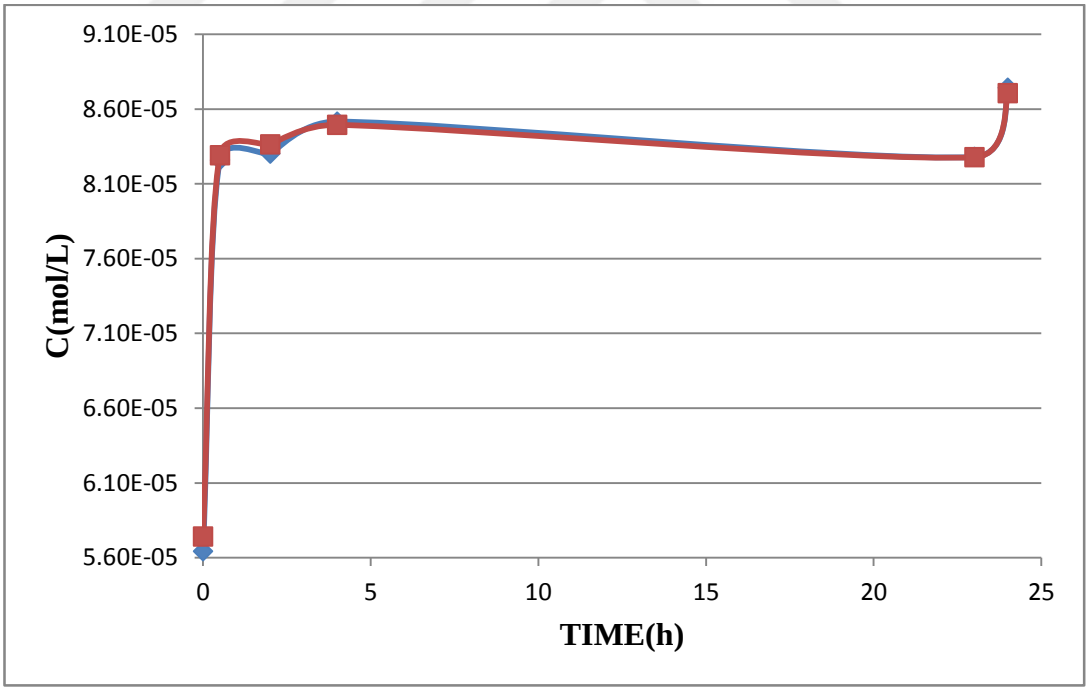


Figure 5.31. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD in (2:1 ratio) complex phosphate buffer (25ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

A decrease in the concentration of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid with the increase in the temperature was also in phosphate buffer observed, when the TBA:CD ratio is 2:1(Figure 5.30 and Figure 5.31). As a result complexation ratio decreases with increasing temeperature also in different ratio in different solvents. The complexation process can be thermodynamically more stable at lower temperature at these conditions.

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water at 37ºC are given in Table 5.13, Table 5.14 and Figure 5.14 (Section .5.3.2.1).

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water at 25ºC are given in Table 5.49, Table 5.50 and Figure 5.32.

Table 5.49. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water (25ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	D. water + TBA	0.6597	$4.7989x10^{-5}$
0.5	D.water+TBA+βCD	1.2147	$8.8361x10^{-5}$
2	D.water+TBA+βCD	1.2815	$9.3220x10^{-5}$
4	D.water+TBA+βCD	1.2989	$9.4486x10^{-5}$
23	D.water+TBA+βCD	1.2652	$9.2035x10^{-5}$
24	D.water+TBA+βCD	1.3293	$9.6697x10^{-5}$

Table 5.50. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water (25ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.6667	$4.8498x10^{-5}$
0.5	D.water+TBA+βCD	1.2364	$8.9940x10^{-5}$
2	D.water+TBA+βCD	1.2792	$9.3053x10^{-5}$
4	D.water+TBA+βCD	1.2956	$9.4246x10^{-5}$
23	D.water+TBA+βCD	1.2650	$9.2020x10^{-5}$
24	D.water+TBA+βCD	1.3256	$9.6428x10^{-5}$

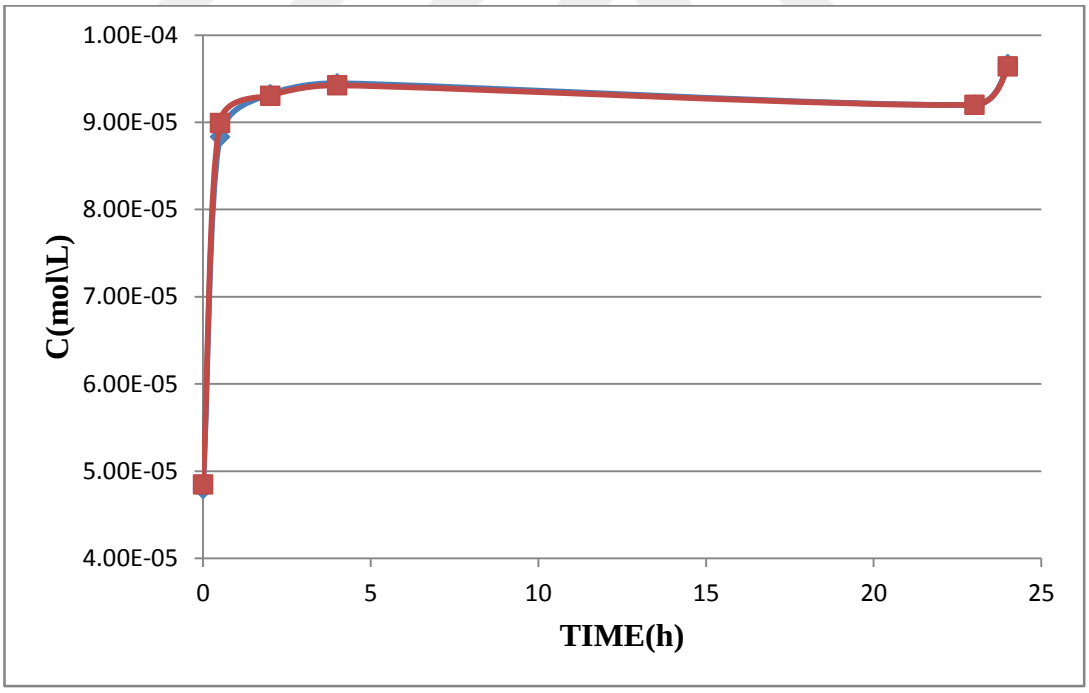


Figure 5.32. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD in (1:1 ratio) complex distilled water (25º) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

A decrease in the concentration of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid with the increase in the temperature was also in distilled water observed, when the TBA:CD ratio is 1:1(Figure 5.14 and Figure 5.32). As a result complexation ratio decreases with increasing temeperature also in different ratio in different solvents. The complexation process can be thermodynamically more stable at lower temperature at these conditions.

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer at 37ºC are given in Table 5.15, Table 5.16 and Figure 5.15 (Section 5.3.2.1).

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer at 25ºC are given in Table 5.51, Table 5.52 and Figure 5.33.

Table 5.51. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer (25ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.5918	$5.7102x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	1.0738	$1.0361x10^{-4}$
2	Phosphate Bf+TBA+βCD	1.1815	$1.1400x10^{-4}$
4	Phosphate Bf+TBA+βCD	1.2071	$1.1647x10^{-4}$
23	Phosphate Bf+TBA+βCD	1.1777	$1.1363x10^{-4}$
24	Phosphate Bf+TBA+βCD	1.2239	$1.1809x10^{-4}$

Table 5.52. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer (25ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.5945	5.7362×10^{-5}
0.5	Phosphate Bf+TBA+βCD	1.0766	1.0388×10^{-4}
2	Phosphate Bf+TBA+βCD	1.1765	1.1352×10^{-4}
4	Phosphate Bf+TBA+βCD	1.2065	1.1641×10^{-4}
23	Phosphate Bf+TBA+βCD	1.1771	1.1358×10^{-4}
24	Phosphate Bf+TBA+βCD	1.2276	1.1845×10^{-4}

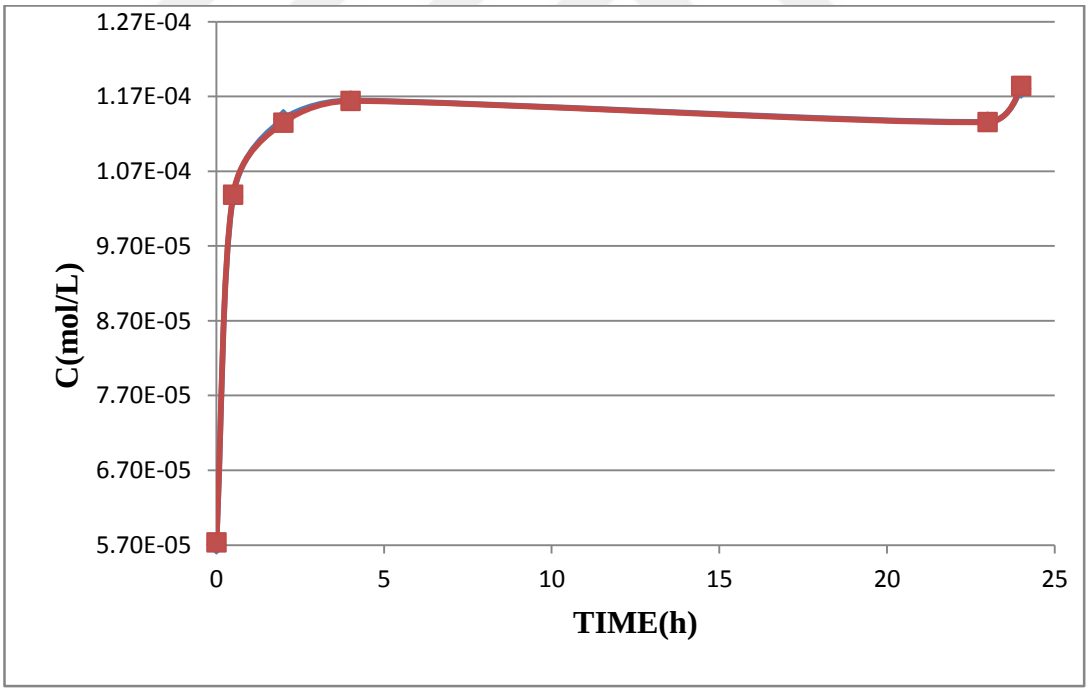


Figure 5.33. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex phosphate buffer (25ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

A decrease in the concentration of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid with the increase in the temperature was also in phosphate buffer observed, when the TBA:CD ratio is 1:1(Figure 5.15 and Figure 5.33). As a result complexation ratio decreases with increasing temeperature also in different ratio in different solvents. The complexation process can be thermodynamically more stable at lower temperature at these conditions.

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water at 37ºC are given in Table 5.21, Table 5.22 and Figure 5.18 (Section 5.3.2.2).

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water at 25ºC are given in Table 5.53, Table 5.54 and Figure 5.34.

Table 5.53. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water (25ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	D. water + TBA	0.6552	$4.7661x10^{-5}$
0.5	D.water+TBA+βCD	1.2889	$9.3759x10^{-5}$
2	D.water+TBA+βCD	1.3201	$9.6028x10^{-5}$
4	D.water+TBA+βCD	1.3495	$9.8167x10^{-5}$
23	D.water+TBA+βCD	1.3036	$9.4828x10^{-5}$
24	D.water+TBA+βCD	1.3708	$9.9716x10^{-5}$

Table 5.54. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water (25ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.6433	$4.6796x10^{-5}$
0.5	D.water+TBA+βCD	1.2849	$9.3468x10^{-5}$
2	D.water+TBA+βCD	1.3178	$9.5861x10^{-5}$
4	D.water+TBA+βCD	1.3487	$9.8109x10^{-5}$
23	D.water+TBA+βCD	1.3033	$9.4806x10^{-5}$
24	D.water+TBA+βCD	1.3638	$9.9207x10^{-5}$

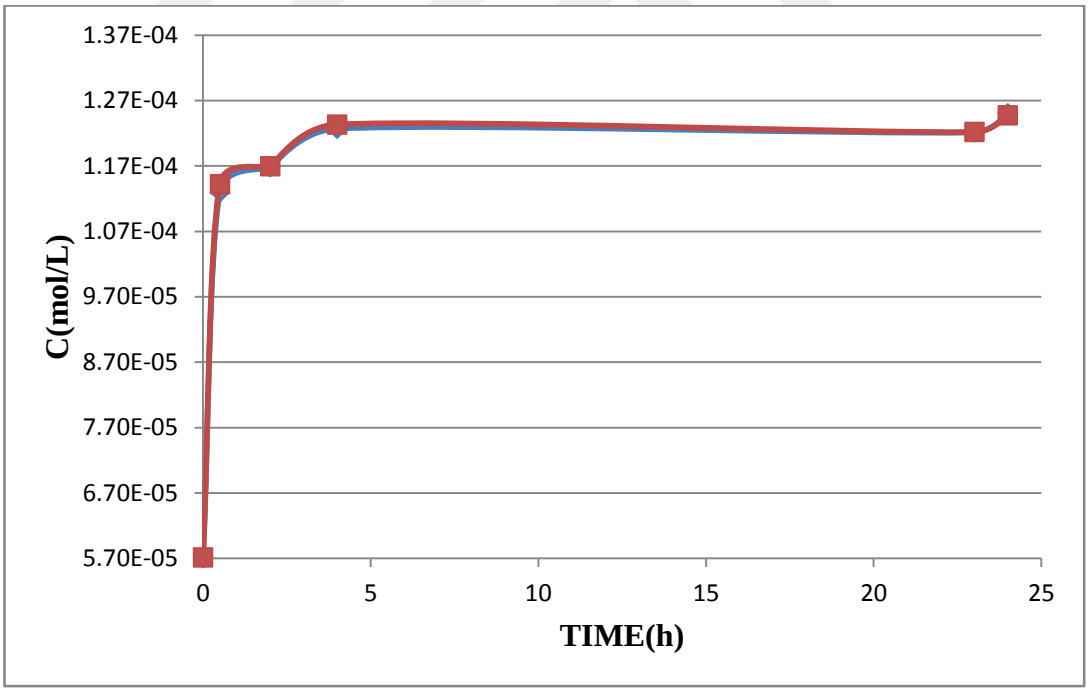


Figure 5.34. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD in (1:2 ratio) complex distilled water (25ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

A decrease in the concentration of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid with the increase in the temperature was also in distilled water observed, when the TBA:CD ratio is 1:2 (Figure 5.18 and Figure 5.34). As a result complexation ratio decreases with increasing temeperature also in different ratio in different solvents. The complexation process can be thermodynamically more stable at lower temperature at these conditions.

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer at 37ºC are given in Table 5.23, Table 5.24 and Figure 5.19 (Section 5.3.2.2).

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer at 25ºC are given in Table 5.55, Table 5.56 and Figure 5.35.

Table 5.55. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer (25ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.5914	$5.7063x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	1.1712	$1.1301x10^{-4}$
2	Phosphate Bf+TBA+βCD	1.2108	$1.1683x10^{-4}$
4	Phosphate Bf+TBA+βCD	1.2718	$1.2271x10^{-4}$
23	Phosphate Bf+TBA+βCD	1.2659	$1.2214x10^{-4}$
24	Phosphate Bf+TBA+βCD	1.2961	$1.2506x10^{-4}$

Table 5.56. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer (25ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.5924	$5.7159x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	1.1837	$1.1421x10^{-4}$
2	Phosphate Bf+TBA+βCD	1.2123	$1.1697x10^{-4}$
4	Phosphate Bf+TBA+βCD	1.2783	$1.2334x10^{-4}$
23	Phosphate Bf+TBA+βCD	1.2663	$1.2218x10^{-4}$
24	Phosphate Bf+TBA+βCD	1.2929	$1.2475x10^{-4}$

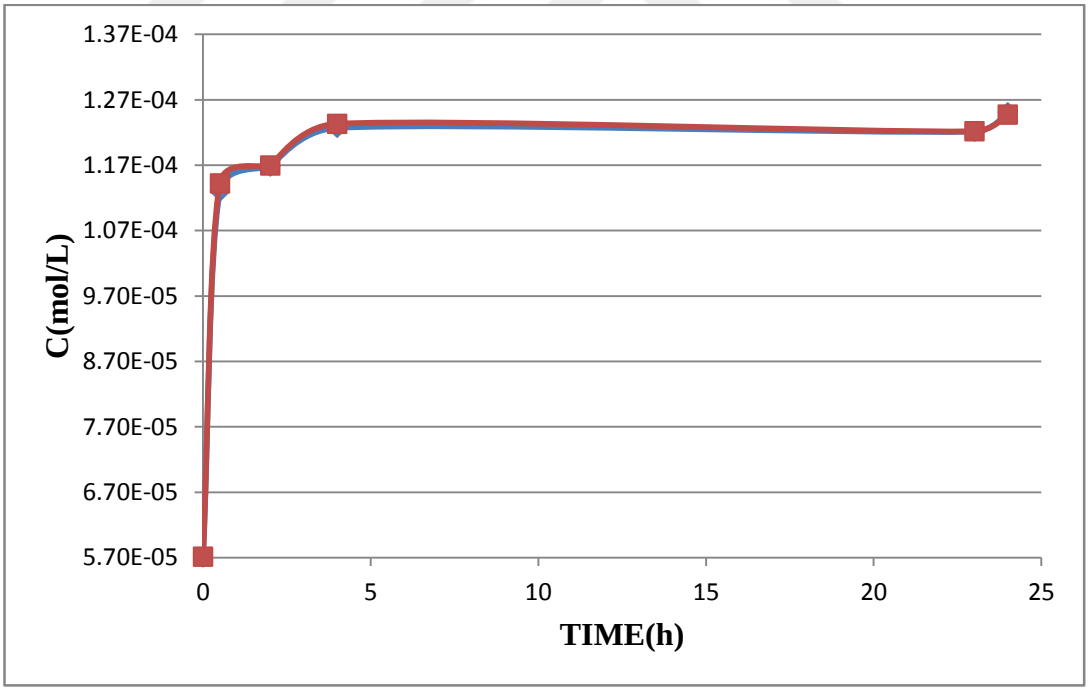


Figure 5.35. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex phosphate buffer (25ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

A decrease in the concentration of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid with the increase in the temperature was also in phosphate buffer observed, when the TBA:CD ratio is 1:2 (Figure 5.19 and Figure 5.35). As a result complexation ratio decreases with increasing temperature also in different ratio in different solvents. The complexation process can be thermodynamically more stable at lower temperature at these conditions.

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water at 37ºC are given in Table 5.25, Table 5.26 and Figure 5.20 (Section 5.3.2.2).

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water at 25ºC are given in Table 5.57, Table 5.58 and Figure 5.36.

Table 5.57. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water (25ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	D. water + TBA	0.6605	$4.8047x10^{-5}$
0.5	D.water+TBA+βCD	1.3277	$9.6581x10^{-5}$
2	D.water+TBA+βCD	1.369	$9.9585x10^{-5}$
4	D.water+TBA+βCD	1.3839	$1.0067x10^{-4}$
23	D.water+TBA+βCD	1.3443	$9.7789x10^{-5}$
24	D.water+TBA+βCD	1.405	$1.0220x10^{-4}$

Table 5.58. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water water (25ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.6595	$4.7974x10^{-5}$
0.5	D.water+TBA+βCD	1.3383	$9.7352x10^{-5}$
2	D.water+TBA+βCD	1.369	$9.9585x10^{-5}$
4	D.water+TBA+βCD	1.3837	$1.0065x10^{-4}$
23	D.water+TBA+βCD	1.3455	$9.7876x10^{-5}$
24	D.water+TBA+βCD	1.4057	$1.0226x10^{-4}$

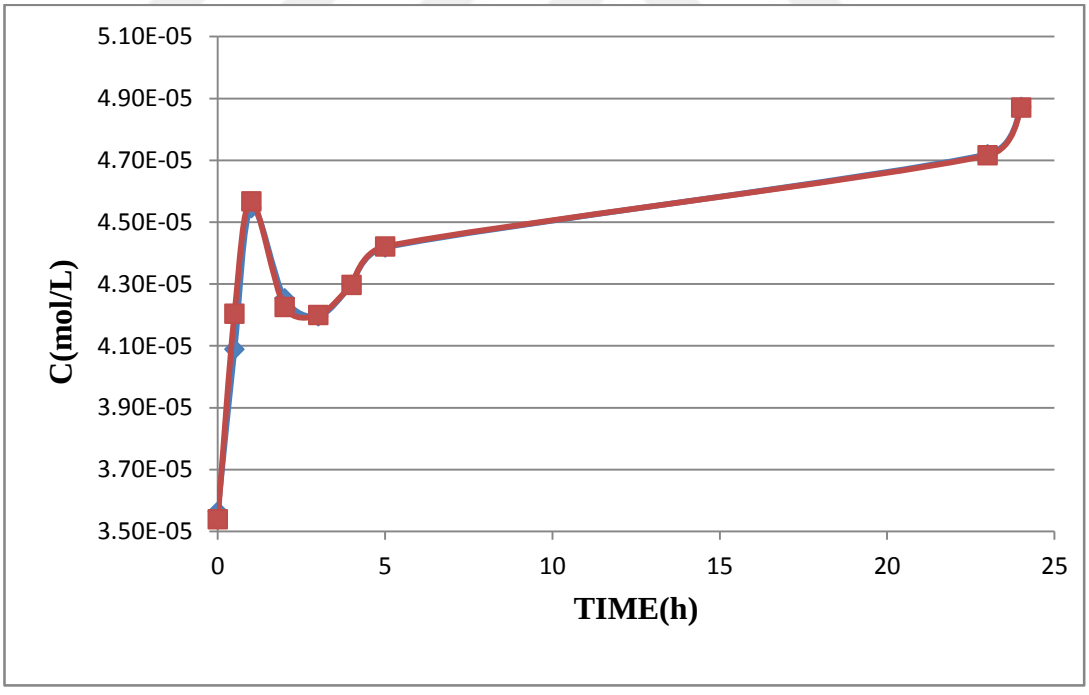


Figure 5.36. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex distilled water (25ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

A decrease in the concentration of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid with the increase in the temperature was also in distilled water observed, when the TBA:CD ratio is 1:4 (Figure 5.20 and Figure 5.36). As a result complexation ratio decreases with increasing temeperature also in different ratio in different solvents. The complexation process can be thermodynamically more stable at lower temperature at these conditions.

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer at 37ºC are given in Table 5.27, Table 5.28 and Figure 5.21 (Section 5.3.2.2).

The results for the measurements of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer at 25ºC are given in Table 5.59, Table 5.60 and Figure 5.37.

Table 5.59. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer (25ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.5959	$5.7497x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	1.2952	$1.2497x10^{-4}$
2	Phosphate Bf+TBA+βCD	1.2477	$1.2039x10^{-4}$
4	Phosphate Bf+TBA+βCD	1.2995	$1.2539x10^{-4}$
23	Phosphate Bf+TBA+βCD	1.266	$1.2215x10^{-4}$
24	Phosphate Bf+TBA+βCD	1.3148	$1.2686x10^{-4}$

Table 5.60. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer (25ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.5959	$5.7497x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	1.2944	$1.2489x10^{-4}$
2	Phosphate Bf+TBA+βCD	1.2485	$1.2047x10^{-4}$
4	Phosphate Bf+TBA+βCD	1.2955	$1.2500x10^{-4}$
23	Phosphate Bf+TBA+βCD	1.2669	$1.2224x10^{-4}$
24	Phosphate Bf+TBA+βCD	1.3158	$1.2696x10^{-4}$

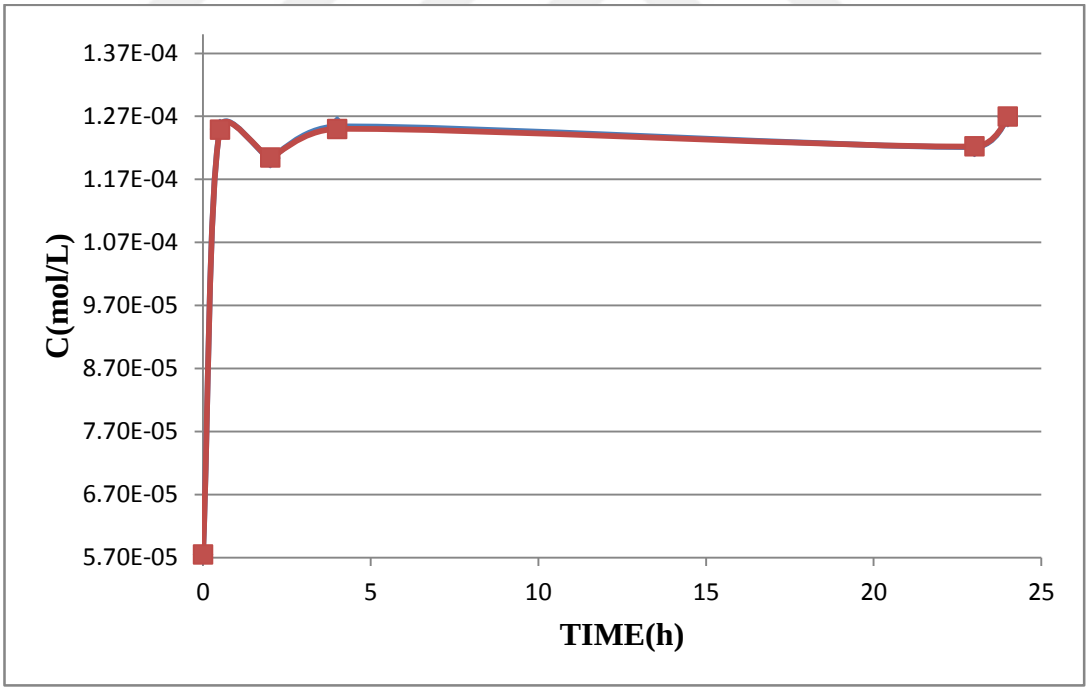


Figure 5.37. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex phosphate buffer (25ºC) (1st & 2nd trial) (blue line: 1st mtrial, red line: 2nd trial)

A decrease in the concentration of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid with the increase in the temperature was also in phosphate buffer observed, when the TBA:CD ratio is 1:4 (Figure 5.21 and Figure 5.37). As a result complexation ratio decreases with increasing temeperature also in different ratio in different solvents. The complexation process can be thermodynamically more stable at lower temperature at these conditions.

5.3.2.4. TBA: Cyclodextrin ratio

In this section, the effect of the TBA:β-CD ratio on the rate of complexation was investigated. Two derivatives, 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid and 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid- were studied.

The same procedure, which was applied in the determination of the effects of the factos, was applied in this section. The 2-thiobarbituric acid derivative-β-CD complex was studied at 24 hours mixing time as explained in Section 4.4.4.1. Absorbance values at 190 nm, where characteristic peak of thiobarbituric acid can be seen, were measured to determine the concentration of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid and 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid- in distilled water and phosphate buffer. The measurements were done for two trials. In each measuremet, the same solution was measured three times and the verage absorbance was calculated as described in Section (4.3.1.1.1).

The data of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid were found in the Sections 5.3.2.2. (Time Effect) and 5.3.2.3 (Temperature Effect) Tables (5.13-5.60) Figures (5.14-5.37).

The maximum absorbance and concentration at 24 hours for 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex in distilled water and phosphate buffer at 25ºC and 37ºC for each thiobarbituric acid-β-CD ratio were given in Tables 5.13-5.60.

Table 5.61.The maximum absorbance and concentration at 24 hours for 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex in distilled water for each ratio at 37ºC

Ratio (TBA:CD)	**A**	**C(mol/L)**
1:1	0.6022	$4.3824x10^{-5}$
1:2	0.6414	$4.6658x10^{-5}$
1:4	0.6697	$4.8717x10^{-5}$
2:1	0.6264	$4.5566x10^{-5}$
4:1	0.6011	$4.3726x10^{-5}$

There are no big differences between concentration results.

Table 5.62. The maximum absorbance and concentration at 24 hours for 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex in distilled water for each ratio at 25ºC

Ratio (TBA:CD)	**A**	**C(mol/L)**
1:1	1.3275	$9.6563x10^{-5}$
1:2	1.3673	$9.9462x10^{-5}$
1:4	1.4054	$1.0223x10^{-4}$
2:1	1.3069	$9.5068x10^{-5}$
4:1	1.2142	$8.8325x10^{-5}$

The highest concentration was obtained when the TBA:CD concentration was 1:4.

Table 5.63. The maximum absorbance and concentration at 24 hours for 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex in phosphate buffer for each ratio at 37ºC

Ratio (TBA:CD)	**A**	**C(mol/L)**
1:1	0.6921	$6.6775x10^{-5}$
1:2	0.7209	$6.9553x10^{-5}$
1:4	1.2751	$1.2303x10^{-4}$
2:1	0.7171	$6.9192x10^{-5}$
4:1	0.6954	$6.7098x10^{-5}$

The highest concentration was obtained when the TBA:CD concentration was 1:4.

Table 5.64. The maximum absorbance and concentration at 24 hours for 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD complex in phosphate buffer for each ratio at 25ºC

Ratio (TBA:CD)	**A**	**C(mol/L)**
1:1	1.2258	$1.1827x10^{-4}$
1:2	1.2945	$1.2491x10^{-4}$
1:4	1.3153	$1.2691x10^{-4}$
2:1	0.9043	$8.7254x10^{-5}$
4:1	0.8248	$7.7579x10^{-5}$

The highest concentration was obtained when the TBA:CD concentration was 1:4.

Considering the Tables, it has been found that highest solubility of TBA in distilled water can be obtained when TBA:CD concentration is 1:4 at the temperatures 25ºC and 37ºC. In

phosphate buffer, highest concentration of TBA can be obtained at the temperatures 25ºC and 37ºC when TBA:CD concentration is 1:4.

5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex was also studied at different ratios at different temperatures (25ºC and 37ºC) and in different solvents (distilled water and phosphate buffer).

The results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex (1:1 ratio), studied in distilled water at 37ºC were given in Table 5.65, Table 5.66 and Figure 5.38.

Table 5.65. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water (37ºC) (1st trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.5193	$1.9554x10^{-5}$
0.5	D. water+TBA+βCD	0.5585	$2.1030x10^{-5}$
1	D. water+TBA+βCD	0.6841	$2.5758x10^{-5}$
2	D. water+TBA+βCD	0.8811	$3.3176x10^{-5}$
3	D. water+TBA+βCD	0.8888	$3.3466x10^{-5}$
23	D. water+TBA+βCD	0.9046	$3.4061x10^{-5}$
24	D. water+TBA+βCD	0.9284	$3.4959x10^{-5}$

Table 5.66. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water (37ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water+TBA	0.5136	$1.9338x10^{-5}$
0.5	D. water+TBA+βCD	0.5588	$2.1040x10^{-5}$
1	D. water+TBA+βCD	0.6825	$2.5699x10^{-5}$
2	D. water+TBA+βCD	0.8798	$3.3127x10^{-5}$
3	D. water+TBA+βCD	0.8865	$3.3381x10^{-5}$
23	D. water+TBA+βCD	0.9049	$3.4074x10^{-5}$
24	D. water+TBA+βCD	0.9290	$3.4981x10^{-5}$

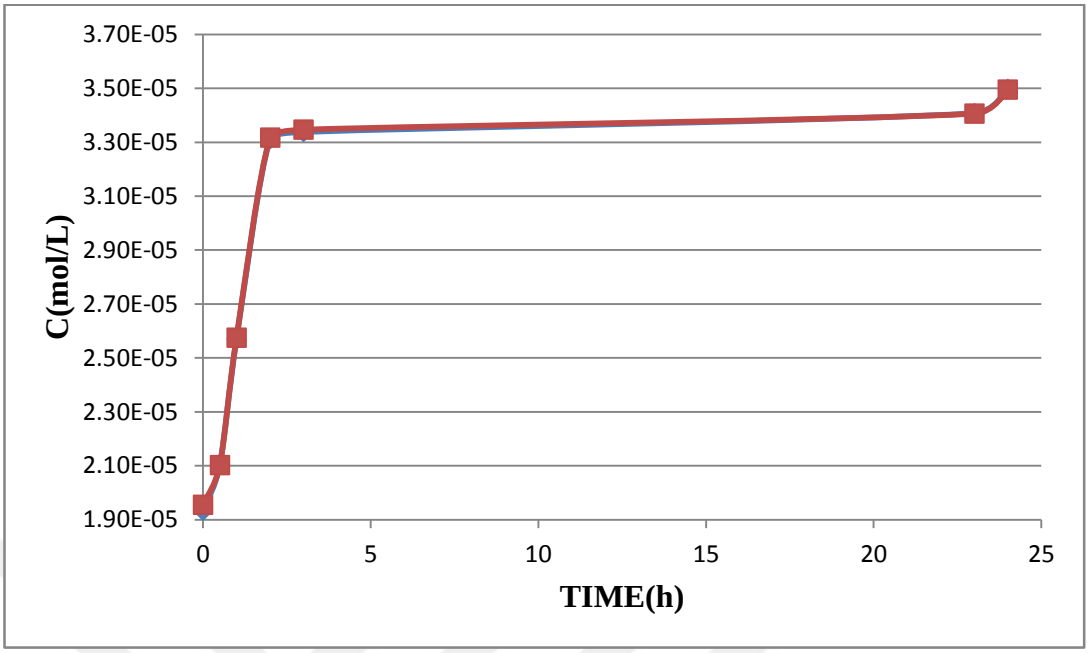


Figure 5.38. Concentration vs. time graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water (37ºC) (1st & 2nd trial)

The results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex(1:2 ratio), studied in distilled water at 37ºC were given in Table 5.67, Table 5.68 and Figure 5.39.

Table 5.67. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water (37ºC) (1st trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.3682	$1.3863x10^{-5}$
0.5	D. water+TBA+βCD	0.5098	$1.9196x10^{-5}$
1	D. water+TBA+βCD	0.5698	$2.1456x10^{-5}$
2	D. water+TBA+βCD	0.7401	$2.7866x10^{-5}$
3	D. water+TBA+βCD	0.9182	$3.4575x10^{-5}$
23	D. water+TBA+βCD	0.8688	$3.2713x10^{-5}$
24	D. water+TBA+βCD	0.9476	$3.5682x10^{-5}$

Table 5.68. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water (37ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.3696	$1.3915x10^{-5}$
0.5	D. water+TBA+βCD	0.5117	$1.9266x10^{-5}$
1	D. water+TBA+βCD	0.5700	$2.1461x10^{-5}$
2	D. water+TBA+βCD	0.7363	$2.7723x10^{-5}$
3	D. water+TBA+βCD	0.9183	$3.4577x10^{-5}$
23	D. water+TBA+βCD	0.8792	$3.3106x10^{-5}$
24	D. water+TBA+βCD	0.9455	$3.5601x10^{-5}$

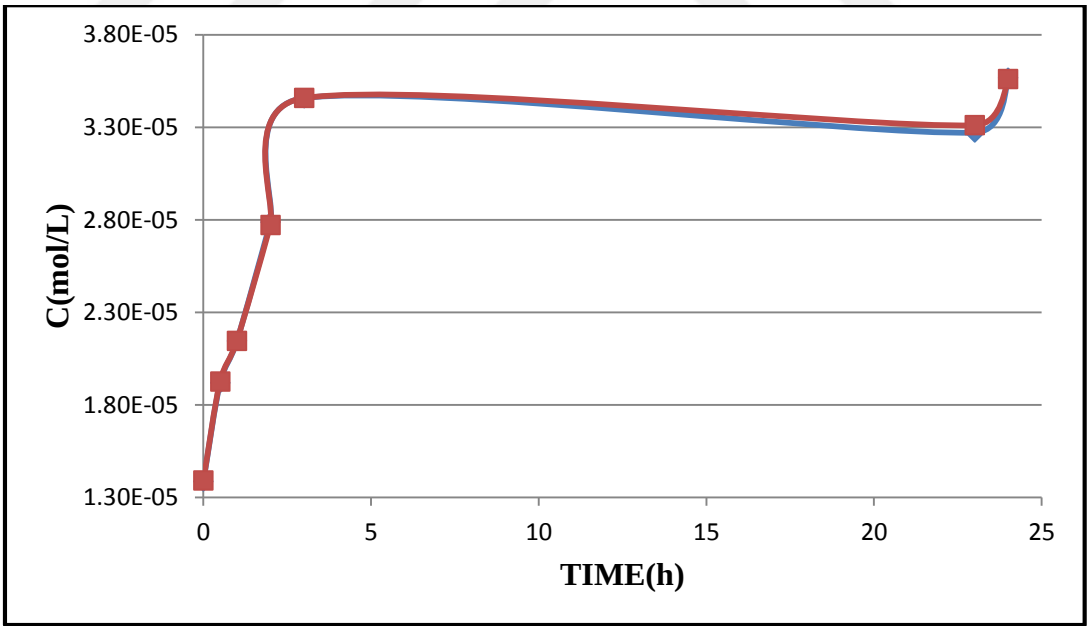


Figure 5.39. Concentration vs.time graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD in (1:2 ratio) complex in distilled water (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex(1:4 ratio), studied in distilled water at 37ºC were given in Table 5.69, Table 5.70 and Figure 5.40.

Table 5.69. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water (37ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	D. water + TBA	0.3905	$1.4702x10^{-5}$
0.5	D. water+TBA+βCD	0.4812	$1.8118x10^{-5}$
1	D. water+TBA+βCD	0.5909	$2.2248x10^{-5}$
2	D. water+TBA+βCD	0.8389	$3.1589x10^{-5}$
3	D. water+TBA+βCD	0.9498	$3.5765x10^{-5}$
23	D. water+TBA+βCD	0.7949	$2.9932x10^{-5}$
24	D. water+TBA+βCD	0.9878	$3.7194x10^{-5}$

Table 5.70. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water (37ºC) (2nd trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	D. water + TBA	0.3934	$1.4812x10^{-5}$
0.5	D. water+TBA+βCD	0.4842	$1.8231x10^{-5}$
1	D. water+TBA+βCD	0.5903	$2.2228x10^{-5}$
2	D. water+TBA+βCD	0.8369	$3.1513x10^{-5}$
3	D. water+TBA+βCD	0.9487	$3.5723x10^{-5}$
23	D. water+TBA+βCD	0.7942	$2.9904x10^{-5}$
24	D. water+TBA+βCD	0.9861	$3.7130x10^{-5}$

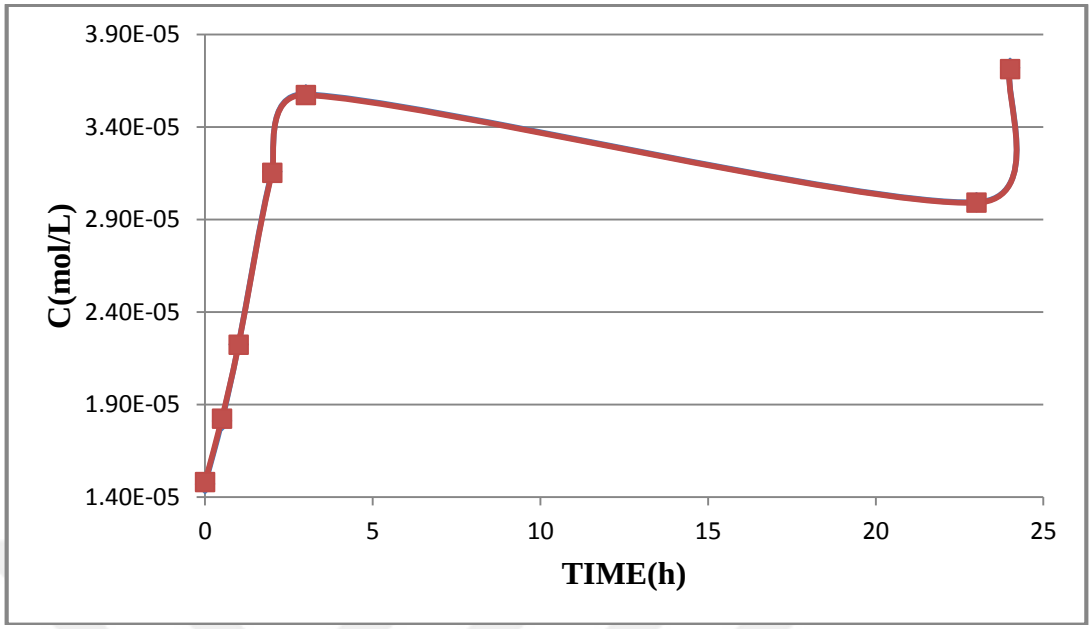


Figure 5.40. Concentration vs. time graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD in (1:4 ratio) complex in distilled water (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The maximum absorbance and concentration at 24 hours 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex in distilled water at 37ºC for each thiobarbituric acid-CD ratios were given in Table 5.71.

Table 5.71.The maximum absorbance and concentration values at 24 hours for the 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex in distilled water for each ratio at 37ºC

Ratio (TBA:CD)	**A**	**C(mol/L)**
1:1	0.9287	$3.4786x10^{-5}$
1:2	0.9466	$3.5642x10^{-5}$
1:4	0.7779	$2.9292x10^{-5}$

There no big differences between concentration results.

The results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex(1:1 ratio), studied in phosphate buffer at 37ºC were given in Table 5.72, Table 5.73 and Figure 5.41.

Table 5.72. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer (37ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.3982	$2.7142x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.4576	$3.1191x10^{-5}$
1	Phosphate Bf+TBA+βCD	0.5689	$3.8777x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.7696	$5.2457x10^{-5}$
3	Phosphate Bf+TBA+βCD	0.8877	$6.0507x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.8757	$5.9689x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.9141	$6.2307x10^{-5}$

Table 5.73. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer (37ºC) (2nd trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.3963	$2.7012x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.4560	$3.1082x10^{-5}$
1	Phosphate Bf+TBA+βCD	0.5734	$3.9084x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.7716	$5.2594x10^{-5}$
3	Phosphate Bf+TBA+βCD	0.8869	$6.0453x10^{-05}$
23	Phosphate Bf+TBA+βCD	0.8777	$5.9826x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.9139	$6.2293x10^{-5}$

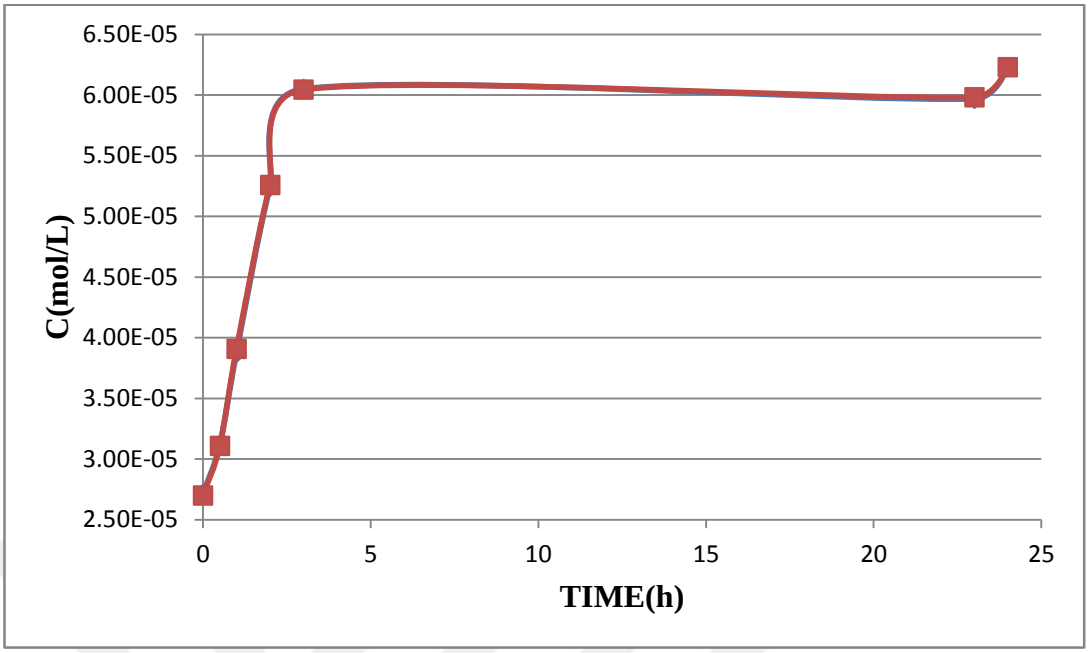


Figure 5.41. Concentration vs. time graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD in (1:1 ratio) complex in phosphate buffer (37ºC) (1st & 2nd trial)

The results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex(1:2 ratio), studied in phosphate buffer at 37ºC were given in Table 5.74, Table 5.75 and Figure 5.42.

Table 5.74. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer (37ºC) (1st trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.4623	$3.1511x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.5559	$3.7891x10^{-5}$
1	Phosphate Bf+TBA+βCD	0.5711	$3.8927x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.6900	$4.7032x10^{-5}$
3	Phosphate Bf+TBA+βCD	0.7679	$5.2341x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.7360	$5.0167x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.8831	$6.0194x10^{-5}$

Table 5.75. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer (37ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.4626	3.1532×10^{-5}
0.5	Phosphate Bf+TBA+βCD	0.5613	3.8259×10^{-5}
1	Phosphate Bf+TBA+βCD	0.5728	3.9043×10^{-5}
2	Phosphate Bf+TBA+βCD	0.6891	4.6970×10^{-5}
3	Phosphate Bf+TBA+βCD	0.7737	5.2737×10^{-5}
23	Phosphate Bf+TBA+βCD	0.7374	5.0262×10^{-5}
24	Phosphate Bf+TBA+βCD	0.8853	6.0344×10^{-5}

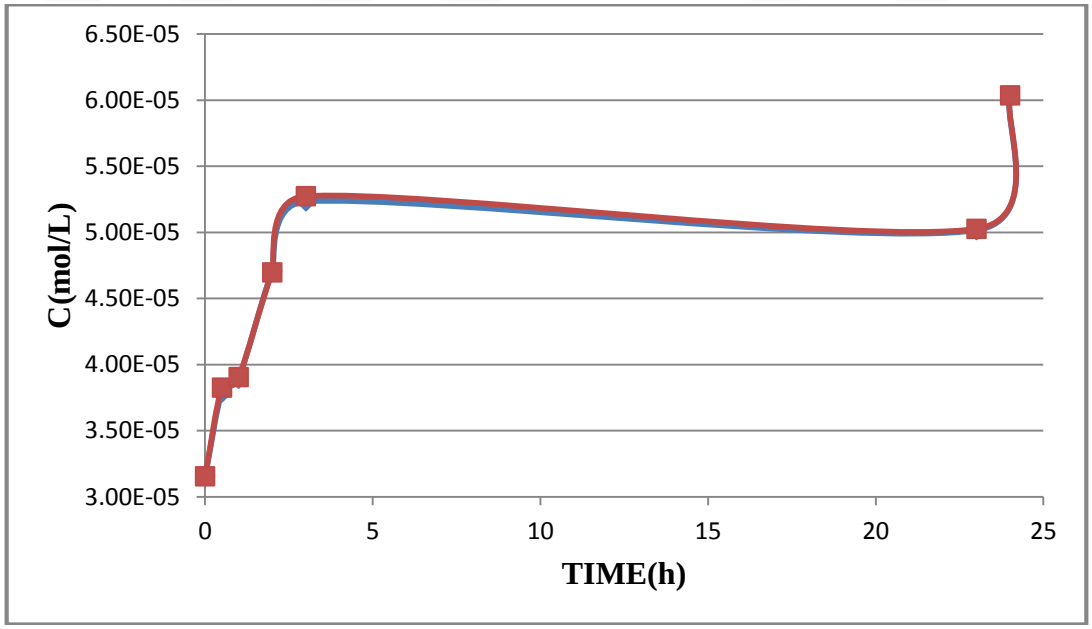


Figure 5.42. Concentration vs. time graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD in (1:2 ratio) complex in phosphate buffer (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex(1:4 ratio), studied in phosphate buffer at 37ºC were given in Table 5.76, Table 5.77 and Figure 5.43.

Table 5.76. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer (37ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.4776	$3.2554x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.5491	$3.7428x10^{-5}$
1	Phosphate Bf+TBA+βCD	0.5574	$3.7993x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.6263	$4.269x10^{-5}$
3	Phosphate Bf+TBA+βCD	0.8777	$5.9826x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.7913	$5.3936x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.8651	$5.8967x10^{-5}$

Table 5.77. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer (37ºC) (2nd trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	Phosphate Bf + TBA	0.4762	$3.2459x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.5485	$3.7387x10^{-5}$
1	Phosphate Bf+TBA+βCD	0.5656	$3.8552x10^{-05}$
2	Phosphate Bf+TBA+βCD	0.6264	$4.2696x10^{-5}$
3	Phosphate Bf+TBA+βCD	0.8775	$5.9812x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.7909	$5.3909x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.8631	$5.8830x10^{-5}$

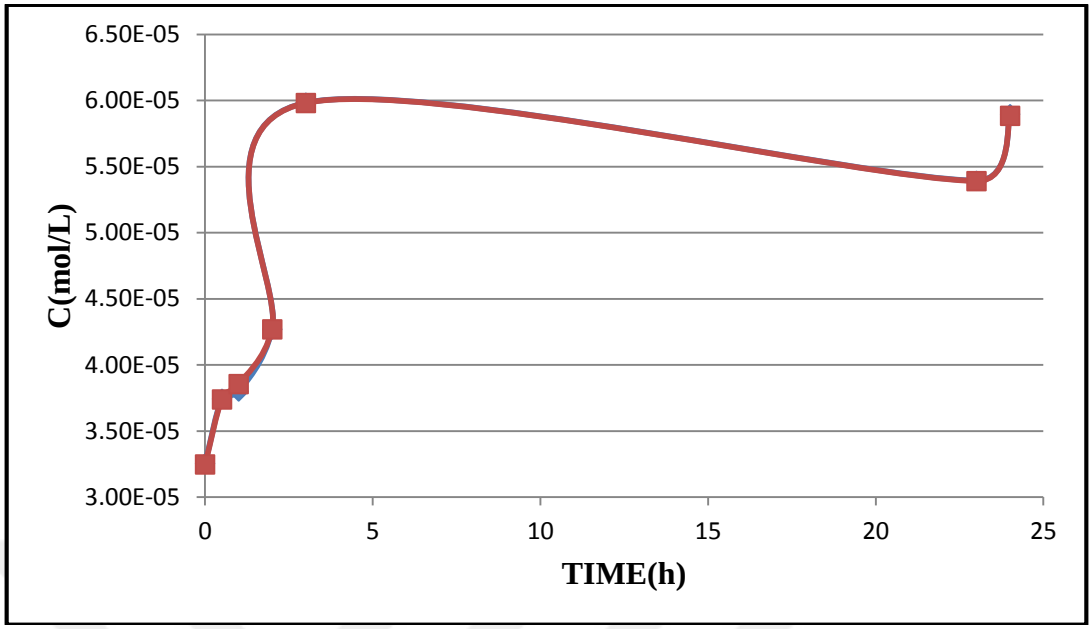


Figure 5.43. Concentration vs. time graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD in (1:4 ratio) complex in phosphate buffer (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial

The maximum absorbance and concentration at 24 hours 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex in phosphate buffer at 37ºC for each thiobarbituric acid-CD ratio were given in Table 5.78.

Table 5.78. The maximum absorbance and concentration at 24 hours for the 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex in phosphate buffer for each ratio at 37ºC

Ratio (TBA:CD)	**A**	**C(mol/L)**
1:1	0.914	$6.23x10^{-5}$
1:2	0.8842	$6.0269x10^{-5}$
1:4	0.8767	$5.9819x10^{-5}$

The highest concentration was obtained when the TBA:CD concentration was 1:1.

The results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex(1:1 ratio), studied in distilled water at 25ºC were given in Table 5.79, Table 5.80 and Figure 5.44.

Table 5.79. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water (25ºC) (1st trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.3938	$1.4827x10^{-5}$
0.5	D. water+TBA+βCD	0.5405	$2.0351x10^{-5}$
1	D. water+TBA+βCD	0.7778	$2.9288x10^{-5}$
2	D. water+TBA+βCD	0.8570	$3.2268x10^{-5}$
3	D. water+TBA+βCD	0.8837	$3.3276x10^{-5}$
23	D. water+TBA+βCD	0.9676	$3.6433x10^{-5}$
24	D. water+TBA+βCD	0.8442	$3.1788x10^{-5}$

Table 5.80. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water (25ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.3858	$1.4525x10^{-5}$
0.5	D. water+TBA+βCD	0.5321	$2.0034x10^{-5}$
1	D. water+TBA+βCD	0.7715	$2.9049x10^{-5}$
2	D. water+TBA+βCD	0.8591	$3.2347x10^{-5}$
3	D. water+TBA+βCD	0.8752	$3.2956x10^{-5}$
23	D. water+TBA+βCD	0.9717	$3.6587x10^{-5}$
24	D. water+TBA+βCD	0.8410	$3.1666x10^{-5}$

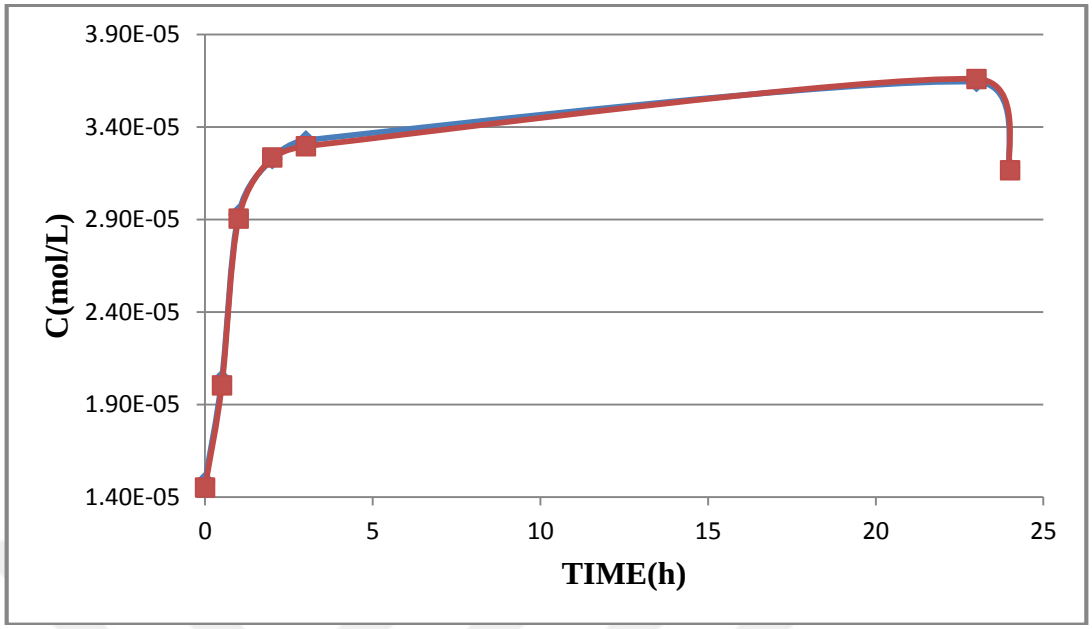


Figure 5.44. Concentration vs. time graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD in (1:1 ratio)complex in distilled water (25ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex(1:2 ratio), studied in distilled water at 25ºC were given in Table 5.81, Table 5.82 and Figure 5.45.

Table 5.81. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid -β-CD (1:2 ratio) complex in distilled water (25ºC) (1st trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.5375	$2.0238x10^{-5}$
0.5	D. water+TBA+βCD	0.5927	$2.2318x10^{-5}$
1	D. water+TBA+βCD	0.7284	$2.7426x10^{-5}$
2	D. water+TBA+βCD	0.7453	$2.8062x10^{-5}$
3	D. water+TBA+βCD	0.8170	$3.0762x10^{-5}$
23	D. water+TBA+βCD	0.7762	$2.9228x10^{-5}$
24	D. water+TBA+βCD	0.8542	$3.2163x10^{-5}$

Table 5.82. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water (25ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.5365	$2.0202x10^{-5}$
0.5	D. water+TBA+βCD	0.6036	$2.2727x10^{-5}$
1	D. water+TBA+βCD	0.7230	$2.7224x10^{-5}$
2	D. water+TBA+βCD	0.7448	$2.8045x10^{-5}$
3	D. water+TBA+βCD	0.8185	$3.0820x10^{-5}$
23	D. water+TBA+βCD	0.7729	$2.9102x10^{-5}$
24	D. water+TBA+βCD	0.8550	$3.2193x10^{-0}$

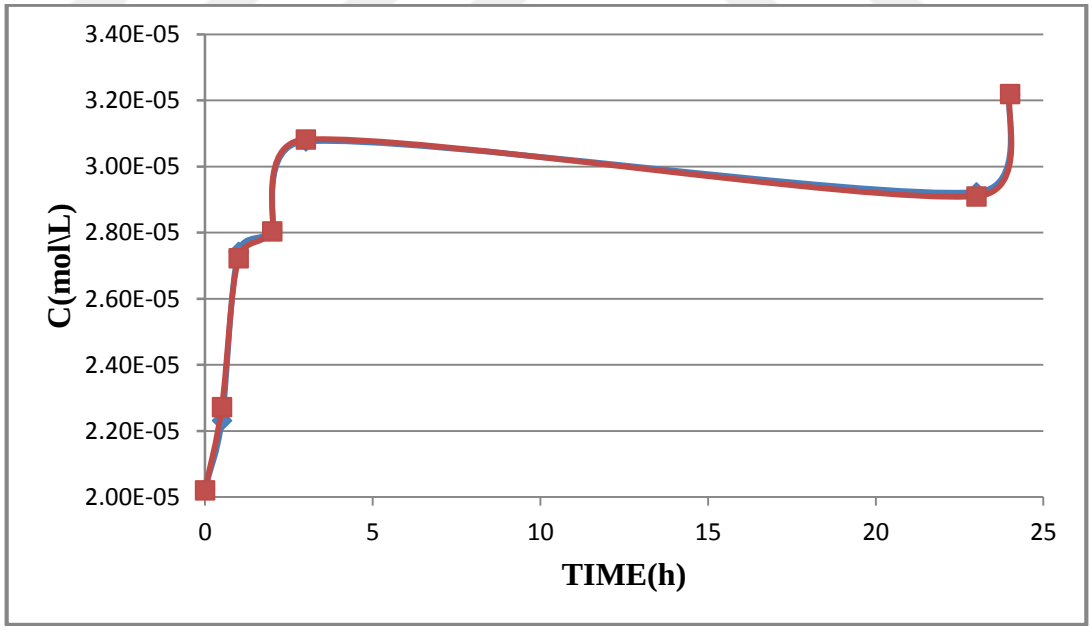


Figure 5.45. Concentration vs. time graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD in (1:2 ratio) complex in distilled water (25ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex(1:4 ratio), studied in distilled water at 25ºC were given in Table 5.83, Table 5.84 and Figure 5.46.

Table 5.83. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water (25ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	D. water + TBA	0.3141	$1.1826x10^{-5}$
0.5	D. water+TBA+βCD	0.4294	$1.6167x10^{-5}$
1	D. water+TBA+βCD	0.6228	$2.3451x10^{-5}$
2	D. water+TBA+βCD	0.8115	$3.0556x10^{-5}$
3	D. water+TBA+βCD	0.8244	$3.1043x10^{-5}$
23	D. water+TBA+βCD	0.8786	$3.3084x10^{-5}$
24	D. water+TBA+βCD	0.9128	$3.4371x10^{-5}$

Table 5.84. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water (25ºC) (2nd trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	D. water + TBA	0.3166	$1.1920x10^{-5}$
0.5	D. water+TBA+βCD	0.4392	$1.6536x10^{-5}$
1	D. water+TBA+βCD	0.6228	$2.3451x10^{-5}$
2	D. water+TBA+βCD	0.7968	$3.0002x10^{-5}$
3	D. water+TBA+βCD	0.8235	$3.1007x10^{-5}$
23	D. water+TBA+βCD	0.8820	$3.3211x10^{-5}$
24	D. water+TBA+βCD	0.9060	$3.4113x10^{-5}$

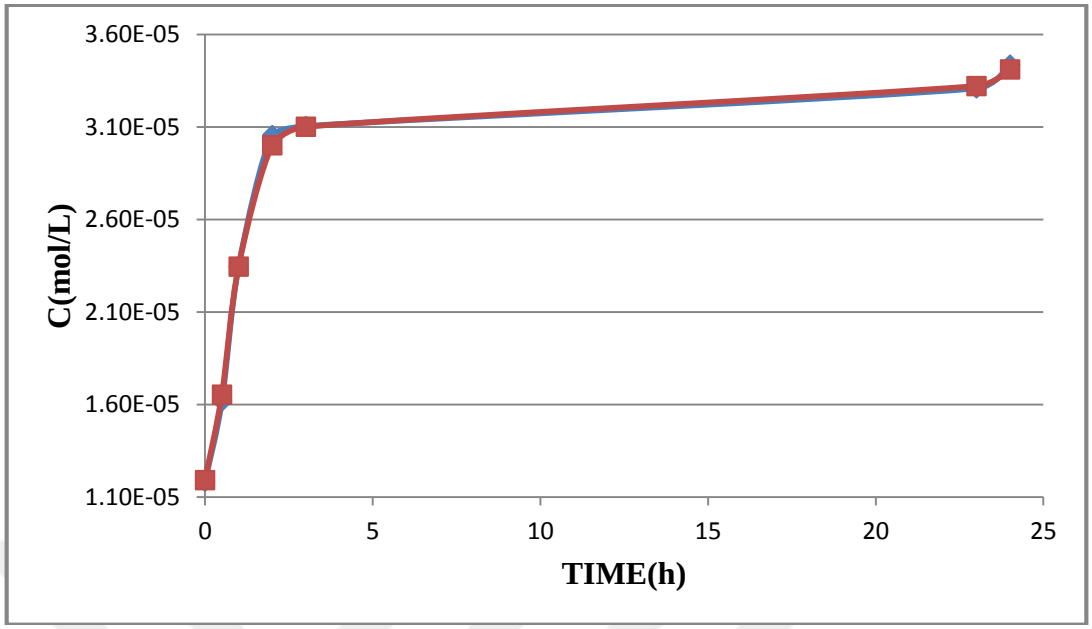


Figure 5.46. . Concentration vs. time graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD in (1:4 ratio) complex in distilled water (25ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The maximum absorbance and concentration at 24 hours 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex in distilled water at 25ºC for each thiobarbituric acid-CD ratio were given in Table 5.85.

Table 5.85. The maximum absorbance and concentration at 24 hours for the 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex distilled water in each ratio at 25ºC

Ratio (TBA:CD)	**A**	**C(mol/L)**
1:1	0.9697	$3.651x10^{-5}$
1:2	0.8546	$3.2178x10^{-5}$
1:4	0.9094	$3.4242x10^{-5}$

The highest concentration was obtained when the TBA:CD concentration was 1:1.

The results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex(1:1 ratio), studied in phosphate buffer at 25ºC were given in Table 5.86, Table 5.87 and Figure 5.47.

Table 5.86. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer (25ºC) (1st trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.5218	$3.5567x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.5637	$3.8423x10^{-5}$
1	Phosphate Bf+TBA+βCD	0.6686	$4.5573x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.7683	$5.2369x10^{-5}$
3	Phosphate Bf+TBA+βCD	0.8188	$5.5811x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.8715	$5.9403x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.8613	$5.8708x10^{-5}$

Table 5.87. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer (25ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.5211	$3.5519x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.5634	$3.8402x10^{-5}$
1	Phosphate Bf+TBA+βCD	0.6696	$4.5641x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.7723	$5.2641x10^{-5}$
3	Phosphate Bf+TBA+βCD	0.8175	$5.5722x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.8791	$5.9921x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.8628	$5.8810x10^{-5}$

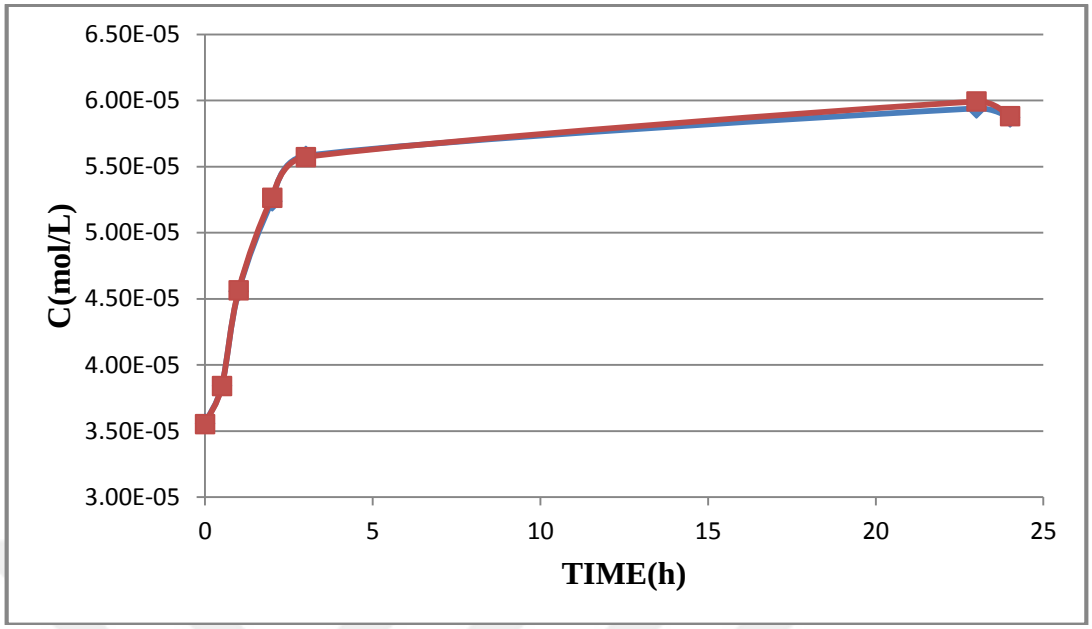


Figure 5.47. Concentration vs. time graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD in (1:1 ratio) complex in phosphate buffer (25ºC) (1st & 2nd trial))(blue line: 1st trial, red line :2nd trial)

The results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex(1:2 ratio), studied in phosphate buffer at 25ºC were given in Table 5.88, Table 5.89 and Figure 5.48.

Table 5.88. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD(1:2 ratio) complex in phosphate buffer (25ºC) (1st trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.6807	$4.6398x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.6911	$4.7107x10^{-5}$
1	Phosphate Bf+TBA+βCD	0.8596	$5.8592x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.9177	$6.2552x10^{-5}$
3	Phosphate Bf+TBA+βCD	0.9147	$6.2347x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.8840	$6.0255x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.9894	$6.7439x10^{-5}$

Table 5.89. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer (25ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	Phosphate Bf + TBA	0.6774	$4.6173x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.7037	$4.7965x10^{-5}$
1	Phosphate Bf+TBA+βCD	0.8612	$5.8701x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.9160	$6.2436x10^{-5}$
3	Phosphate Bf+TBA+βCD	0.9154	$6.2395x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.8811	$6.0057x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.9914	$6.7575x10^{-5}$

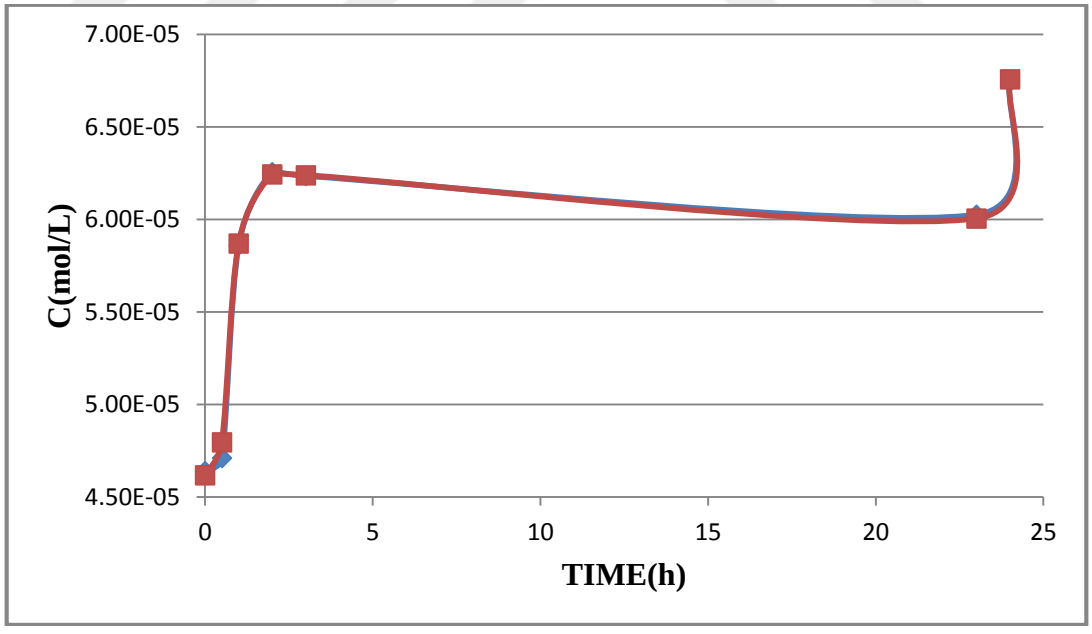


Figure 5.48. Concentration vs. time graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD in (1:2 ratio) complex in phosphate buffer (25ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex(1:4 ratio), studied in phosphate buffer at 25ºC were given in Table 5.90, Table 5.91 and Figure 5.49.

Table 5.90. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer (25ºC) (1st trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.4819	$3.2847x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.5799	$3.9527x10^{-5}$
1	Phosphate Bf+TBA+βCD	0.7160	$4.8804x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.8102	$5.5225x10^{-5}$
3	Phosphate Bf+TBA+βCD	0.9124	$6.2191x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.9725	$6.6287x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.9451	$6.4420x10^{-5}$

Table 5.91. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer (25ºC) (2nd trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.4790	$3.2649x10^{-5}$
0.5	Phosphate Bf+TBA+βCD	0.5804	$3.9561x10^{-5}$
1	Phosphate Bf+TBA+βCD	0.7150	$4.8736x10^{-5}$
2	Phosphate Bf+TBA+βCD	0.8098	$5.5197x10^{-5}$
3	Phosphate Bf+TBA+βCD	0.9137	$6.2279x10^{-5}$
23	Phosphate Bf+TBA+βCD	0.9744	$6.6417x10^{-5}$
24	Phosphate Bf+TBA+βCD	0.9537	$6.5006x10^{-5}$

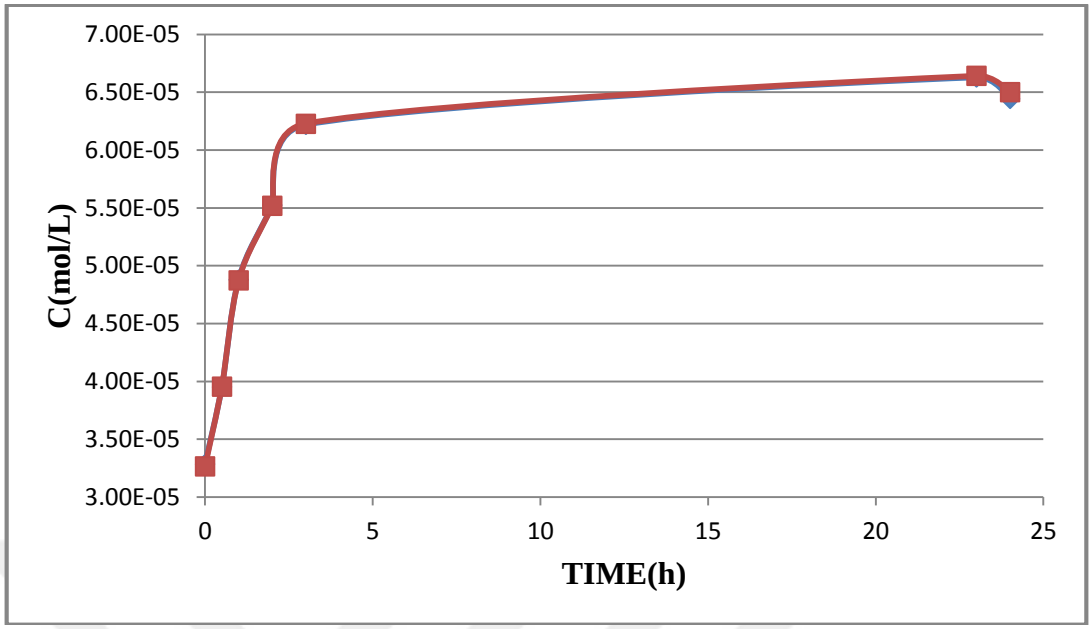


Figure 5.49. Concentration vs. time graph of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD in (1:4 ratio) complex in phosphate buffer (25ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The maximum absorbance and concentration at 24 hours 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex in phosphate buffer at 25ºC for each thiobarbituric acid-CD ratio were given in Table 5.92.

Table 5.92. The maximum absorbance and concentration at 24 hours for the 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD complex phosphate buffer in each ratio at 25ºC

Ratio (TBA:CD)	**A**	**C(mol/L)**
1:1	0.8753	$5.9662x10^{-5}$
1:2	0.9904	$6.7507x10^{-5}$
1:4	0.9735	$6.6352x10^{-5}$

The highest concentation was obtained when the TBA:CD concentration was 1:2.

Considering the Tables, it has been found that highest solubility of TBA in distilled water can be obtained when TBA:CD concentration is 1:1 at the temperatures 25ºC and 37ºC. In

phosphate buffer, highest concentration of TBA can be obtained at 25ºC when TBA:CD concentration is 1:2 and at 37ºC when TBA:CD concentration is 1:1.

5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid (1:4 ratio at 25ºC) was foun to be the highest in this study.

5.3.2.5. Effect of Structrure of β-CD

Two derivatives of cyclodextrin, β-CD (Figure 2.9) and 2-hydroxypropyl-β-CD, HPβ-CD (Figure 2.14) were used for complexation. To be able to determine the effect of the structure of cyclodextrin on the complexation ratio, two processes, which were carried out at the same conditions except cyclodextrin type were chosen and the concemtration of TBA in the aqueous solution was determined after mixing TBA and CD for 24 hours as explained in Section 4.4.4.1. Again the absorbance values at 190 nm were measured and measurements were done for two trials. In each measurement, the same solution was measured three times and the average absorbance was calculated as described in Section (4.3.1.1.1).

Mixing processes were conducted both in distilled water and phosphate buffer. The temperature was chosen as 37ºC.

The results of the processes conducted with HPβ-CD in distilled water at 37ºC are given in Table 5.93, Table 5.94 and Figure 5.50.

Table 5.93. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-2-hydroxypropyl-β-CD (1:1 ratio) complex in distilled water (37ºC) (1st trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.6452	4.6934×10^{-5}
0.5	D.water+TBA+HPβCD	1.0859	7.8992×10^{-5}
2	D.water+TBA+HPβCD	0.6651	4.8381×10^{-5}
4	D.water+TBA+HPβCD	0.7415	5.3939×10^{-5}
23	D.water+TBA+HPβCD	0.7314	5.3204×10^{-5}
24	D.water+TBA+HPβCD	0.7734	5.6260×10^{-5}

Table 5.94. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-2-hydroxypropyl-β-CD (1:1 ratio) complex in distilled water (37ºC) (2nd trial)

Time (h)	Type of solution	A	C (mol/L)
0	D. water + TBA	0.6529	4.7494×10^{-5}
0.5	D.water+TBA+HPβCD	1.0889	7.9210×10^{-5}
2	D.water+TBA+HPβCD	0.6654	4.8403×10^{-5}
4	D.water+TBA+HPβCD	0.7554	5.4950×10^{-5}
23	D.water+TBA+HPβCD	0.7325	5.3284×10^{-5}
24	D.water+TBA+HPβCD	0.771	5.6085×10^{-5}

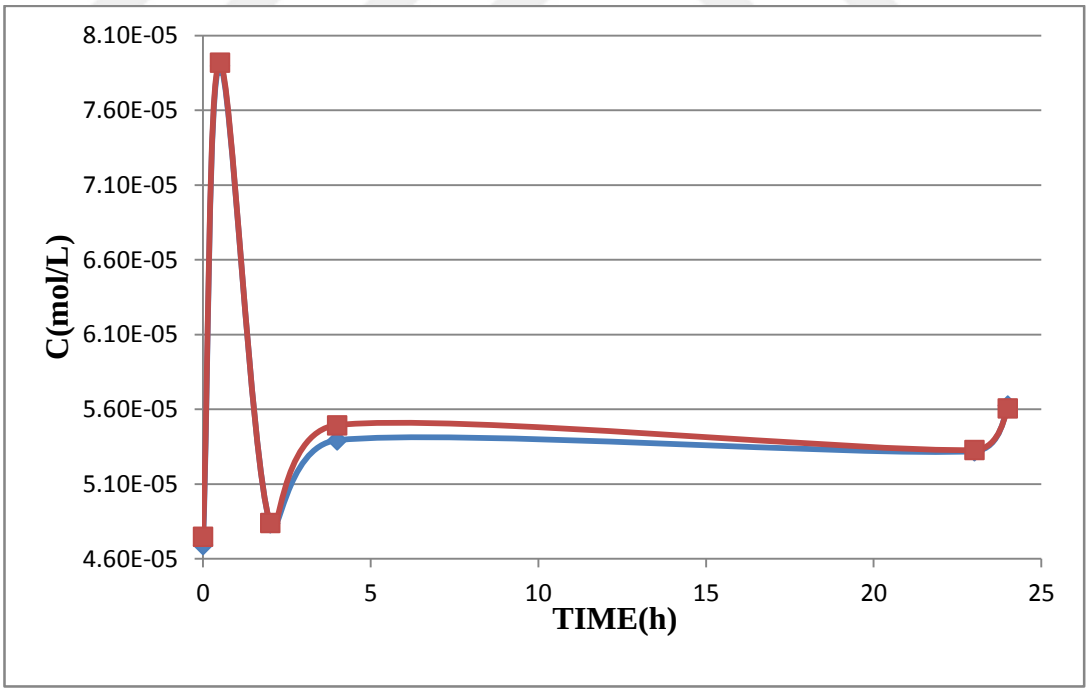


Figure 5.50. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2thiobarbituric acid-2-hydroxypropyl-β-CD complex (1:1 ratio) in distilled water (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The maximum concentration of TBA in distilled water was obtained after half an hour mixing, and then its concentration in distilled water decreased. The highest concentration of TBA in distilled water containing β-CD was obtained as $4.8717x10^{-5}$ mol/L after 24 hours.

The results of the processes conducted with HPβ-CD in phosphate buffer at 37ºC are given in Table 5.95, Table 5.96 and Figure 5.51.

Table 5.95. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-2-hydroxypropyl-β-CD (1:1 ratio) complex in phosphate buffer (37ºC) (1^{st} trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.5923	$5.7150x10^{-5}$
0.5	Phosphate Bf+TBA+HPβCD	1.1602	$1.1195x10^{-4}$
2	Phosphate Bf+TBA+HPβCD	0.7569	$7.3032x10^{-5}$
4	Phosphate Bf+TBA+HPβCD	0.7931	$7.6525x10^{-5}$
23	Phosphate Bf+TBA+HPβCD	0.7677	$7.4074x10^{-5}$
24	Phosphate Bf+TBA+HPβCD	0.8196	$7.9081x10^{-5}$

Table 5.96. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-2-hydroxypropyl-β-CD (1:1 ratio) complex in phosphate buffer (37ºC) (2^{nd} trial)

Time (h)	**Type of solution**	**A**	**C (mol/L)**
0	Phosphate Bf + TBA	0.5921	$5.7130x10^{-5}$
0.5	Phosphate Bf+TBA+HPβCD	1.1618	$1.1210x10^{-4}$
2	Phosphate Bf+TBA+HPβCD	0.7556	$7.2906x10^{-5}$
4	Phosphate Bf+TBA+HPβCD	0.7895	$7.6177x10^{-5}$
23	Phosphate Bf+TBA+HPβCD	0.7668	$7.3987x10^{-5}$
24	Phosphate Bf+TBA+HPβCD	0.8107	$7.8223x10^{-5}$

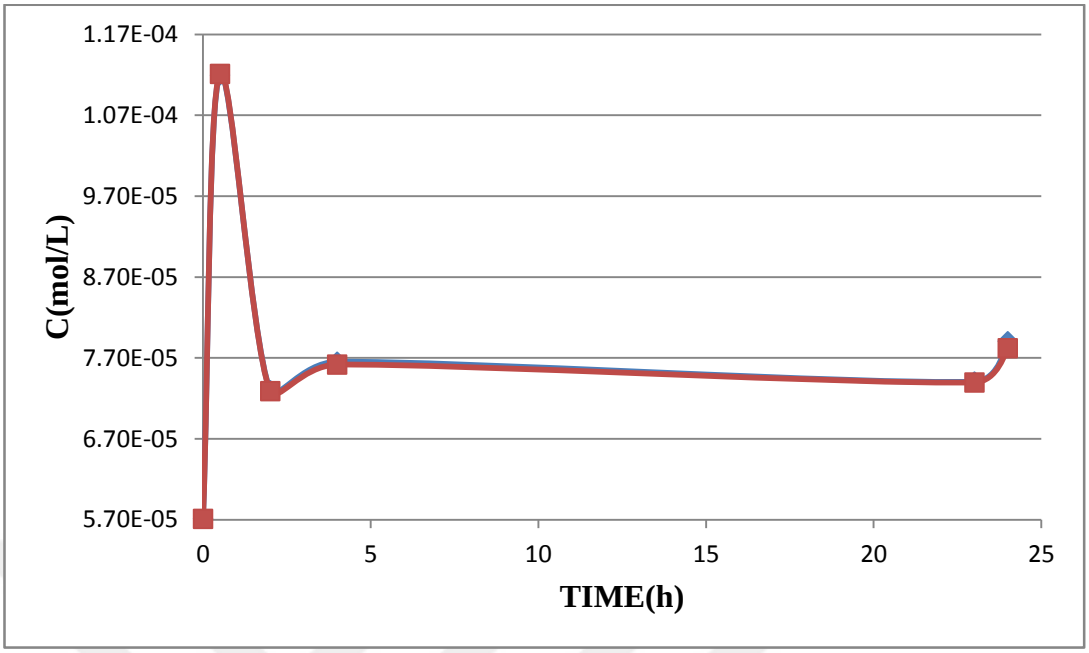


Figure 5.51. Concentration vs. time graph of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-2-hydroxypropyl-β-CD complex (1:1 ratio) in phosphate buffer (37ºC) (1st & 2nd trial) (blue line: 1st trial, red line: 2nd trial)

The maximum concentration of TBA in distilled water and phosphate buffer was obtained after half an hour mixing, and then its concentration in the solutions decreased. The highest concentration of TBA containing β-CD was obtained as 4.8717×10^{-5} mol/L after 24 hours in distilled water and 1.2303×10^{-4} mol/L after 24 hours in phosphate buffer.

By regarding the results, it was decided that the complex formed with β-CD is more stable than the complex formed with HPβ-CD, since the concentration of TBA decreases in the solution with HPβ-CD after half an hour very sharply.Additionally the highest concentration of TBA was obtained in the solution with β-CD.

5.4. THERMODYNAMIC CALCULATIONS USING UV-SPECTROSCOPY RESULTS

The phase solubility study was implemented to specified binding/complexation constant K_{25} and K_{37} of β-CD-TBA complexes. Phase solubility studies of binary systems (TBA- β-CD) were accomplished to show the effect of complexation ability of different carrier systems. The configuration of phase solubility profiles (Figure 5.52 and 5.53).

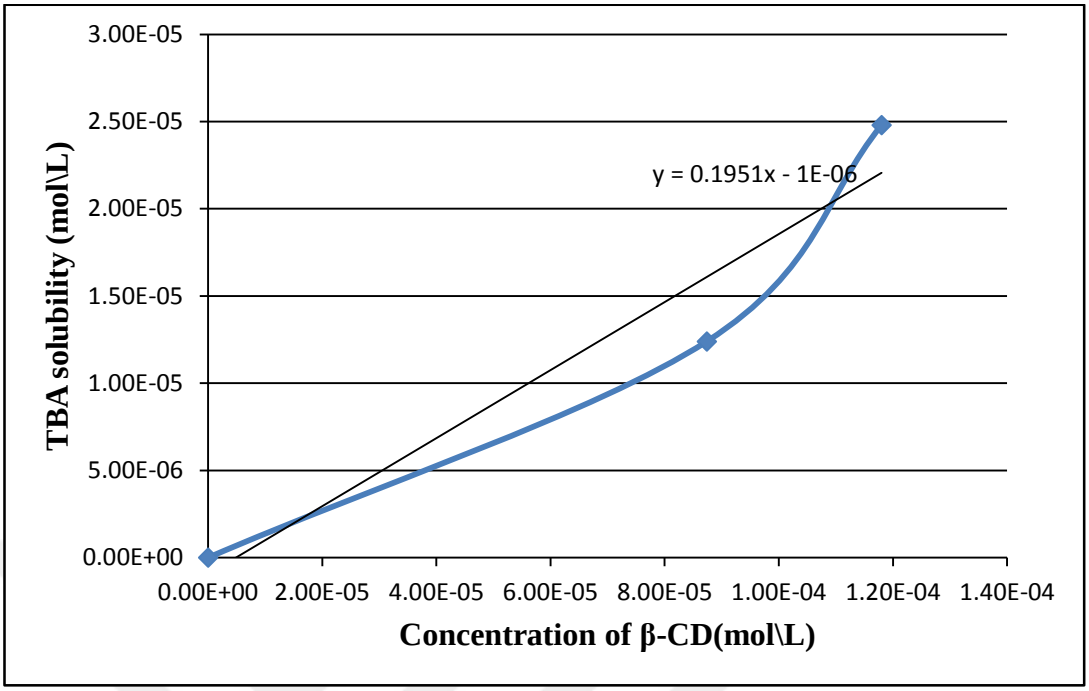


Figure 5.52. Phase solubility profile of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid with β-CD in phosphate buffer at 25°C

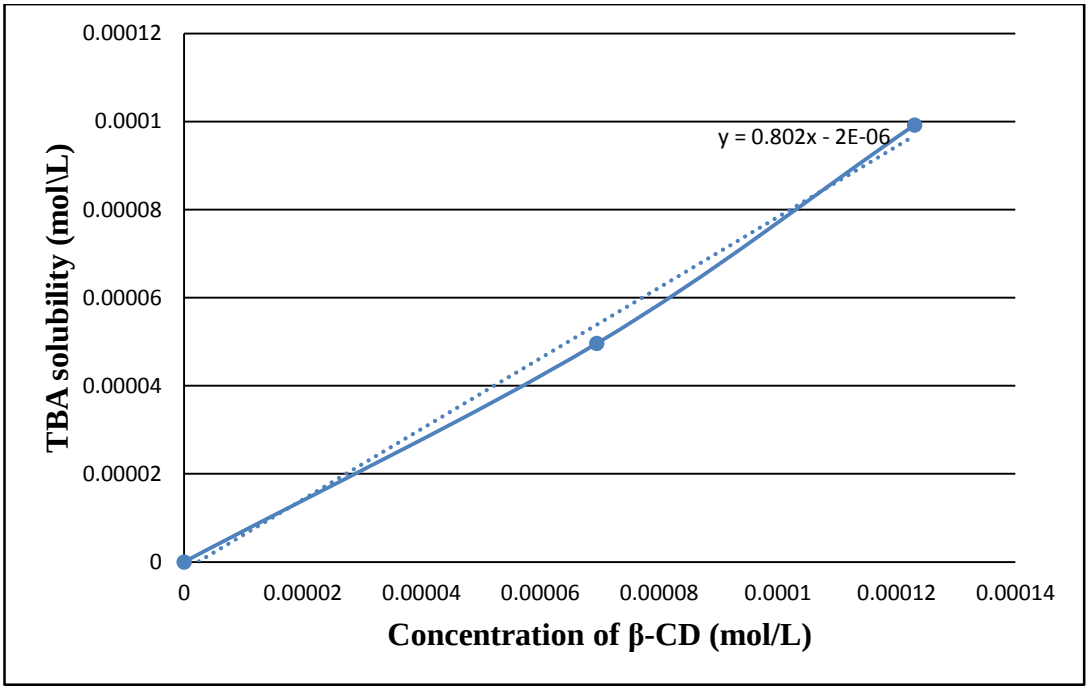


Figure 5.53. Phase solubility profile of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid with β-CD in phosphate buffer at 37°C

The profiles was showed different values of intercept and slope as temperature and pH of media were accused. Stability constant (K) was calculated by intercept and slope of linear part of profile.

High stability constants K_{25} and K_{37} were detected as $0.4068M^{-1}$ and $6.44M^{-1}$ at 25°C and 37°C in phosphate buffer and pH 2.4. Thermodynamic parameters of reactions the free energy change (ΔG°), the enthalpy change (ΔH°) and the entropy change (ΔS°) was obtained from temperature dependence of stability constant. Calculated values are reported in Table 5.97.

Table 5.97. Thermodynamic functions for 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid in phosphate buffer

ΔG° (J/mol)	**ΔH° (J/mol)**	**ΔS° (J/molK)**
$2.2295x10^3$	$186.62x10^3$	618.45

6. CONCLUSIONS AND FUTURE WORK

6.1. CONCLUSIONS

First of all, *o*-substituted phenylthiourea derivatives were synthesized to perform the syntheses of *o*-substituted-2-thiobarbituric acid derivatives. For the synthesis of *o*-substituted-phenylthiourea derivatives, *o*-substituted aniline, hydrochloric acid, ammoniumthiocyanate were used. Then, methyl or 5-5-dimethyl-*o*-substituted-2-thiobarbituric acid derivatives were synthesized by refluxing methylmalonic acid or dimethylmalonic acid and the corresponding *o*-substituted-phenylthiourea in acetyl chloride for 24 hours.

After synthesis of 5-methyl- or 5-5-dimethyl-*o*-substituted-2-thiobarbituric acid derivatives, HPLC and NMR analyses were performed in order to determine occurrence of the reactions and the purity of the products. These results were shown and discussed in the discussion part.

To study the complexation of thiobarbiturates and cyclodextrin, the thiobarbituric acids and cyclodextrin derivatives were mixed at specific temperature for a specific period of time and the complexation process of the thiobarbituric acid and cyclodextrin derivatives were followed by HPLC and UV-absorption analyses.

In HPLC analysis, samples were taken from the mixture solution after a specified time and were given to a reversed phase column to observe the separation of diastereomers, but separation cannot be achieved under specified conditions.

Complex formation between thiobarbiturates and cyclodextrin was followed by UV-spectroscopy. The complexation processes were performed in different solvents such as 0.1 M HCl solution and buffer solutions at different pH values and different temperatures.

The synthesized thiourea derivatives, *o*-tolylthiourea and *o*-fluorophenylthiourea were analyzed by HPLC for their purity. The 5-methyl and 5,5-dimethyl-*o*-substituted-2-thiobarbituric acid derivatives, 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid and 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid were characterizd by HPLC and were checked for their purity by HPLC. To observe the formation of diastereomeric complexes of

thiobarbituric acid derivative with β-CD, the samples from the solution in which complexation process was carried out were taken and given to the reversed phase HPLC column.At least two peaks belonging to two different diastereomers were expected to be seen, however only one peak was seen as in Figure 5.5 and Figure 5.6. The mole ratio of thiobarbituric acid:cyclodextrin was changed and all the solutions (thiobarbituric acid:cyclodextrin (by mole): 1:0.25 ratio; 1:0.5 ratio; 1:0.75 ratio; 1:1 ratio; 1:2 ratio; 1:4 ratio) were analyzed by HPLC. No separation can be observed under specified conditions.

In the UV-absorption analyses, first the UV-spectra of thiobarbituric acid derivatives and cyclodextrin derivatives were taken. Thiobarbituric acid and cyclodextrin were mixed for a specific period of time, then the increase in absorption was measured, which is due to increase in the concentration of thiobarbituric acid. Thiobarbituric acid-cyclodextrin complex is more soluble in water, than thiobarbituric itself, thus increase in the absorption of thiobarbituric acid was observed. The effect of ratio of thiobarbituric acid: cyclodextrin, mixing time, temperature, structure of cyclodextrin and solvents used in the mixing were studied.

First saturated solutions of 1-(*o*-aryl)-2-thiobarbituric acid derivatives in different solvents (distilled water, HCl solution, phosphate buffer and TEA buffer) The pH values of HCl, phosphate buffer, distilled water and TEA buffer solutions were 1.0, 2.4, 3.0 and 4.2 respectively.The graphs of the absorbance vs. concentration of these thiobarbituric acid derivatives in these solutions were plotted (Figure 5.7-5.12) and from the data of these graphs, molar absorptivity values of thiobarbituric acids were found as 26557 M^{-1} $cm^{-1}$and 14767 M^{-1} cm^{-1} for 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid, in distilled water and phosphate buffer, respectively, and as 13747 M^{-1} cm^{-1}, 10364 M^{-1} cm^{-1}, 488.01 M^{-1} cm^{-1} and 360.28 M^{-1} cm^{-1} for 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid in distilled water, phosphate buffer, 0.1M HCl and TEA buffer, respectively (calculation methods were described in Section 4.4.1.1).The concentrations of thibarbiturates in the solvents were compared to decide in which solvent the complexation ratio is the highest. The concentrations were approximately between $5x10^{-5}$ M and $7x10^{-5}$ M in distilled water and phosphate buffer, whereas in other solutions the highest concentrations of TBA were found approximately as $1x10^{-3}$ M. But HCl and TEA buffer solutions were not clear and measurements were done with difficulty. In this study, distilled water and phosphate buffer were used as solvents in other complexation studies.

Effect of mixing time on the concentration was also studied. For this reason, the absorbance of thiobarbituric acid at 190 nm was followed at specific time intervals. Samples from the mixing solution were taken at specific hours and their UV-analyses were done. The aim is to determine the mixing time, at which maximum concentration was achieved and also to determine if the complex is stable with time or not. As seen from all graphs, in the first three hours there is a sharp increase in the concentration of TBA, and the maximum concentration was achieved after 24 hours. After 24 hours, a decrease in the concentration of TBA was observed, so the complexation process seems not to be stable after that time. Therefore it was concluded to perform other processes to determine the effects on the complexation process in 24 hours period.

Besides, temperature effect on the complexation was investigated. All conditions were kept constant except temperature. UV-absorption values of the solutions at two different temperatures 25ºC and 37ºC were compared. First the thiobarbituric acid derivative-β-CD complex was studied at 24 hours mixing time at 37ºC and 25ºC in distilled water and phosphate buffer in 5 different ratios (thiobarbituric acid derivative:β-CD=4:1; 2:1; 1:1; 1:2; 1:4) as explained in Section 4.4.1.1. Absorbance values at 190 nm, where characteristic peak of thiobarbituric acid can be seen, were measured to determine the concentration of thiobarbituric acid derivative. The measurements were done for two trials. In each measurement, the same solution was measured three times, and the average absorbance was calculated as described in Section (4.3.1.1.1). As a result complexation ratio decreases with increasing tmeprature distilled water and phosphate buffer.

The effect of the TBA:β-CD ratio on the rate of complexation was investigated. Two derivatives, 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid and 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid- were studied. 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid has been found that highest solubility of TBA in distilled water can be obtained when TBA:CD concentration is 1:4 at the temperatures 25ºC and 37ºC. In phosphate buffer, highest concentration of TBA can be obtained at the temperatures 25ºC and 37ºC when TBA:CD concentration is 1:4. 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid has been foud to have the highest solubility in distilled water when TBA:CD ratio is 1:1 at the temperatures 25ºC and 37ºC. In phosphate buffer, highest concentration of TBA can be obtained at 25ºC when TBA:CD ratio is 1:2 and at 37ºC when TBA:CD concentration is 1:1.

Two derivatives of cyclodextrin, β-CD (Figure 2.9) and 2-hydroxypropyl-β-CD, HPβ-CD (Figure 2.14) were used for complexation to determine the effect of the structure o the process. To be able to determine the effect of the structure of cyclodextrin on the complexation ratio, two processes, which were carried out at the same conditions except cyclodextrin type were chosen and the concentration of TBA in the aqueous solution was determined after mixing TBA and CD for 24 hours as explained in Section 4.4.4.1. According to the results, 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid was decided to form a more stable complex formed with β-CD than with HPβ-CD, since the concentration of TBA decreases in the solution with HPβ-CD after half an hour very sharply. Additionally a higher concentration of TBA was obtained in the solution with β-CD.

6.2. FUTURE WORK

Based on the results, different cyclodextrin derivatives and buffer solutions can be examined as a future study to obtain a higher solubility of thiobarbiturates in aqueous solutions. Effect of substitutents on the cyclodextrin may be investigated for their function in complex formation. Buffer solutions with higher pH values may be used. Different derivatives of thiobarbituric acid may be synthesized and structure of the thiobarbituric acid on the complexation may be also examined. Different techniques such as Scannnig Electron Microscope and NMR may be used to define the complex formed. Furthermore, different columns may be used to resolve diastereomeric complexes in the HPLC column. Additionally physiochemical calculattions can be repeated with more data.

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APPENDIX A: 5,5-DIMETHYL-1-(-*O*-TOLYL)-2-TBA (37°C)

Table A.1. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD(1:1 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.4948	$1.8630x10^{-5}$
0	D.water+TBA (2)	0.5324	$2.0046x10^{-5}$
0	D.water+TBA (3)	0.5656	$2.1296x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.5587	$2.1038x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.5588	$2.1040x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.5973	$2.2489x10^{-5}$
1	D.water+TBA+βCD (1)	0.6454	$2.4301x10^{-5}$
1	D.water+TBA+βCD (2)	0.6802	$2.5611x10^{-5}$
1	D.water+TBA+βCD (3)	0.6849	$2.5788x10^{-5}$
2	D.water+TBA+βCD (1)	0.6897	$2.5971x10^{-5}$
2	D.water+TBA+βCD (2)	0.8916	$3.3573x10^{-5}$
2	D.water+TBA+βCD (3)	0.8679	$3.2679x10^{-5}$
3	D.water+TBA+βCD (1)	0.8979	$3.3808x10^{-5}$
3	D.water+TBA+βCD (2)	0.8752	$3.2954x10^{-5}$
3	D.water+TBA+βCD (3)	0.9104	$3.4279x10^{-5}$
23	D.water+TBA+βCD (1)	0.8067	$3.0374x10^{-5}$
23	D.water+TBA+βCD (2)	0.9012	$3.3935x10^{-5}$
23	D.water+TBA+βCD (3)	0.9086	$3.4211x10^{-5}$
24	D.water+TBA+βCD (1)	0.9213	$3.4690x10^{-5}$
24	D.water+TBA+βCD (2)	0.9368	$3.5273x10^{-5}$
24	D.water+TBA+βCD (3)	0.9730	$3.6638x10^{-5}$

Table A.2. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.5384	2.0271×10^{-5}
0	D.water+TBA (2)	0.5002	1.8835×10^{-5}
0	D.water+TBA (3)	0.4711	1.7739×10^{-5}
0.5	D.water+TBA+βCD (1)	0.5289	1.9914×10^{-5}
0.5	D.water+TBA+βCD (2)	0.5514	2.0763×10^{-5}
0.5	D.water+TBA+βCD (3)	0.5656	2.1298×10^{-5}
1	D.water+TBA+βCD (1)	0.6838	2.5748×10^{-5}
1	D.water+TBA+βCD (2)	0.6843	2.5767×10^{-5}
1	D.water+TBA+βCD (3)	0.7743	2.9154×10^{-5}
2	D.water+TBA+βCD (1)	0.7989	3.0082×10^{-5}
2	D.water+TBA+βCD (2)	0.8544	3.2170×10^{-5}
2	D.water+TBA+βCD (3)	0.8686	3.2707×10^{-5}
3	D.water+TBA+βCD (1)	0.8800	3.3134×10^{-5}
3	D.water+TBA+βCD (2)	0.8976	3.3797×10^{-5}
3	D.water+TBA+βCD (3)	0.9909	3.7310×10^{-5}
23	D.water+TBA+βCD (1)	0.8317	3.1318×10^{-5}
23	D.water+TBA+βCD (2)	0.9014	3.3942×10^{-5}
23	D.water+TBA+βCD (3)	0.9077	3.4177×10^{-5}
24	D.water+TBA+βCD (1)	0.9212	3.4688×10^{-5}
24	D.water+TBA+βCD (2)	0.9356	3.5228×10^{-5}
24	D.water+TBA+βCD (3)	1.0252	3.8604×10^{-5}

Table A.3. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.3950	$2.6924x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.4014	$2.7360x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.3691	$2.5158x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (1)	0.4593	$3.1307x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (2)	0.4559	$3.1075x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (3)	0.5009	$3.4142x10^{-5}$
1	Phosphate Bf+TBA+βCD (1)	0.5061	$3.4497x10^{-5}$
1	Phosphate Bf+TBA+βCD (2)	0.5852	$3.9888x10^{-5}$
1	Phosphate Bf+TBA+βCD (3)	0.5527	$3.7673x10^{-5}$
2	Phosphate Bf+TBA+βCD (1)	0.7599	$5.1796x10^{-5}$
2	Phosphate Bf+TBA+βCD (2)	0.7794	$5.3125x10^{-5}$
2	Phosphate Bf+TBA+βCD (3)	0.9056	$6.1727x10^{-5}$
3	Phosphate Bf+TBA+βCD (1)	0.8207	$5.5940x10^{-5}$
3	Phosphate Bf+TBA+βCD (2)	0.8890	$6.0596x10^{-5}$
3	Phosphate Bf+TBA+βCD (3)	0.8864	$6.0419x10^{-5}$
23	Phosphate Bf+TBA+βCD (1)	0.8658	$5.9014x10^{-5}$
23	Phosphate Bf+TBA+βCD (2)	0.8838	$6.0241x10^{-5}$
23	Phosphate Bf+TBA+βCD (3)	0.9438	$6.4331x10^{-5}$
24	Phosphate Bf+TBA+βCD (1)	0.9152	$6.2382x10^{-5}$
24	Phosphate Bf+TBA+βCD (2)	0.9129	$6.2225x10^{-5}$
24	Phosphate Bf+TBA+βCD (3)	1.0356	$7.0588x10^{-5}$

Table A.4. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.3714	$2.5315x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.4211	$2.8703x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.3532	$2.4075x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (1)	0.3934	$2.6815x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (2)	0.4556	$3.1054x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (3)	0.4564	$3.1109x10^{-5}$
1	Phosphate Bf+TBA+βCD (1)	0.4663	$3.1784x10^{-5}$
1	Phosphate Bf+TBA+βCD (2)	0.5900	$4.0215x10^{-5}$
1	Phosphate Bf+TBA+βCD (3)	0.5568	$3.7952x10^{-5}$
2	Phosphate Bf+TBA+βCD (1)	0.7633	$5.2028x10^{-5}$
2	Phosphate Bf+TBA+βCD (2)	0.9639	$6.5701x10^{-5}$
2	Phosphate Bf+TBA+βCD (3)	0.7848	$5.3493x10^{-5}$
3	Phosphate Bf+TBA+βCD (1)	0.8885	$6.0562x10^{-5}$
3	Phosphate Bf+TBA+βCD (2)	0.8139	$5.5477x10^{-5}$
3	Phosphate Bf+TBA+βCD (3)	0.8853	$6.0344x10^{-5}$
23	Phosphate Bf+TBA+βCD (1)	0.7947	$5.4168x10^{-5}$
23	Phosphate Bf+TBA+βCD (2)	0.8950	$6.1005x10^{-5}$
23	Phosphate Bf+TBA+βCD (3)	0.8603	$5.8639x10^{-5}$
24	Phosphate Bf+TBA+βCD (1)	0.9107	$6.2075x10^{-5}$
24	Phosphate Bf+TBA+βCD (2)	0.9171	$6.2511x10^{-5}$
24	Phosphate Bf+TBA+βCD (3)	0.8845	$6.0289x10^{-5}$

Table A.5. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (0.8 mM) complex in distilled water (1st trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	D.water+TBA (1)	0.3275	$1.2330x10^{-5}$
0	D.water+TBA (2)	0.3527	$1.3281x10^{-5}$
0	D.water+TBA (3)	0.3289	$1.2385x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.3061	$1.1524x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.3912	$1.4729x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.3680	$1.3857x10^{-5}$
1	D.water+TBA+βCD (1)	0.3703	$1.3942x10^{-5}$
1	D.water+TBA+βCD (2)	0.4593	$1.7293x10^{-5}$
1	D.water+TBA+βCD (3)	0.4894	$1.8426x10^{-5}$
2	D.water+TBA+βCD (1)	0.5334	$2.0085x10^{-5}$
2	D.water+TBA+βCD (2)	0.5190	$1.9543x10^{-5}$
2	D.water+TBA+βCD (3)	0.4136	$1.5574x10^{-5}$
3	D.water+TBA+βCD (1)	0.6867	$2.5856x10^{-5}$
3	D.water+TBA+βCD (2)	0.6510	$2.4511x10^{-5}$
3	D.water+TBA+βCD (3)	0.7150	$2.6923x10^{-5}$
23	D.water+TBA+βCD (1)	0.6515	$2.4530x10^{-5}$
23	D.water+TBA+βCD (2)	0.7586	$2.8565x10^{-5}$
23	D.water+TBA+βCD (3)	0.7871	$2.9636x10^{-5}$
24	D.water+TBA+βCD (1)	0.7714	$2.9045x10^{-5}$
24	D.water+TBA+βCD (2)	0.7981	$3.0052x10^{-5}$

24	D.water+TBA+βCD (3)	0.8717	$3.2824x10^{-5}$
25	D.water+TBA+βCD (1)	0.8361	$3.1483x10^{-5}$
25	D.water+TBA+βCD (2)	0.8208	$3.0905x10^{-5}$
25	D.water+TBA+βCD (3)	0.8701	$3.2762x10^{-5}$
26	D.water+TBA+βCD (1)	0.9165	$3.4509x10^{-5}$
26	D.water+TBA+βCD (2)	0.8989	$3.3846x10^{-5}$
26	D.water+TBA+βCD (3)	0.8038	$3.0265x10^{-5}$
27	D.water+TBA+βCD (1)	0.9212	$3.4686x10^{-5}$
27	D.water+TBA+βCD (2)	0.8157	$3.0713x10^{-5}$
27	D.water+TBA+βCD (3)	0.9381	$3.5322x10^{-5}$
28	D.water+TBA+βCD (1)	0.8108	$3.0529x10^{-5}$
28	D.water+TBA+βCD (2)	0.8276	$3.1163x10^{-5}$
28	D.water+TBA+βCD (3)	0.8449	$3.1813x10^{-5}$
47	D.water+TBA+βCD (1)	0.8095	$3.0480x10^{-5}$
47	D.water+TBA+βCD (2)	0.8124	$3.0591x10^{-5}$
47	D.water+TBA+βCD (3)	0.8763	$3.2997x10^{-5}$
48	D.water+TBA+βCD (1)	0.8351	$3.1444x10^{-5}$
48	D.water+TBA+βCD (2)	0.8301	$3.1257x10^{-5}$
48	D.water+TBA+βCD (3)	0.8843	$3.3296x10^{-5}$

Table A.6. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (0.8 mM) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.3736	$1.4066x10^{-5}$
0	D.water+TBA (2)	0.3251	$1.2240x10^{-5}$
0	D.water+TBA (3)	0.3257	$1.2262x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.3831	$1.4424x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.3717	$1.3996x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.4286	$1.6139x10^{-5}$
1	D.water+TBA+βCD (1)	0.4162	$1.5670x10^{-5}$
1	D.water+TBA+βCD (2)	0.4642	$1.7479x10^{-5}$
1	D.water+TBA+βCD (3)	0.4896	$1.8436x10^{-5}$
2	D.water+TBA+βCD (1)	0.5311	$1.9997x10^{-5}$
2	D.water+TBA+βCD (2)	0.5167	$1.9454x10^{-5}$
2	D.water+TBA+βCD (3)	0.6185	$2.3288x10^{-5}$
3	D.water+TBA+βCD (1)	0.6505	$2.4494x10^{-5}$
3	D.water+TBA+βCD (2)	0.8087	$3.0451x10^{-5}$
3	D.water+TBA+βCD (3)	0.6860	$2.5829x10^{-5}$
23	D.water+TBA+βCD (1)	0.8254	$3.1078x10^{-5}$
23	D.water+TBA+βCD (2)	0.7820	$2.9444x10^{-5}$
23	D.water+TBA+βCD (3)	0.7656	$2.8827x10^{-5}$
24	D.water+TBA+βCD (1)	0.7726	$2.9092x10^{-5}$
24	D.water+TBA+βCD (2)	0.7861	$2.9600x10^{-5}$

24	D.water+TBA+βCD (3)	0.8490	$3.1969x10^{-5}$
25	D.water+TBA+βCD (1)	0.8099	$3.0495x10^{-5}$
25	D.water+TBA+βCD (2)	0.8417	$3.1692x10^{-5}$
25	D.water+TBA+βCD (3)	0.8934	$3.3641x10^{-5}$
26	D.water+TBA+βCD (1)	0.9122	$3.4347x10^{-5}$
26	D.water+TBA+βCD (2)	0.8501	$3.2009x10^{-5}$
26	D.water+TBA+βCD (3)	0.8987	$3.3839x10^{-5}$
27	D.water+TBA+βCD (1)	0.9390	$3.5356x10^{-5}$
27	D.water+TBA+βCD (2)	0.9222	$3.4725x10^{-5}$
27	D.water+TBA+βCD (3)	0.8330	$3.1366x10^{-5}$
28	D.water+TBA+βCD (1)	0.8456	$3.1841x10^{-5}$
28	D.water+TBA+βCD (2)	0.8950	$3.3699x10^{-5}$
28	D.water+TBA+βCD (3)	0.8290	$3.1216x10^{-5}$
47	D.water+TBA+βCD (1)	0.8077	$3.0412x10^{-5}$
47	D.water+TBA+βCD (2)	0.7871	$2.9638x10^{-5}$
47	D.water+TBA+βCD (3)	0.8142	$3.0657x10^{-5}$
48	D.water+TBA+βCD (1)	0.8265	$3.1120x10^{-5}$
48	D.water+TBA+βCD (2)	0.8304	$3.1269x10^{-5}$
48	D.water+TBA+βCD (3)	0.9154	$3.4469x10^{-5}$

Table A.7. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (0.8 mM) complex in phosphate buffer (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.4035	$2.7503x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.4204	$2.8655x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.4173	$2.8444x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.4857	$3.3106x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.4815	$3.2820x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.4454	$3.0359x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.5684	$3.8743x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.4940	$3.3672x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.5614	$3.8266x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.6285	$4.2840x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.6029	$4.1095x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.5677	$3.8695x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.6909	$4.7093x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.6755	$4.6043x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	0.7811	$5.3241x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.7868	$5.3630x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.7880	$5.3711x10^{-5}$
23	Phosphate Bf+BA+βCD (3)	0.6596	$4.4959x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	0.7604	$5.1830x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.8029	$5.4727x10^{-5}$

24	Phosphate Bf+BA+βCD (3)	0.8052	$5.4884x10^{-5}$
25	Phosphate Bf+BA+βCD (1)	0.7676	$5.2321x10^{-5}$
25	Phosphate Bf+BA+βCD (2)	0.7503	$5.1142x10^{-5}$
25	Phosphate Bf+BA+βCD (3)	0.7496	$5.1094x10^{-5}$
26	Phosphate Bf+BA+βCD (1)	0.8062	$5.4952x10^{-5}$
26	Phosphate Bf+BA+βCD (2)	0.7376	$5.0276x10^{-5}$
26	Phosphate Bf+BA+βCD (3)	0.8227	$5.6077x10^{-5}$
27	Phosphate Bf+BA+βCD (1)	0.7883	$5.3732x10^{-5}$
27	Phosphate Bf+BA+βCD (2)	0.7888	$5.3766x10^{-5}$
27	Phosphate Bf+BA+βCD (3)	0.8139	$5.5477x10^{-5}$
28	Phosphate Bf+BA+βCD (1)	0.8726	$5.9478x10^{-5}$
28	Phosphate Bf+BA+βCD (2)	0.8058	$5.4925x10^{-5}$
28	Phosphate Bf+BA+βCD (3)	0.8064	$5.4966x10^{-5}$
47	Phosphate Bf+BA+βCD (1)	0.7832	$5.3384x10^{-5}$
47	Phosphate Bf+BA+βCD (2)	0.7750	$5.2825x10^{-5}$
47	Phosphate Bf+BA+βCD (3)	0.7506	$5.1162x10^{-5}$
48	Phosphate Bf+BA+βCD (1)	0.8350	$5.6915x10^{-5}$
48	Phosphate Bf+BA+βCD (2)	0.7814	$5.3262x10^{-5}$
48	Phosphate Bf+BA+βCD (3)	0.8167	$5.5668x10^{-5}$

Table A.8. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (0.8 mM) complex in phosphate buffer (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.4209	$2.8689x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.4055	$2.7640x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.4197	$2.8607x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.4805	$3.2752x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.4112	$2.8028x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.4836	$3.2963x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.4548	$3.1000x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.5762	$3.9275x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.5481	$3.7359x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.6146	$4.1892x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.6159	$4.1981x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.8247	$5.6213x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.8154	$5.5579x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.6804	$4.6377x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	0.6953	$4.7393x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.7862	$5.3589x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.7873	$5.3664x10^{-5}$
23	Phosphate Bf+BA+βCD (3)	0.9686	$6.6021x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	0.8058	$5.4925x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.8031	$5.4741x10^{-5}$

24	Phosphate Bf+BA+βCD (3)	1.0112	$6.8925x10^{-5}$
25	Phosphate Bf+BA+βCD (1)	0.9988	$6.8080x10^{-5}$
25	Phosphate Bf+BA+βCD (2)	0.7687	$5.2396x10^{-5}$
25	Phosphate Bf+BA+βCD (3)	0.7582	$5.1680x10^{-5}$
26	Phosphate Bf+BA+βCD (1)	0.8083	$5.5095x10^{-5}$
26	Phosphate Bf+BA+βCD (2)	0.8209	$5.5954x10^{-5}$
26	Phosphate Bf+BA+βCD (3)	1.1044	$7.5278x10^{-5}$
27	Phosphate Bf+BA+βCD (1)	1.0469	$7.1358x10^{-5}$
27	Phosphate Bf+BA+βCD (2)	0.7857	$5.3555x10^{-5}$
27	Phosphate Bf+BA+βCD (3)	0.7889	$5.3773x10^{-5}$
28	Phosphate Bf+BA+βCD (1)	0.8114	$5.5306x10^{-5}$
28	Phosphate Bf+BA+βCD (2)	0.8079	$5.5068x10^{-5}$
28	Phosphate Bf+BA+βCD (3)	0.4746	$3.2350x10^{-5}$
47	Phosphate Bf+BA+βCD (1)	0.7718	$5.2607x10^{-5}$
47	Phosphate Bf+BA+βCD (2)	0.7834	$5.3398x10^{-5}$
47	Phosphate Bf+BA+βCD (3)	1.0959	$7.4698x10^{-5}$
48	Phosphate Bf+BA+βCD (1)	0.8272	$5.6383x10^{-5}$
48	Phosphate Bf+BA+βCD (2)	0.8486	$5.7842x10^{-5}$
48	Phosphate Bf+BA+βCD (3)	1.0119	$6.8973x10^{-5}$

Table A.9. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.3102	$1.1679x10^{-5}$
0	D.water+TBA (2)	0.3835	$1.4441x10^{-5}$
0	D.water+TBA (3)	0.3528	$1.3285x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.4339	$1.6338x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.5004	$1.8842x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.5192	$1.9550x10^{-5}$
1	D.water+TBA+βCD (1)	0.5527	$2.0812x10^{-5}$
1	D.water+TBA+βCD (2)	0.5869	$2.2100x10^{-5}$
1	D.water+TBA+βCD (3)	0.7033	$2.6481x10^{-5}$
2	D.water+TBA+βCD (1)	0.7433	$2.7989x10^{-5}$
2	D.water+TBA+βCD (2)	0.6942	$2.6138x10^{-5}$
2	D.water+TBA+βCD (3)	0.7368	$2.7742x10^{-5}$
3	D.water+TBA+βCD (1)	0.8808	$3.3166x10^{-5}$
3	D.water+TBA+βCD (2)	0.9232	$3.4763x10^{-5}$
3	D.water+TBA+βCD (3)	0.9132	$3.4386x10^{-5}$
23	D.water+TBA+βCD (1)	0.7749	$2.9179x10^{-5}$
23	D.water+TBA+βCD (2)	0.8600	$3.2381x10^{-5}$
23	D.water+TBA+βCD (3)	0.8775	$3.3042x10^{-5}$
24	D.water+TBA+βCD (1)	0.8387	$3.1581x10^{-5}$
24	D.water+TBA+βCD (2)	0.9635	$3.6279x10^{-5}$
24	D.water+TBA+βCD (3)	0.9317	$3.5083x10^{-5}$

Table A.10. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.3803	$1.4320x10^{-5}$
0	D.water+TBA (2)	0.3081	$1.1601x10^{-5}$
0	D.water+TBA (3)	0.3588	$1.3509x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.4029	$1.5171x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.4959	$1.8671x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.5275	$1.9861x10^{-5}$
1	D.water+TBA+βCD (1)	0.5539	$2.0855x10^{-5}$
1	D.water+TBA+βCD (2)	0.5861	$2.2070x10^{-5}$
1	D.water+TBA+βCD (3)	0.7476	$2.8149x10^{-5}$
2	D.water+TBA+βCD (1)	0.6560	$2.4702x10^{-5}$
2	D.water+TBA+βCD (2)	0.7305	$2.7507x10^{-5}$
2	D.water+TBA+βCD (3)	0.7420	$2.7940x10^{-5}$
3	D.water+TBA+βCD (1)	0.8726	$3.2858x10^{-5}$
3	D.water+TBA+βCD (2)	0.9281	$3.4946x10^{-5}$
3	D.water+TBA+βCD (3)	0.9085	$3.4208x10^{-5}$
23	D.water+TBA+βCD (1)	0.7974	$3.0024x10^{-5}$
23	D.water+TBA+βCD (2)	0.8540	$3.2157x10^{-5}$
23	D.water+TBA+βCD (3)	0.9044	$3.4053x10^{-5}$
24	D.water+TBA+βCD (1)	0.8718	$3.2826x10^{-5}$
24	D.water+TBA+βCD (2)	0.9648	$3.6329x10^{-5}$
24	D.water+TBA+βCD (3)	0.9261	$3.4870x10^{-5}$

Table A.11. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.5177	$3.5287x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.4692	$3.1981x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.4554	$3.1041x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.5033	$3.4306x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.5728	$3.9043x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.53895	$3.6736x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.5605	$3.8205x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.5817	$3.9650x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.67835	$4.6237x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.68595	$4.6756x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.6939	$4.7297x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.74485	$5.0770x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.7614	$5.1898x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.77435	$5.2781x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	0.8205	$5.5927x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.7455	$5.0815x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.7948	$5.4175x10^{-5}$
23	Phosphate Bf+BA+βCD (3)	0.72645	$4.9516x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	0.886	$6.0391x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.8802	$5.9996x10^{-5}$
24	Phosphate Bf+BA+βCD (3)	0.9	$6.1346x10^{-5}$

Table A.12. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.4649	$3.1688x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.4944	$3.3699x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.4602	$3.1368x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.5530	$3.7693x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.4946	$3.3713x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.5695	$3.8818x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.5823	$3.9691x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.5633	$3.8395x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.6169	$4.2049x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.6865	$4.6793x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.6918	$4.7154x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.8150	$5.5552x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.7946	$5.4161x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.9087	$6.1939x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	0.7527	$5.1305x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.7261	$4.9492x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.7486	$5.1026x10^{-5}$
23	Phosphate Bf+BA+βCD (3)	0.9680	$6.5981x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	0.8818	$6.0105x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.9508	$6.4808x10^{-5}$
24	Phosphate Bf+BA+βCD (3)	0.8887	$6.0575x10^{-5}$

Table A.13. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD(1:4 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.3186	$1.1997x10^{-5}$
0	D.water+TBA (2)	0.3974	$1.4962x10^{-5}$
0	D.water+TBA (3)	0.3836	$1.4443x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.4451	$1.6760x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.5172	$1.9475x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.6323	$2.3809x10^{-5}$
1	D.water+TBA+βCD (1)	0.6098	$2.2960x10^{-5}$
1	D.water+TBA+βCD (2)	0.7668	$2.8874x10^{-5}$
1	D.water+TBA+βCD (3)	0.5720	$2.1537x10^{-5}$
2	D.water+TBA+βCD (1)	0.7267	$2.7364x10^{-5}$
2	D.water+TBA+βCD (2)	0.8437	$3.1768x10^{-5}$
2	D.water+TBA+βCD (3)	0.8342	$3.1410x10^{-5}$
3	D.water+TBA+βCD (1)	0.9971	$3.7546x10^{-5}$
3	D.water+TBA+βCD (2)	0.9025	$3.3982x10^{-5}$
3	D.water+TBA+βCD (3)	0.7683	$2.8930x10^{-5}$
23	D.water+TBA+βCD (1)	0.7919	$2.9819x10^{-5}$
23	D.water+TBA+βCD (2)	0.8682	$3.2692x10^{-5}$
23	D.water+TBA+βCD (3)	0.7979	$3.0043x10^{-5}$
24	D.water+TBA+βCD (1)	0.9957	$3.7491x10^{-5}$
24	D.water+TBA+βCD (2)	0.8374	$3.1530x10^{-5}$
24	D.water+TBA+βCD (3)	0.9798	$3.6894x10^{-5}$

Table A.14. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.3946	1.4859×10^{-5}
0	D.water+TBA (2)	0.3222	1.2131×10^{-5}
0	D.water+TBA (3)	0.3921	1.4763×10^{-5}
0.5	D.water+TBA+βCD (1)	0.4842	1.8232×10^{-5}
0.5	D.water+TBA+βCD (2)	0.4884	1.8391×10^{-5}
0.5	D.water+TBA+βCD (3)	0.4841	1.8229×10^{-5}
1	D.water+TBA+βCD (1)	0.5738	2.1604×10^{-5}
1	D.water+TBA+βCD (2)	0.5077	1.9115×10^{-5}
1	D.water+TBA+βCD (3)	0.6068	2.2849×10^{-5}
2	D.water+TBA+βCD (1)	0.8432	3.1749×10^{-5}
2	D.water+TBA+βCD (2)	0.6090	2.2932×10^{-5}
2	D.water+TBA+βCD (3)	0.8306	3.1276×10^{-5}
3	D.water+TBA+βCD (1)	0.9499	3.5766×10^{-5}
3	D.water+TBA+βCD (2)	0.8050	3.0312×10^{-5}
3	D.water+TBA+βCD (3)	0.9475	3.5678×10^{-5}
23	D.water+TBA+βCD (1)	0.6978	2.6274×10^{-5}
23	D.water+TBA+βCD (2)	0.7938	2.9889×10^{-5}
23	D.water+TBA+βCD (3)	0.7947	2.9922×10^{-5}
24	D.water+TBA+βCD (1)	0.9757	3.6740×10^{-5}
24	D.water+TBA+βCD (2)	0.8919	3.3582×10^{-5}
24	D.water+TBA+βCD (3)	0.9964	3.7517×10^{-5}

Table A.15. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.4734	$3.2268x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.4818	$3.2840x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.4242	$2.8914x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.4651	$3.1702\ x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.5525	$3.7659x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.5457	$3.7196x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.5557	$3.7877x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.5591	$3.8109x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.6075	$4.1408x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.6415	$4.3726x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.6110	$4.1647x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.8253	$5.6254x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.7764	$5.2921x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.8622	$5.8769x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	0.8931	$6.0875x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.8596	$5.8592x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.7946	$5.4161x10^{-5}$
23	Phosphate Bf+BA+βCD (3)	0.7879	$5.3705x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	1.0191	$6.9464x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.8784	$5.9873x10^{-5}$
24	Phosphate Bf+BA+βCD (3)	0.8518	$5.8060x10^{-5}$

Table A.16. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.4701	$3.2043x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.4548	$3.1000x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.4822	$3.2868x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.5454	$3.7175x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.4816	$3.2827x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.5516	$3.7598x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.5614	$3.8266x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.5379	$3.6664x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.5697	$3.8832x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.5346	$3.6439x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.6434	$4.3855x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.6093	$4.1531x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.6751	$4.6016x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.8620	$5.8755x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	0.8929	$6.0862x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.7508	$5.1176x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.7895	$5.3814x10^{-5}$
23	Phosphate Bf+BA+βCD (3)	0.7922	$5.3998x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	0.8750	$5.9641x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.8513	$5.8026x10^{-5}$
24	Phosphate Bf+BA+βCD (3)	0.9136	$6.2273x10^{-5}$

APPENDIX B: 5,5-DIMETHYL-1-(-*O*-TOLYL)-2-TBA (25°C)

Table B.1. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.3903	$1.4697x10^{-5}$
0	D.water+TBA (2)	0.3972	$1.4957x10^{-5}$
0	D.water+TBA (3)	0.3709	$1.3966x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.53515	$2.0151x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.5458	$2.0552x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.6127	$2.3071x10^{-5}$
1	D.water+TBA+βCD (1)	0.7759	$2.9216x10^{-5}$
1	D.water+TBA+βCD (2)	0.64765	$2.4387x10^{-5}$
1	D.water+TBA+βCD (3)	0.7797	$2.9359x10^{-5}$
2	D.water+TBA+βCD (1)	0.85275	$3.2110x10^{-5}$
2	D.water+TBA+βCD (2)	0.8611	$3.2425x10^{-5}$
2	D.water+TBA+βCD (3)	0.771	$2.9032x10^{-5}$
3	D.water+TBA+βCD (1)	0.88835	$3.3451x10^{-5}$
3	D.water+TBA+βCD (2)	0.87905	$3.3101x10^{-5}$
3	D.water+TBA+βCD (3)	0.9143	$3.4428x10^{-5}$
23	D.water+TBA+βCD (1)	0.98005	$3.6904x10^{-5}$
23	D.water+TBA+βCD (2)	1.03955	$3.9144x10^{-5}$
23	D.water+TBA+βCD (3)	0.95505	$3.5962x10^{-5}$
24	D.water+TBA+βCD (1)	0.84845	$3.1948x10^{-5}$
24	D.water+TBA+βCD (2)	0.83995	$3.1628x10^{-5}$
24	D.water+TBA+βCD (3)	0.95705	$3.6038x10^{-5}$

Table B.2. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water (2nd trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	D.water+TBA (1)	0.4097	$1.5427x10^{-5}$
0	D.water+TBA (2)	0.3618	$1.3622x10^{-5}$
0	D.water+TBA (3)	0.4310	$1.6229x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.5383	$2.0270x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.5258	$1.9797x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.5810	$2.1877x10^{-5}$
1	D.water+TBA+βCD (1)	0.6203	$2.3355x10^{-5}$
1	D.water+TBA+βCD (2)	0.7734	$2.9120x10^{-5}$
1	D.water+TBA+βCD (3)	0.7696	$2.8977x10^{-5}$
2	D.water+TBA+βCD (1)	0.7798	$2.9363x10^{-5}$
2	D.water+TBA+βCD (2)	0.8642	$3.2539x10^{-5}$
2	D.water+TBA+βCD (3)	0.8540	$3.2155x10^{-5}$
3	D.water+TBA+βCD (1)	0.8763	$3.2995x10^{-5}$
3	D.water+TBA+βCD (2)	1.1123	$4.1883x10^{-5}$
3	D.water+TBA+βCD (3)	0.8736	$3.2895x10^{-5}$
23	D.water+TBA+βCD (1)	0.8968	$3.3769x10^{-5}$
23	D.water+TBA+βCD (2)	0.9594	$3.6124x10^{-5}$
23	D.water+TBA+βCD (3)	0.9840	$3.7050x10^{-5}$
24	D.water+TBA+βCD (1)	0.8462	$3.1862x10^{-5}$
24	D.water+TBA+βCD (2)	0.8358	$3.1472x10^{-5}$
24	D.water+TBA+βCD (3)	1.0207	$3.8432x10^{-5}$

Table B.3. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD(1:1 ratio) complex in phosphate buffer (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.61895	$4.2189x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5	$3.4081x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5436	$3.7053x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.53265	$3.6306x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.5647	$3.8491x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.56255	$3.8344x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.5927	$4.0399x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.666	$4.5396x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.67115	$4.5747x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.7771	$5.2968x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.7594	$5.1762x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.87435	$5.9597x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.9691	$6.6055x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.8093	$5.5163x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	0.8283	$5.6458x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.79735	$5.4349x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.8603	$5.8639x10^{-5}$
23	Phosphate Bf+BA+βCD (3)	0.8826	$6.0159x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	0.86655	$5.9066x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.80425	$5.4819x10^{-5}$
24	Phosphate Bf+BA+βCD (3)	0.85605	$5.8350x10^{-5}$

Table B.4. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.6513	$4.4394x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5359	$3.6528x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5062	$3.4503x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.5957	$4.0604x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.5647	$3.8491x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.5622	$3.8320x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.6627	$4.5171x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.6764	$4.6105x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.7235	$4.9315x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.7850	$5.3507x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.7597	$5.1782x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.9237	$6.2961x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.8276	$5.6411x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.8075	$5.5041x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	1.0191	$6.9464x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.8705	$5.9335x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.8877	$6.0507x10^{-5}$
23	Phosphate Bf+BA+βCD (3)	0.9446	$6.4386x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	0.8668	$5.9083x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.9355	$6.3765x10^{-5}$
24	Phosphate Bf+BA+βCD (3)	0.8589	$5.8544x10^{-5}$

Table B.5. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.5359	$2.0177x10^{-5}$
0	D.water+TBA (2)	0.5038	$1.8971x10^{-5}$
0	D.water+TBA (3)	0.5390	$2.0296x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.5344	$2.0123x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.5976	$2.2501x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.5878	$2.2134x10^{-5}$
1	D.water+TBA+βCD (1)	0.5780	$2.1763x10^{-5}$
1	D.water+TBA+βCD (2)	0.7132	$2.6854x10^{-5}$
1	D.water+TBA+βCD (3)	0.7436	$2.7998x10^{-5}$
2	D.water+TBA+βCD (1)	0.8574	$3.2285x10^{-5}$
2	D.water+TBA+βCD (2)	0.7414	$2.7917x10^{-5}$
2	D.water+TBA+βCD (3)	0.7491	$2.8207x10^{-5}$
3	D.water+TBA+βCD (1)	0.8134	$3.0627x10^{-5}$
3	D.water+TBA+βCD (2)	0.8961	$3.3743x10^{-5}$
3	D.water+TBA+βCD (3)	0.8206	$3.0898x10^{-5}$
23	D.water+TBA+βCD (1)	0.7817	$2.9433x10^{-5}$
23	D.water+TBA+βCD (2)	0.7707	$2.9021x10^{-5}$
23	D.water+TBA+βCD (3)	0.9073	$3.4164x10^{-5}$
24	D.water+TBA+βCD (1)	0.8512	$3.2050x10^{-5}$
24	D.water+TBA+βCD (2)	0.8572	$3.2276x10^{-5}$
24	D.water+TBA+βCD (3)	0.8778	$3.3053x10^{-5}$

Table B.6. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.4675	1.760×10^{-5}
0	D.water+TBA (2)	0.5378	2.025×10^{-5}
0	D.water+TBA (3)	0.5352	2.015×10^{-5}
0.5	D.water+TBA+βCD (1)	0.4751	1.789×10^{-5}
0.5	D.water+TBA+βCD (2)	0.6306	2.375×10^{-5}
0.5	D.water+TBA+βCD (3)	0.5765	2.171×10^{-5}
1	D.water+TBA+βCD (1)	0.5761	2.169×10^{-5}
1	D.water+TBA+βCD (2)	0.7335	2.762×10^{-5}
1	D.water+TBA+βCD (3)	0.7126	2.683×10^{-5}
2	D.water+TBA+βCD (1)	0.7412	2.791×10^{-5}
2	D.water+TBA+βCD (2)	0.7484	2.818×10^{-5}
2	D.water+TBA+βCD (3)	0.8507	3.203×10^{-5}
3	D.water+TBA+βCD (1)	0.8124	3.059×10^{-5}
3	D.water+TBA+βCD (2)	0.8524	3.210×10^{-5}
3	D.water+TBA+βCD (3)	0.8246	3.105×10^{-5}
23	D.water+TBA+βCD (1)	0.7607	2.864×10^{-5}
23	D.water+TBA+βCD (2)	0.8200	3.088×10^{-5}
23	D.water+TBA+βCD (3)	0.7850	2.956×10^{-5}
24	D.water+TBA+βCD (1)	0.8410	3.167×10^{-5}
24	D.water+TBA+βCD (2)	0.8580	3.231×10^{-5}
24	D.water+TBA+βCD (3)	0.8520	3.208×10^{-5}

Table B.7. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer (1st trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	Phosphate Buffer+TBA (1)	0.6868	$4.6813x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5944	$4.0515x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.6746	$4.5982x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.8678	$5.9151x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.6759	$4.6070x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.7063	$4.8143x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.8629	$5.8817x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.8563	$5.8367x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	1.0165	$6.9286x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.9719	$6.6246x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.8999	$6.1339x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.9355	$6.3765x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.9066	$6.1795x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.9228	$6.2900x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	1.0198	$6.9511x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.9529	$6.4951x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.8880	$6.0528x10^{-5}$
23	Phosphate Bf+BA+βCD (3)	0.8800	$5.9982x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	0.9620	$6.5572x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.9936	$6.7725x10^{-5}$
24	Phosphate Bf+BA+βCD (3)	0.9852	$6.7153x10^{-5}$

Table B.8. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.4900	$3.3399x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.6942	$4.7318x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.6606	$4.5028x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.5716	$3.8961x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.7044	$4.8013x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.7030	$4.7918x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.8585	$5.8517x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.8638	$5.8878x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.7794	$5.3125x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.8022	$5.467x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.9359	$6.3793x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.8962	$6.1086x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.9063	$6.1775x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.9244	$6.3009x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	0.9592	$6.5381x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.8858	$6.0378x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.8763	$5.9730x10^{-5}$
23	Phosphate Bf+BA+βCD (3)	0.9832	$6.7017x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	0.9929	$6.7678x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.9898	$6.7466x10^{-5}$
24	Phosphate Bf+BA+βCD (3)	1.1012	$7.5060x10^{-5}$

Table B.9. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.3078	$1.1588x10^{-5}$
0	D.water+TBA (2)	0.3594	$1.3531x10^{-5}$
0	D.water+TBA (3)	0.3203	$1.2061x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.3395	$1.2782x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.4326	$1.6289x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.4261	$1.6043x10^{-5}$
1	D.water+TBA+βCD (1)	0.4723	$1.7784x10^{-5}$
1	D.water+TBA+βCD (2)	0.6128	$2.3075x10^{-5}$
1	D.water+TBA+βCD (3)	0.6328	$2.3826x10^{-5}$
2	D.water+TBA+βCD (1)	0.6894	$2.5959x10^{-5}$
2	D.water+TBA+βCD (2)	0.7906	$2.9768x10^{-5}$
2	D.water+TBA+βCD (3)	0.8324	$3.1344x10^{-5}$
3	D.water+TBA+βCD (1)	0.8325	$3.1346x10^{-5}$
3	D.water+TBA+βCD (2)	0.8163	$3.0738x10^{-5}$
3	D.water+TBA+βCD (3)	0.9017	$3.3953x10^{-5}$
23	D.water+TBA+βCD (1)	0.8277	$3.1165x10^{-5}$
23	D.water+TBA+βCD (2)	0.8957	$3.3726x10^{-5}$
23	D.water+TBA+βCD (3)	0.8615	$3.2440x10^{-5}$
24	D.water+TBA+βCD (1)	0.8935	$3.3643x10^{-5}$
24	D.water+TBA+βCD (2)	0.9178	$3.4558x10^{-5}$
24	D.water+TBA+βCD (3)	0.9078	$3.4183x10^{-5}$

Table B.10. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.3111	$1.1713x10^{-5}$
0	D.water+TBA (2)	0.4173	$1.5713x10^{-5}$
0	D.water+TBA (3)	0.3220	$1.2125x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.4045	$1.5231x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.4430	$1.6679x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.4354	$1.6393x10^{-5}$
1	D.water+TBA+βCD (1)	0.6120	$2.3045x10^{-5}$
1	D.water+TBA+βCD (2)	0.6336	$2.3858x10^{-5}$
1	D.water+TBA+βCD (3)	0.5953	$2.2414x10^{-5}$
2	D.water+TBA+βCD (1)	0.7744	$2.9158x10^{-5}$
2	D.water+TBA+βCD (2)	0.6806	$2.5626x10^{-5}$
2	D.water+TBA+βCD (3)	0.8192	$3.0847x10^{-5}$
3	D.water+TBA+βCD (1)	0.8337	$3.1393x10^{-5}$
3	D.water+TBA+βCD (2)	0.9622	$3.6230x10^{-5}$
3	D.water+TBA+βCD (3)	0.8133	$3.0623x10^{-5}$
23	D.water+TBA+βCD (1)	0.8649	$3.2568x10^{-5}$
23	D.water+TBA+βCD (2)	0.9463	$3.5633x10^{-5}$
23	D.water+TBA+βCD (3)	0.8991	$3.3854x10^{-5}$
24	D.water+TBA+βCD (1)	0.9511	$3.5814x10^{-5}$
24	D.water+TBA+βCD (2)	0.9359	$3.5241x10^{-5}$
24	D.water+TBA+βCD (3)	0.8760	$3.2986x10^{-5}$

Table B.11. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.5194	$3.5403x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.4693	$3.1988x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5357	$3.6514x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.5616	$3.8280x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.4224	$2.8791x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.5981	$4.0768x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.7081	$4.8265x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.7239	$4.9342x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.7452	$5.0794x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.9062	$6.1768x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.8415	$5.7358x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.7791	$5.3105x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.9600	$6.5435x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.9060	$6.1754x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	0.9187	$6.2620x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.8274	$5.6397x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.9759	$6.6519x10^{-5}$
23	Phosphate Bf+BA+βCD (3)	0.9691	$6.6055x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	1.0336	$7.0452x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.9473	$6.4570x10^{-5}$
24	Phosphate Bf+BA+βCD (3)	0.9429	$6.4270x10^{-5}$

Table B.12. Absorbance & concentration results of 5,5-dimethyl-1-(*o*-tolyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.4934	$3.3631x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.4646	$3.1668x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.4051	$2.7612x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.4455	$3.0366x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.5616	$3.828x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.5993	$4.0849x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.5712	$3.8934x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.7099	$4.8388x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.7201	$4.9083x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.8404	$5.7283x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.7791	$5.3105x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.8666	$5.9069x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.9186	$6.2613x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.9282	$6.3268x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	0.9089	$6.1952x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.9793	$6.6751x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.8917	$6.078x10^{-5}$
23	Phosphate Bf+BA+βCD (3)	0.9694	$6.6076x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	0.9108	$6.2082x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.9518	$6.4876x10^{-5}$
24	Phosphate Bf+BA+βCD (3)	0.9556	$6.5135x10^{-5}$

APPENDIX C: 5-METHYL-1-(*O*-FLUOROPHENYL)-2-TBA (37°C)

Table C.1. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.49755	$3.6193x10^{-5}$
0	D.water+TBA (2)	0.41015	$2.9836x10^{-5}$
0	D.water+TBA (3)	0.84975	$6.1813x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.70555	$5.1324x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.577	$4.1973x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.56165	$4.0856x10^{-5}$
1	D.water+TBA+βCD (1)	0.5916	$4.3035x10^{-5}$
1	D.water+TBA+βCD (2)	0.6283	$4.5705x10^{-5}$
1	D.water+TBA+βCD (3)	0.59375	$4.3191x10^{-5}$
2	D.water+TBA+βCD (1)	0.61085	$4.4435x10^{-5}$
2	D.water+TBA+βCD (2)	0.5778	$4.2031x10^{-5}$
2	D.water+TBA+βCD (3)	0.594	$4.3209x10^{-5}$
3	D.water+TBA+βCD (1)	0.54915	$3.9947x10^{-5}$
3	D.water+TBA+βCD (2)	0.55135	$4.0107x10^{-5}$
3	D.water+TBA+βCD (3)	0.57185	$4.1598x10^{-5}$
23	D.water+TBA+βCD (1)	0.5402	$3.9296x10^{-5}$
23	D.water+TBA+βCD (2)	0.5816	$4.2307x10^{-5}$
23	D.water+TBA+βCD (3)	0.54655	$3.9758x10^{-5}$
24	D.water+TBA+βCD (1)	0.5578	$4.0576x10^{-5}$
24	D.water+TBA+βCD (2)	0.52095	$3.7896x10^{-5}$
24	D.water+TBA+βCD (3)	0.5576	$4.0562x10^{-5}$

Table C.2. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.4109	2.9890×10^{-5}
0	D.water+TBA (2)	0.4858	3.5339×10^{-5}
0	D.water+TBA (3)	0.4914	3.5746×10^{-5}
0.5	D.water+TBA+βCD (1)	0.56755	4.1285×10^{-5}
0.5	D.water+TBA+βCD (2)	0.5648	4.1085×10^{-5}
0.5	D.water+TBA+βCD (3)	0.56685	4.1234×10^{-5}
1	D.water+TBA+βCD (1)	0.58835	4.2798×10^{-5}
1	D.water+TBA+βCD (2)	0.6177	4.4933×10^{-5}
1	D.water+TBA+βCD (3)	0.5952	4.3297×10^{-5}
2	D.water+TBA+βCD (1)	0.60325	4.3882×10^{-5}
2	D.water+TBA+βCD (2)	0.5309	3.8619×10^{-5}
2	D.water+TBA+βCD (3)	0.6004	4.3675×10^{-5}
3	D.water+TBA+βCD (1)	0.54405	3.9576×10^{-5}
3	D.water+TBA+βCD (2)	0.5481	3.9871×10^{-5}
3	D.water+TBA+βCD (3)	0.49855	3.6266×10^{-5}
23	D.water+TBA+βCD (1)	0.5454	3.9674×10^{-5}
23	D.water+TBA+βCD (2)	0.4918	3.5775×10^{-5}
23	D.water+TBA+βCD (3)	0.53835	3.9161×10^{-5}
24	D.water+TBA+βCD (1)	0.4957	3.6059×10^{-5}
24	D.water+TBA+βCD (2)	0.5414	3.9383×10^{-5}
24	D.water+TBA+βCD (3)	0.4887	3.5550×10^{-5}

Table C.3. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.5384	$5.1949x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.501	$4.8340x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.53485	$5.1607x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.60665	$5.8534x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.5914	$5.7063x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.62975	$6.0763x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.6766	$6.5284x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.74405	$7.1792x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.70385	$6.7913x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.65635	$6.3330x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.6343	$6.1202x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.6795	$6.5563x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.61925	$5.9750x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.6415	$6.1897x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	0.6833	$6.5930x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.5671	$5.4718x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.64085	$6.1834x10^{-5}$
23	Phosphate Bf+BA+βCD (3)	0.55935	$5.3970x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	0.5733	$5.5316x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.59965	$5.7859x10^{-5}$
24	Phosphate Bf+BA+βCD (3)	0.59545	$5.7454x10^{-5}$

Table C.4. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.459	$4.4288x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5513	$5.3194x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5182	$5.0000x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.56065	$5.4096x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.58785	$5.6720x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.64325	$6.2066x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.60965	$5.8824x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.69105	$6.6678x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.69665	$6.7218x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.6003	$5.7922x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.6596	$6.3643x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.66605	$6.4266x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.62885	$6.0676x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.6009	$5.7980x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	0.63035	$6.0821x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.6314	$6.0922x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.57965	$5.5929x10^{-5}$
23	Phosphate Bf+BA+βCD (3)	0.55765	$5.3806x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	0.57765	$5.5736x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.56345	$5.4366x10^{-5}$
24	Phosphate Bf+BA+βCD (3)	0.60365	$5.8245x10^{-5}$

Table C.5. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.4976	$3.6197x10^{-5}$
0	D.water+TBA (2)	0.4878	$3.5484x10^{-5}$
0	D.water+TBA (3)	0.4148	$3.0174x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.5184	$3.7710x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.6119	$4.4512x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.4921	$3.5797x10^{-5}$
1	D.water+TBA+βCD (1)	0.6069	$4.4148x10^{-5}$
1	D.water+TBA+βCD (2)	0.6118	$4.4504x10^{-5}$
1	D.water+TBA+βCD (3)	0.6098	$4.4359x10^{-5}$
2	D.water+TBA+βCD (1)	0.5709	$4.1529x10^{-5}$
2	D.water+TBA+βCD (2)	0.5784	$4.2075x10^{-5}$
2	D.water+TBA+βCD (3)	0.5351	$3.8925x10^{-5}$
3	D.water+TBA+βCD (1)	0.5696	$4.1434x10^{-5}$
3	D.water+TBA+βCD (2)	0.5698	$4.1449x10^{-5}$
3	D.water+TBA+βCD (3)	0.5548	$4.0358x10^{-5}$
4	D.water+TBA+βCD (1)	0.5878	$4.2758x10^{-5}$
4	D.water+TBA+βCD (2)	0.5884	$4.2802x10^{-5}$
4	D.water+TBA+βCD (3)	0.5513	$4.0103x10^{-5}$
5	D.water+TBA+βCD (1)	0.5998	$4.3631x10^{-5}$
5	D.water+TBA+βCD (2)	0.5990	$4.3573x10^{-5}$
5	D.water+TBA+βCD (3)	0.5801	$4.2198x10^{-5}$
23	D.water+TBA+βCD (1)	0.6204	$4.5130x10^{-5}$
23	D.water+TBA+βCD (2)	0.6211	$4.5181x10^{-5}$

23	D.water+TBA+βCD (3)	0.6198	$4.5086x10^{-5}$
24	D.water+TBA+βCD (1)	0.6403	$4.6577x10^{-5}$
24	D.water+TBA+βCD (2)	0.6417	$4.6679x10^{-5}$
24	D.water+TBA+βCD (3)	0.6420	$4.6701x10^{-5}$
25	D.water+TBA+βCD (1)	0.6399	$4.6548x10^{-5}$
25	D.water+TBA+βCD (2)	0.6387	$4.6461x10^{-5}$
25	D.water+TBA+βCD (3)	0.6378	$4.6396x10^{-5}$
26	D.water+TBA+βCD (1)	0.6299	$4.5821x10^{-5}$
26	D.water+TBA+βCD (2)	0.6288	$4.5741x10^{-5}$
26	D.water+TBA+βCD (3)	0.6010	$4.3719x10^{-5}$
28	D.water+TBA+βCD (1)	0.6103	$4.4395x10^{-5}$
28	D.water+TBA+βCD (2)	0.6104	$4.4402x10^{-5}$
28	D.water+TBA+βCD (3)	0.6099	$4.4366x10^{-5}$
47	D.water+TBA+βCD (1)	0.5998	$4.3631x10^{-5}$
47	D.water+TBA+βCD (2)	0.5989	$4.3566x10^{-5}$
47	D.water+TBA+βCD (3)	0.5786	$4.2089x10^{-5}$
48	D.water+TBA+βCD (1)	0.5798	$4.2176x10^{-5}$
48	D.water+TBA+βCD (2)	0.5701	$4.1471x10^{-5}$
48	D.water+TBA+βCD (3)	0.5781	$4.2053x10^{-5}$
72	D.water+TBA+βCD (1)	0.5888	$4.2831x10^{-5}$
72	D.water+TBA+βCD (2)	0.5895	$4.2882x10^{-5}$
72	D.water+TBA+βCD (3)	0.5703	$4.1485x10^{-5}$
96	D.water+TBA+βCD (1)	0.5417	$3.9405x10^{-5}$
96	D.water+TBA+βCD (2)	0.5418	$3.9412x10^{-5}$
96	D.water+TBA+βCD (3)	0.5399	$3.9274x10^{-5}$

Table C.6. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.4818	$3.5048x10^{-5}$
0	D.water+TBA (2)	0.4814	$3.5019x10^{-5}$
0	D.water+TBA (3)	0.4774	$3.4728x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.5528	$4.0212x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.4945	$3.5971x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.5546	$4.0343x10^{-5}$
1	D.water+TBA+βCD (1)	0.6178	$4.4941x10^{-5}$
1	D.water+TBA+βCD (2)	0.6096	$4.4344x10^{-5}$
1	D.water+TBA+βCD (3)	0.6102	$4.4388x10^{-5}$
2	D.water+TBA+βCD (1)	0.5773	$4.1995x10^{-5}$
2	D.water+TBA+βCD (2)	0.5761	$4.1907x10^{-5}$
2	D.water+TBA+βCD (3)	0.5269	$3.8328x10^{-5}$
3	D.water+TBA+βCD (1)	0.5677	$4.1296x10^{-5}$
3	D.water+TBA+βCD (2)	0.5699	$4.1456x10^{-5}$
3	D.water+TBA+βCD (3)	0.5540	$4.0300x10^{-5}$
4	D.water+TBA+βCD (1)	0.5896	$4.2889x10^{-5}$
4	D.water+TBA+βCD (2)	0.5881	$4.2780x10^{-5}$
4	D.water+TBA+βCD (3)	0.5777	$4.2024x10^{-5}$
5	D.water+TBA+βCD (1)	0.5991	$4.3580x10^{-5}$
5	D.water+TBA+βCD (2)	0.5997	$4.3624x10^{-5}$
5	D.water+TBA+βCD (3)	0.5703	$4.1485x10^{-5}$
23	D.water+TBA+βCD (1)	0.6203	$4.5123x10^{-5}$
23	D.water+TBA+βCD (2)	0.6213	$4.5195x10^{-5}$

23	D.water+TBA+βCD (3)	0.6014	$4.3748x10^{-5}$
24	D.water+TBA+βCD (1)	0.6405	$4.6592x10^{-5}$
24	D.water+TBA+βCD (2)	0.6419	$4.6694x10^{-5}$
24	D.water+TBA+βCD (3)	0.6422	$4.6716x10^{-5}$
25	D.water+TBA+βCD (1)	0.6390	$4.6483x10^{-5}$
25	D.water+TBA+βCD (2)	0.6399	$4.6548x10^{-5}$
25	D.water+TBA+βCD (3)	0.6377	$4.6388x10^{-5}$
26	D.water+TBA+βCD (1)	0.6298	$4.5814x10^{-5}$
26	D.water+TBA+βCD (2)	0.6291	$4.5763x10^{-5}$
26	D.water+TBA+βCD (3)	0.6001	$4.3653x10^{-5}$
28	D.water+TBA+βCD (1)	0.6198	$4.5086x10^{-5}$
28	D.water+TBA+βCD (2)	0.6107	$4.4424x10^{-5}$
28	D.water+TBA+βCD (3)	0.6088	$4.4286x10^{-5}$
47	D.water+TBA+βCD (1)	0.5995	$4.3610x10^{-5}$
47	D.water+TBA+βCD (2)	0.5990	$4.3573x10^{-5}$
47	D.water+TBA+βCD (3)	0.5713	$4.1558x10^{-5}$
48	D.water+TBA+βCD (1)	0.5788	$4.2104x10^{-5}$
48	D.water+TBA+βCD (2)	0.5799	$4.2184x10^{-5}$
48	D.water+TBA+βCD (3)	0.5703	$4.1485x10^{-5}$
72	D.water+TBA+βCD (1)	0.5881	$4.2780x10^{-5}$
72	D.water+TBA+βCD (2)	0.5896	$4.2889x10^{-5}$
72	D.water+TBA+βCD (3)	0.5701	$4.1471x10^{-5}$
96	D.water+TBA+βCD (1)	0.5405	$3.9318x10^{-5}$
96	D.water+TBA+βCD (2)	0.5422	$3.9441x10^{-5}$
96	D.water+TBA+βCD (3)	0.5417	$3.9405x10^{-5}$

Table C.7. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.5286	$5.1003x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5396	$5.2065x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5148	$4.9672x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	1.2139	$1.1713x10^{-4}$
0.5	Phosphate Bf+BA+βCD (2)	0.6332	$6.1096x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.6340	$6.1173x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.6778	$6.5399x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.6796	$6.5573x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.6592	$6.3605x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.6392	$6.1675x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.6397	$6.1723x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.780	$7.5261x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.6217	$5.9986x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.6208	$5.9900x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	0.6098	$5.8838x10^{-5}$
4	Phosphate Bf+BA+βCD (1)	0.6696	$6.4608x10^{-5}$
4	Phosphate Bf+BA+βCD (2)	0.6687	$6.4521x10^{-5}$
4	Phosphate Bf+BA+βCD (3)	0.6888	$6.6461x10^{-5}$
5	Phosphate Bf+BA+βCD (1)	0.6818	$6.5785x10^{-5}$
5	Phosphate Bf+BA+βCD (2)	0.6882	$6.6403x10^{-5}$
5	Phosphate Bf+BA+βCD (3)	0.6704	$6.4685x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.7012	$6.7657x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.7014	$6.7677x10^{-5}$

23	Phosphate Bf+BA+βCD (3)	0.7102	$6.8526x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	0.7202	$6.9491x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.7213	$6.9597x10^{-5}$
24	Phosphate Bf+BA+βCD (3)	0.7001	$6.7551x10^{-5}$
25	Phosphate Bf+BA+βCD (1)	0.7109	$6.8593x10^{-5}$
25	Phosphate Bf+BA+βCD (2)	0.7199	$6.9462x10^{-5}$
25	Phosphate Bf+BA+βCD (3)	0.7188	$6.9355x10^{-5}$
26	Phosphate Bf+BA+βCD (1)	0.7088	$6.8391x10^{-5}$
26	Phosphate Bf+BA+βCD (2)	0.7069	$6.8207x10^{-5}$
26	Phosphate Bf+BA+βCD (3)	0.7047	$6.7995x10^{-5}$
28	Phosphate Bf+BA+βCD (1)	0.6998	$6.7522x10^{-5}$
28	Phosphate Bf+BA+βCD (2)	0.6889	$6.6470x10^{-5}$
28	Phosphate Bf+BA+βCD (3)	0.6918	$6.6750x10^{-5}$
47	Phosphate Bf+BA+βCD (1)	0.6758	$6.5206x10^{-5}$
47	Phosphate Bf+BA+βCD (2)	0.6713	$6.4772x10^{-5}$
47	Phosphate Bf+BA+βCD (3)	0.6699	$6.4637x10^{-5}$
48	Phosphate Bf+BA+βCD (1)	0.6513	$6.2843x10^{-5}$
48	Phosphate Bf+BA+βCD (2)	0.6504	$6.2756x10^{-5}$
48	Phosphate Bf+BA+βCD (3)	0.6548	$6.3180x10^{-5}$
72	Phosphate Bf+BA+βCD (1)	0.5989	$5.7787x10^{-5}$
72	Phosphate Bf+BA+βCD (2)	0.6001	$5.7902x10^{-5}$
72	Phosphate Bf+BA+βCD (3)	0.5999	$5.7883x10^{-5}$
96	Phosphate Bf+BA+βCD (1)	0.5714	$5.5133x10^{-5}$
96	Phosphate Bf+BA+βCD (2)	0.5802	$5.5982x10^{-5}$
96	Phosphate Bf+BA+βCD (3)	0.5716	$5.5152x10^{-5}$

Table C.8. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.5543	$5.3483x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5298	$5.1119x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5286	$5.1003x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	0.6096	$5.8819x10^{-5}$
0.5	Phosphate Bf+BA+βCD (2)	0.5907	$5.6995x10^{-5}$
0.5	Phosphate Bf+BA+βCD (3)	0.6479	$6.2514x10^{-5}$
1	Phosphate Bf+BA+βCD (1)	0.6817	$6.5776x10^{-5}$
1	Phosphate Bf+BA+βCD (2)	0.6799	$6.5602x10^{-5}$
1	Phosphate Bf+BA+βCD (3)	0.6149	$5.9330x10^{-5}$
2	Phosphate Bf+BA+βCD (1)	0.6109	$5.8944x10^{-5}$
2	Phosphate Bf+BA+βCD (2)	0.6423	$6.1974x10^{-5}$
2	Phosphate Bf+BA+βCD (3)	0.6474	$6.2466x10^{-5}$
3	Phosphate Bf+BA+βCD (1)	0.6211	$5.9929x10^{-5}$
3	Phosphate Bf+BA+βCD (2)	0.6213	$5.9948x10^{-5}$
3	Phosphate Bf+BA+βCD (3)	0.6014	$5.8028x10^{-5}$
4	Phosphate Bf+BA+βCD (1)	0.7001	$6.7551x10^{-5}$
4	Phosphate Bf+BA+βCD (2)	0.6699	$6.4637x10^{-5}$
4	Phosphate Bf+BA+βCD (3)	0.6608	$6.3759x10^{-5}$
5	Phosphate Bf+BA+βCD (1)	0.6820	$6.5805x10^{-5}$
5	Phosphate Bf+BA+βCD (2)	0.6874	$6.6326x10^{-5}$
5	Phosphate Bf+BA+βCD (3)	0.6714	$6.4782x10^{-5}$
23	Phosphate Bf+BA+βCD (1)	0.7015	$6.7686x10^{-5}$
23	Phosphate Bf+BA+βCD (2)	0.7016	$6.7696x10^{-5}$

23	Phosphate Bf+BA+βCD (3)	0.7103	$6.8535x10^{-5}$
24	Phosphate Bf+BA+βCD (1)	0.7217	$6.9635x10^{-5}$
24	Phosphate Bf+BA+βCD (2)	0.7201	$6.9481x10^{-5}$
24	Phosphate Bf+BA+βCD (3)	0.7199	$6.9462x10^{-5}$
25	Phosphate Bf+BA+βCD (1)	0.7108	$6.8584x10^{-5}$
25	Phosphate Bf+BA+βCD (2)	0.7118	$6.8680x10^{-5}$
25	Phosphate Bf+BA+βCD (3)	0.7198	$6.9452x10^{-5}$
26	Phosphate Bf+BA+βCD (1)	0.7098	$6.8487x10^{-5}$
26	Phosphate Bf+BA+βCD (2)	0.7102	$6.8526x10^{-5}$
26	Phosphate Bf+BA+βCD (3)	0.7058	$6.8101x10^{-5}$
28	Phosphate Bf+BA+βCD (1)	0.6970	$6.7252x10^{-5}$
28	Phosphate Bf+BA+βCD (2)	0.6972	$6.7271x10^{-5}$
28	Phosphate Bf+BA+βCD (3)	0.6911	$6.6683x10^{-5}$
47	Phosphate Bf+BA+βCD (1)	0.6760	$6.5226x10^{-5}$
47	Phosphate Bf+BA+βCD (2)	0.6715	$6.4792x10^{-5}$
47	Phosphate Bf+BA+βCD (3)	0.6696	$6.4608x10^{-5}$
48	Phosphate Bf+BA+βCD (1)	0.6517	$6.2881x10^{-5}$
48	Phosphate Bf+BA+βCD (2)	0.6501	$6.2727x10^{-5}$
48	Phosphate Bf+BA+βCD (3)	0.6549	$6.3190x10^{-5}$
72	Phosphate Bf+BA+βCD (1)	0.5971	$5.7613x10^{-5}$
72	Phosphate Bf+BA+βCD (2)	0.6011	$5.7999x10^{-5}$
72	Phosphate Bf+BA+βCD (3)	0.6001	$5.7902x10^{-5}$
96	Phosphate Bf+BA+βCD (1)	0.5717	$5.5162x10^{-5}$
96	Phosphate Bf+BA+βCD (2)	0.5801	$5.5973x10^{-5}$
96	Phosphate Bf+BA+βCD (3)	0.5715	$5.5143x10^{-5}$

Table C.9. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.4109	2.9890×10^{-5}
0	D.water+TBA (2)	0.4896	3.5615×10^{-5}
0	D.water+TBA (3)	0.4902	3.5659×10^{-5}
0.5	D.water+TBA+βCD (1)	0.5703	4.1485×10^{-5}
0.5	D.water+TBA+βCD (2)	0.4966	3.6124×10^{-5}
0.5	D.water+TBA+βCD (3)	0.5539	4.0292×10^{-5}
1	D.water+TBA+βCD (1)	0.6247	4.5443×10^{-5}
1	D.water+TBA+βCD (2)	0.6213	4.5195×10^{-5}
1	D.water+TBA+βCD (3)	0.6288	4.5741×10^{-5}
2	D.water+TBA+βCD (1)	0.5818	4.2322×10^{-5}
2	D.water+TBA+βCD (2)	0.5876	4.2744×10^{-5}
2	D.water+TBA+βCD (3)	0.5104	3.7128×10^{-5}
3	D.water+TBA+βCD (1)	0.5748	4.1813×10^{-5}
3	D.water+TBA+βCD (2)	0.5788	4.2104×10^{-5}
3	D.water+TBA+βCD (3)	0.5044	3.6692×10^{-5}
4	D.water+TBA+βCD (1)	0.5881	4.2780×10^{-5}
4	D.water+TBA+βCD (2)	0.5903	4.2940×10^{-5}
4	D.water+TBA+βCD (3)	0.5910	4.2991×10^{-5}
5	D.water+TBA+βCD (1)	0.6061	4.4090×10^{-5}
5	D.water+TBA+βCD (2)	0.6057	4.4061×10^{-5}
5	D.water+TBA+βCD (3)	0.6103	4.4395×10^{-5}
23	D.water+TBA+βCD (1)	0.6478	4.7123×10^{-5}
23	D.water+TBA+βCD (2)	0.6498	4.7268×10^{-5}

23	D.water+TBA+βCD (3)	0.6317	4.5952×10^{-5}
24	D.water+TBA+βCD (1)	0.6699	4.8731×10^{-5}
24	D.water+TBA+βCD (2)	0.6698	4.8723×10^{-5}
24	D.water+TBA+βCD (3)	0.6887	5.0098×10^{-5}
25	D.water+TBA+βCD (1)	0.6587	4.7916×10^{-5}
25	D.water+TBA+βCD (2)	0.6560	4.7720×10^{-5}
25	D.water+TBA+βCD (3)	0.6413	4.6650×10^{-5}
26	D.water+TBA+βCD (1)	0.6599	4.8003×10^{-5}
26	D.water+TBA+βCD (2)	0.6587	4.7916×10^{-5}
26	D.water+TBA+βCD (3)	0.6167	4.4861×10^{-5}
28	D.water+TBA+βCD (1)	0.6317	4.5952×10^{-5}
28	D.water+TBA+βCD (2)	0.6318	4.5959×10^{-5}
28	D.water+TBA+βCD (3)	0.6298	4.5814×10^{-5}
47	D.water+TBA+βCD (1)	0.6013	4.3740×10^{-5}
47	D.water+TBA+βCD (2)	0.6004	4.3675×10^{-5}
47	D.water+TBA+βCD (3)	0.6015	4.3755×10^{-5}
48	D.water+TBA+βCD (1)	0.5813	4.2286×10^{-5}
48	D.water+TBA+βCD (2)	0.5814	4.2293×10^{-5}
48	D.water+TBA+βCD (3)	0.5817	4.2315×10^{-5}
72	D.water+TBA+βCD (1)	0.6001	4.3653×10^{-5}
72	D.water+TBA+βCD (2)	0.6013	4.3740×10^{-5}
72	D.water+TBA+βCD (3)	0.6002	4.3660×10^{-5}
96	D.water+TBA+βCD (1)	0.5421	3.9434×10^{-5}
96	D.water+TBA+βCD (2)	0.5422	3.9441×10^{-5}
96	D.water+TBA+βCD (3)	0.5455	3.9681×10^{-5}

Table C.10. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.4857	$3.5331x10^{-5}$
0	D.water+TBA (2)	0.4875	$3.5462x10^{-5}$
0	D.water+TBA (3)	0.4798	$3.4902x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.5298	$3.8539x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.5602	$4.0751x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.5956	$4.3326x10^{-5}$
1	D.water+TBA+βCD (1)	0.6297	$4.5806x10^{-5}$
1	D.water+TBA+βCD (2)	0.6247	$4.5443x10^{-5}$
1	D.water+TBA+βCD (3)	0.6068	$4.4141x10^{-5}$
2	D.water+TBA+βCD (1)	0.5711	$4.1544x10^{-5}$
2	D.water+TBA+βCD (2)	0.5807	$4.2242x10^{-5}$
2	D.water+TBA+βCD (3)	0.5788	$4.2104x10^{-5}$
3	D.water+TBA+βCD (1)	0.5747	$4.1805x10^{-5}$
3	D.water+TBA+βCD (2)	0.5798	$4.2176x10^{-5}$
3	D.water+TBA+βCD (3)	0.5105	$3.7135x10^{-5}$
4	D.water+TBA+βCD (1)	0.5905	$4.2955x10^{-5}$
4	D.water+TBA+βCD (2)	0.5909	$4.2984x10^{-5}$
4	D.water+TBA+βCD (3)	0.5818	$4.2322x10^{-5}$
5	D.water+TBA+βCD (1)	0.6058	$4.4068x10^{-5}$
5	D.water+TBA+βCD (2)	0.6071	$4.4162x10^{-5}$
5	D.water+TBA+βCD (3)	0.6104	$4.4402x10^{-5}$
23	D.water+TBA+βCD (1)	0.6477	$4.7116x10^{-5}$
23	D.water+TBA+βCD (2)	0.6488	$4.7196x10^{-5}$

23	D.water+TBA+βCD (3)	0.6302	$4.5843x10^{-5}$
24	D.water+TBA+βCD (1)	0.6688	$4.8651x10^{-5}$
24	D.water+TBA+βCD (2)	0.6702	$4.8752x10^{-5}$
24	D.water+TBA+βCD (3)	0.6503	$4.7305x10^{-5}$
25	D.water+TBA+βCD (1)	0.6589	$4.7930x10^{-5}$
25	D.water+TBA+βCD (2)	0.6558	$4.7705x10^{-5}$
25	D.water+TBA+βCD (3)	0.6013	$4.3740x10^{-5}$
26	D.water+TBA+βCD (1)	0.6591	$4.7945x10^{-5}$
26	D.water+TBA+βCD (2)	0.6592	$4.7952x10^{-5}$
26	D.water+TBA+βCD (3)	0.6413	$4.6650x10^{-5}$
28	D.water+TBA+βCD (1)	0.6313	$4.5923x10^{-5}$
28	D.water+TBA+βCD (2)	0.6319	$4.5966x10^{-5}$
28	D.water+TBA+βCD (3)	0.6288	$4.5741x10^{-5}$
47	D.water+TBA+βCD (1)	0.6018	$4.3777x10^{-5}$
47	D.water+TBA+βCD (2)	0.6005	$4.3682x10^{-5}$
47	D.water+TBA+βCD (3)	0.6013	$4.3740x10^{-5}$
48	D.water+TBA+βCD (1)	0.5816	$4.2307x10^{-5}$
48	D.water+TBA+βCD (2)	0.5809	$4.2256x10^{-5}$
48	D.water+TBA+βCD (3)	0.5820	$4.2337x10^{-5}$
72	D.water+TBA+βCD (1)	0.6015	$4.3755x10^{-5}$
72	D.water+TBA+βCD (2)	0.6004	$4.3675x10^{-5}$
72	D.water+TBA+βCD (3)	0.6011	$4.3726x10^{-5}$
96	D.water+TBA+βCD (1)	0.5433	$3.9521x10^{-5}$
96	D.water+TBA+βCD (2)	0.5420	$3.9427x10^{-5}$
96	D.water+TBA+βCD (3)	0.5441	$3.9580x10^{-5}$

Table C.11. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.5384	5.1949×10^{-5}
0	Phosphate Buffer+TBA (2)	0.5211	5.0280×10^{-5}
0	Phosphate Buffer+TBA (3)	0.5012	4.8360×10^{-5}
0.5	Phosphate Bf+BA+βCD (1)	1.1767	1.1354×10^{-4}
0.5	Phosphate Bf+BA+βCD (2)	1.1696	1.1285×10^{-4}
0.5	Phosphate Bf+BA+βCD (3)	1.1647	1.1238×10^{-4}
1	Phosphate Bf+BA+βCD (1)	1.2021	1.1599×10^{-4}
1	Phosphate Bf+BA+βCD (2)	1.2247	1.1817×10^{-4}
1	Phosphate Bf+BA+βCD (3)	1.2196	1.1768×10^{-4}
2	Phosphate Bf+BA+βCD (1)	1.1818	1.1403×10^{-4}
2	Phosphate Bf+BA+βCD (2)	1.1817	1.1402×10^{-4}
2	Phosphate Bf+BA+βCD (3)	0.9999	9.6478×10^{-5}
3	Phosphate Bf+BA+βCD (1)	1.1717	1.1305×10^{-4}
3	Phosphate Bf+BA+βCD (2)	1.1796	1.1382×10^{-4}
3	Phosphate Bf+BA+βCD (3)	1.1112	1.0722×10^{-4}
4	Phosphate Bf+BA+βCD (1)	1.1999	1.1578×10^{-4}
4	Phosphate Bf+BA+βCD (2)	1.2001	1.1580×10^{-4}
4	Phosphate Bf+BA+βCD (3)	1.1988	1.1567×10^{-4}
5	Phosphate Bf+BA+βCD (1)	1.2021	1.1599×10^{-4}
5	Phosphate Bf+BA+βCD (2)	1.2017	1.1595×10^{-4}
5	Phosphate Bf+BA+βCD (3)	1.2308	1.1876×10^{-4}
23	Phosphate Bf+BA+βCD (1)	1.2412	1.1976×10^{-4}
23	Phosphate Bf+BA+βCD (2)	1.2416	1.1980×10^{-4}

23	Phosphate Bf+BA+βCD (3)	1.2403	$1.1967x10^{-4}$
24	Phosphate Bf+BA+βCD (1)	1.2799	$1.2349x10^{-4}$
24	Phosphate Bf+BA+βCD (2)	1.2698	$1.2252x10^{-4}$
24	Phosphate Bf+BA+βCD (3)	1.2477	$1.2039x10^{-4}$
25	Phosphate Bf+BA+βCD (1)	1.2540	$1.2100x10^{-4}$
25	Phosphate Bf+BA+βCD (2)	1.2518	$1.2078x10^{-4}$
25	Phosphate Bf+BA+βCD (3)	1.2557	$1.2116x10^{-4}$
26	Phosphate Bf+BA+βCD (1)	1.2493	$1.2054x10^{-4}$
26	Phosphate Bf+BA+βCD (2)	1.2399	$1.1964x10^{-4}$
26	Phosphate Bf+BA+βCD (3)	1.2403	$1.1967x10^{-4}$
28	Phosphate Bf+BA+βCD (1)	1.2211	$1.1782x10^{-4}$
28	Phosphate Bf+BA+βCD (2)	1.2218	$1.1789x10^{-4}$
28	Phosphate Bf+BA+βCD (3)	1.2220	$1.1791x10^{-4}$
47	Phosphate Bf+BA+βCD (1)	1.2017	$1.1595x10^{-4}$
47	Phosphate Bf+BA+βCD (2)	1.2018	$1.1596x10^{-4}$
47	Phosphate Bf+BA+βCD (3)	1.2128	$1.1702x10^{-4}$
48	Phosphate Bf+BA+βCD (1)	1.1884	$1.1467x10^{-4}$
48	Phosphate Bf+BA+βCD (2)	1.1871	$1.1454x10^{-4}$
48	Phosphate Bf+BA+βCD (3)	1.1870	$1.1453x10^{-4}$
72	Phosphate Bf+BA+βCD (1)	1.2001	$1.1580x10^{-4}$
72	Phosphate Bf+BA+βCD (2)	1.2012	$1.1590x10^{-4}$
72	Phosphate Bf+BA+βCD (3)	1.2014	$1.1592x10^{-4}$
96	Phosphate Bf+BA+βCD (1)	1.1212	$1.0818x10^{-4}$
96	Phosphate Bf+BA+βCD (2)	1.1303	$1.0906x10^{-4}$
96	Phosphate Bf+BA+βCD (3)	1.1296	$1.0899x10^{-4}$

Table C.12. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.5396	$5.2065x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5217	$5.0338x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5218	$5.0347x10^{-5}$
0.5	Phosphate Bf+BA+βCD (1)	1.1697	$1.1286x10^{-4}$
0.5	Phosphate Bf+BA+βCD (2)	1.1599	$1.1192x10^{-4}$
0.5	Phosphate Bf+BA+βCD (3)	1.1648	$1.1239x10^{-4}$
1	Phosphate Bf+BA+βCD (1)	1.2188	$1.1760x10^{-4}$
1	Phosphate Bf+BA+βCD (2)	1.2116	$1.1690x10^{-4}$
1	Phosphate Bf+BA+βCD (3)	1.2298	$1.1866x10^{-4}$
2	Phosphate Bf+BA+βCD (1)	1.1814	$1.1399x10^{-4}$
2	Phosphate Bf+BA+βCD (2)	1.1861	$1.1444x10^{-4}$
2	Phosphate Bf+BA+βCD (3)	1.1202	$1.0809x10^{-4}$
3	Phosphate Bf+BA+βCD (1)	1.1798	$1.1384x10^{-4}$
3	Phosphate Bf+BA+βCD (2)	1.1777	$1.1363x10^{-4}$
3	Phosphate Bf+BA+βCD (3)	1.1011	$1.0624x10^{-4}$
4	Phosphate Bf+BA+βCD (1)	1.1986	$1.1565x10^{-4}$
4	Phosphate Bf+BA+βCD (2)	1.1997	$1.1576x10^{-4}$
4	Phosphate Bf+BA+βCD (3)	1.1808	$1.1393x10^{-4}$
5	Phosphate Bf+BA+βCD (1)	1.2088	$1.1663x10^{-4}$
5	Phosphate Bf+BA+βCD (2)	1.2002	$1.1580x10^{-4}$
5	Phosphate Bf+BA+βCD (3)	1.2403	$1.1967x10^{-4}$
23	Phosphate Bf+BA+βCD (1)	1.2413	$1.1977x10^{-4}$
23	Phosphate Bf+BA+βCD (2)	1.2417	$1.1981x10^{-4}$

23	Phosphate Bf+BA+βCD (3)	1.2404	$1.1968x10^{-4}$
24	Phosphate Bf+BA+βCD (1)	1.2799	$1.2349x10^{-4}$
24	Phosphate Bf+BA+βCD (2)	1.2795	$1.2346x10^{-4}$
24	Phosphate Bf+BA+βCD (3)	1.2403	$1.1967x10^{-4}$
25	Phosphate Bf+BA+βCD (1)	1.2542	$1.2102x10^{-4}$
25	Phosphate Bf+BA+βCD (2)	1.2513	$1.2074x10^{-4}$
25	Phosphate Bf+BA+βCD (3)	1.2560	$1.2119x10^{-4}$
26	Phosphate Bf+BA+βCD (1)	1.2459	$1.2021x10^{-4}$
26	Phosphate Bf+BA+βCD (2)	1.2501	$1.2062x10^{-4}$
26	Phosphate Bf+BA+βCD (3)	1.2458	$1.2020x10^{-4}$
28	Phosphate Bf+BA+βCD (1)	1.2224	$1.1795x10^{-4}$
28	Phosphate Bf+BA+βCD (2)	1.2228	$1.1799x10^{-4}$
28	Phosphate Bf+BA+βCD (3)	1.2227	$1.1798x10^{-4}$
47	Phosphate Bf+BA+βCD (1)	1.2003	$1.1581x10^{-4}$
47	Phosphate Bf+BA+βCD (2)	1.2020	$1.1598x10^{-4}$
47	Phosphate Bf+BA+βCD (3)	1.2130	$1.1704x10^{-4}$
48	Phosphate Bf+BA+βCD (1)	1.1886	$1.1469x10^{-4}$
48	Phosphate Bf+BA+βCD (2)	1.1872	$1.1455x10^{-4}$
48	Phosphate Bf+BA+βCD (3)	1.1870	$1.1453x10^{-4}$
72	Phosphate Bf+BA+βCD (1)	1.2003	$1.1581x10^{-4}$
72	Phosphate Bf+BA+βCD (2)	1.2114	$1.1689x10^{-4}$
72	Phosphate Bf+BA+βCD (3)	1.2005	$1.1583x10^{-4}$
96	Phosphate Bf+BA+βCD (1)	1.1221	$1.0827x10^{-4}$
96	Phosphate Bf+BA+βCD (2)	1.1301	$1.0904x10^{-4}$
96	Phosphate Bf+BA+βCD (3)	1.2201	$1.1772x10^{-4}$

Table C.13. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:0.25 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.4620	$3.3607x10^{-5}$
0	D.water+TBA (2)	0.4568	$3.3229x10^{-5}$
0	D.water+TBA (3)	0.4558	$3.3156x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.5285	$3.8445x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.5355	$3.8954x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.5298	$3.8539x10^{-5}$
2	D.water+TBA+βCD (1)	0.5417	$3.9405x10^{-5}$
2	D.water+TBA+βCD (2)	0.5419	$3.9420x10^{-5}$
2	D.water+TBA+βCD (3)	0.5599	$4.0729x10^{-5}$
4	D.water+TBA+βCD (1)	0.5598	$4.0722x10^{-5}$
4	D.water+TBA+βCD (2)	0.5572	$4.0532x10^{-5}$
4	D.water+TBA+βCD (3)	0.5560	$4.0445x10^{-5}$
23	D.water+TBA+βCD (1)	0.5701	$4.1471x10^{-5}$
23	D.water+TBA+βCD (2)	0.5713	$4.1558x10^{-5}$
23	D.water+TBA+βCD (3)	0.5114	$3.7201x10^{-5}$
24	D.water+TBA+βCD (1)	0.6006	$4.3690x10^{-5}$
24	D.water+TBA+βCD (2)	0.6017	$4.3770x10^{-5}$
24	D.water+TBA+βCD (3)	0.6010	$4.3719x10^{-5}$

Table C.14. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:0.25 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.4513	$3.2829x10^{-5}$
0	D.water+TBA (2)	0.4596	$3.3433x10^{-5}$
0	D.water+TBA (3)	0.4718	$3.4320x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.5249	$3.8183x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.5205	$3.7863x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.5291	$3.8488x10^{-5}$
2	D.water+TBA+βCD (1)	0.5420	$3.9427x10^{-5}$
2	D.water+TBA+βCD (2)	0.5413	$3.9376x10^{-5}$
2	D.water+TBA+βCD (3)	0.5618	$4.0867x10^{-5}$
4	D.water+TBA+βCD (1)	0.5596	$4.0707x10^{-5}$
4	D.water+TBA+βCD (2)	0.5571	$4.0525x10^{-5}$
4	D.water+TBA+βCD (3)	0.5575	$4.0554x10^{-5}$
23	D.water+TBA+βCD (1)	0.5708	$4.1522x10^{-5}$
23	D.water+TBA+βCD (2)	0.5711	$4.1544x10^{-5}$
23	D.water+TBA+βCD (3)	0.5010	$3.6444x10^{-5}$
24	D.water+TBA+βCD (1)	0.6013	$4.3740x10^{-5}$
24	D.water+TBA+βCD (2)	0.6001	$4.3653x10^{-5}$
24	D.water+TBA+βCD (3)	0.6018	$4.3777x10^{-5}$

Table C.15. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:0.25 ratio) complex in phosphate buffer (1st trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	Phosphate Buffer+TBA (1)	0.5402	$5.2123x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5398	$5.2084x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5315	$5.1283x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (1)	0.5393	$5.2036x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (2)	0.5438	$5.2470x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (3)	0.5972	$5.7623x10^{-5}$
2	Phosphate Bf+TBA+βCD (1)	0.6381	$6.1569x10^{-5}$
2	Phosphate Bf+TBA+βCD (2)	0.6317	$6.0951x10^{-5}$
2	Phosphate Bf+TBA+βCD (3)	0.6396	$6.1714x10^{-5}$
4	Phosphate Bf+TBA+βCD (1)	0.6211	$5.9929x10^{-5}$
4	Phosphate Bf+TBA+βCD (2)	0.6307	$6.0855x10^{-5}$
4	Phosphate Bf+TBA+βCD (3)	0.6390	$6.1656x10^{-5}$
23	Phosphate Bf+TBA+βCD (1)	0.6517	$6.2881x10^{-5}$
23	Phosphate Bf+TBA+βCD (2)	0.6502	$6.2736x10^{-5}$
23	Phosphate Bf+TBA+βCD (3)	0.6513	$6.2843x10^{-5}$
24	Phosphate Bf+TBA+βCD (1)	0.6934	$6.6905x10^{-5}$
24	Phosphate Bf+TBA+βCD (2)	0.6960	$6.7156x10^{-5}$
24	Phosphate Bf+TBA+βCD (3)	0.6999	$6.7532x10^{-5}$

Table C.16. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:0.25 ratio) complex in phosphate buffer (2nd trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	Phosphate Buffer+TBA (1)	0.5084	4.9054×10^{-5}
0	Phosphate Buffer+TBA (2)	0.5413	5.2229×10^{-5}
0	Phosphate Buffer+TBA (3)	0.5399	5.2094×10^{-5}
0.5	Phosphate Bf+TBA+βCD (1)	0.5576	5.1872×10^{-5}
0.5	Phosphate Bf+TBA+βCD (2)	0.5569	5.1804×10^{-5}
0.5	Phosphate Bf+TBA+βCD (3)	0.5547	5.3522×10^{-5}
2	Phosphate Bf+TBA+βCD (1)	0.6315	6.0932×10^{-5}
2	Phosphate Bf+TBA+βCD (2)	0.6397	6.1723×10^{-5}
2	Phosphate Bf+TBA+βCD (3)	0.6355	6.1318×10^{-5}
4	Phosphate Bf+TBA+βCD (1)	0.6213	5.9948×10^{-5}
4	Phosphate Bf+TBA+βCD (2)	0.6312	6.0903×10^{-5}
4	Phosphate Bf+TBA+βCD (3)	0.6394	6.1694×10^{-5}
23	Phosphate Bf+TBA+βCD (1)	0.6520	6.2910×10^{-5}
23	Phosphate Bf+TBA+βCD (2)	0.6522	6.2929×10^{-5}
23	Phosphate Bf+TBA+βCD (3)	0.6501	6.2727×10^{-5}
24	Phosphate Bf+TBA+βCD (1)	0.6986	6.7406×10^{-5}
24	Phosphate Bf+TBA+βCD (2)	0.6916	6.6731×10^{-5}
24	Phosphate Bf+TBA+βCD (3)	0.6901	6.6586×10^{-5}

Table C.17. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:0.5 ratio) complex distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.4544	$3.3054x10^{-5}$
0	D.water+TBA (2)	0.4543	$3.3047x10^{-5}$
0	D.water+TBA (3)	0.4140	$3.0116x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.5543	$4.0322x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.5527	$4.0205x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.5506	$4.0052x10^{-5}$
2	D.water+TBA+βCD (1)	0.5620	$4.0882x10^{-5}$
2	D.water+TBA+βCD (2)	0.5604	$4.0765x10^{-5}$
2	D.water+TBA+βCD (3)	0.5613	$4.0831x10^{-5}$
4	D.water+TBA+βCD (1)	0.5703	$4.1485x10^{-5}$
4	D.water+TBA+βCD (2)	0.5699	$4.1456x10^{-5}$
4	D.water+TBA+βCD (3)	0.5715	$4.1573x10^{-5}$
23	D.water+TBA+βCD (1)	0.5920	$4.3064x10^{-5}$
23	D.water+TBA+βCD (2)	0.5899	$4.2911x10^{-5}$
23	D.water+TBA+βCD (3)	0.5913	$4.3013x10^{-5}$
24	D.water+TBA+βCD (1)	0.6286	$4.5726x10^{-5}$
24	D.water+TBA+βCD (2)	0.6216	$4.5217x10^{-5}$
24	D.water+TBA+βCD (3)	0.6257	$4.5515x10^{-5}$

Table C.18. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:0.5 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.4530	$3.2953x10^{-5}$
0	D.water+TBA (2)	0.4561	$3.3178x10^{-5}$
0	D.water+TBA (3)	0.4030	$2.9315x10^{-5}$
0.5	D.water+TBA+βCD (1)	0.5505	$4.0045x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.5569	$4.0511x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.5502	$4.0023x10^{-5}$
2	D.water+TBA+βCD (1)	0.5621	$4.0889x10^{-5}$
2	D.water+TBA+βCD (2)	0.5605	$4.0773x10^{-5}$
2	D.water+TBA+βCD (3)	0.5611	$4.0816x10^{-5}$
4	D.water+TBA+βCD (1)	0.5713	$4.1558x10^{-5}$
4	D.water+TBA+βCD (2)	0.5618	$4.0867x10^{-5}$
4	D.water+TBA+βCD (3)	0.5702	$4.1478x10^{-5}$
23	D.water+TBA+βCD (1)	0.5922	$4.3078x10^{-5}$
23	D.water+TBA+βCD (2)	0.5917	$4.3042x10^{-5}$
23	D.water+TBA+βCD (3)	0.5713	$4.1558x10^{-5}$
24	D.water+TBA+βCD (1)	0.6298	$4.5814x10^{-5}$
24	D.water+TBA+βCD (2)	0.6270	$4.5610x10^{-5}$
24	D.water+TBA+βCD (3)	0.6258	$4.5523x10^{-5}$

Table C.19. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:0.5 ratio) complex in phosphate buffer (1st trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	Phosphate Buffer+TBA (1)	0.5302	$5.1158x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5388	$5.1988x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5201	$5.0183x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (1)	0.6105	$5.8906x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (2)	0.6197	$5.9794x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (3)	0.7319	$7.0619x10^{-5}$
2	Phosphate Bf+TBA+βCD (1)	0.6526	$6.2968x10^{-5}$
2	Phosphate Bf+TBA+βCD (2)	0.7989	$7.7084x10^{-5}$
2	Phosphate Bf+TBA+βCD (3)	0.6527	$6.2978x10^{-5}$
4	Phosphate Bf+TBA+βCD (1)	0.6417	$6.1916x10^{-5}$
4	Phosphate Bf+TBA+βCD (2)	0.6398	$6.1733x10^{-5}$
4	Phosphate Bf+TBA+βCD (3)	0.6415	$6.1897x10^{-5}$
23	Phosphate Bf+TBA+βCD (1)	0.6648	$6.4145x10^{-5}$
23	Phosphate Bf+TBA+βCD (2)	0.6617	$6.3846x10^{-5}$
23	Phosphate Bf+TBA+βCD (3)	0.6607	$6.3750x10^{-5}$
24	Phosphate Bf+TBA+βCD (1)	0.7184	$6.9317x10^{-5}$
24	Phosphate Bf+TBA+βCD (2)	0.7123	$6.8728x10^{-5}$
24	Phosphate Bf+TBA+βCD (3)	0.7244	$6.9896x10^{-5}$

Table C.20. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:0.5 ratio) complex in phosphate buffer (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.5599	5.4024×10^{-5}
0	Phosphate Buffer+TBA (2)	0.5318	5.1312×10^{-5}
0	Phosphate Buffer+TBA (3)	0.5499	5.3059×10^{-5}
0.5	Phosphate Bf+TBA+βCD (1)	0.6113	5.8983×10^{-5}
0.5	Phosphate Bf+TBA+βCD (2)	0.6678	6.4435×10^{-5}
0.5	Phosphate Bf+TBA+βCD (3)	0.6141	5.9253×10^{-5}
2	Phosphate Bf+TBA+βCD (1)	0.8166	7.8792×10^{-5}
2	Phosphate Bf+TBA+βCD (2)	0.6588	6.3566×10^{-5}
2	Phosphate Bf+TBA+βCD (3)	0.6594	6.3624×10^{-5}
4	Phosphate Bf+TBA+βCD (1)	0.6403	6.1781×10^{-5}
4	Phosphate Bf+TBA+βCD (2)	0.6450	6.2235×10^{-5}
4	Phosphate Bf+TBA+βCD (3)	0.6648	6.4145×10^{-5}
23	Phosphate Bf+TBA+βCD (1)	0.6659	6.4251×10^{-5}
23	Phosphate Bf+TBA+βCD (2)	0.6615	6.3827×10^{-5}
23	Phosphate Bf+TBA+βCD (3)	0.6113	5.8983×10^{-5}
24	Phosphate Bf+TBA+βCD (1)	0.7149	6.8979×10^{-5}
24	Phosphate Bf+TBA+βCD (2)	0.7165	6.9134×10^{-5}
24	Phosphate Bf+TBA+βCD (3)	0.7164	6.9124×10^{-5}

Table C.21. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid 2-hydroxyl- propyl-β-CD (1:1 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.6012	$4.3733x10^{-5}$
0	D.water+TBA (2)	0.6891	$5.0127x10^{-5}$
0	D.water+TBA (3)	0.7011	$5.1000x10^{-5}$
0.5	D.water+TBA+HPβCD (1)	1.0805	$7.8599x10^{-5}$
0.5	D.water+TBA+HPβCD (2)	1.1231	$8.1698x10^{-5}$
0.5	D.water+TBA+HPβCD (3)	1.0912	$7.9377x10^{-5}$
2	D.water+TBA+HPβCD (1)	0.6678	$4.8578x10^{-5}$
2	D.water+TBA+HPβCD (2)	0.6623	$4.8178x10^{-5}$
2	D.water+TBA+HPβCD (3)	0.6083	$4.4250x10^{-5}$
4	D.water+TBA+HPβCD (1)	0.686	$4.9902x10^{-5}$
4	D.water+TBA+HPβCD (2)	0.7418	$5.3961x10^{-5}$
4	D.water+TBA+HPβCD (3)	0.7412	$5.3917x10^{-5}$
23	D.water+TBA+HPβCD (1)	0.7312	$5.3190x10^{-5}$
23	D.water+TBA+HPβCD (2)	0.7315	$5.3212x10^{-5}$
23	D.water+TBA+HPβCD (3)	0.7057	$5.1335x10^{-5}$
24	D.water+TBA+HPβCD (1)	0.7809	$5.6805x10^{-5}$
24	D.water+TBA+HPβCD (2)	0.7047	$5.1262x10^{-5}$
24	D.water+TBA+HPβCD (3)	0.7659	$5.5714x10^{-5}$

Table C.22. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid 2-hydroxyl- propyl-β-CD (1:1 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.6413	4.6650×10^{-5}
0	D.water+TBA (2)	0.6657	4.8425×10^{-5}
0	D.water+TBA (3)	0.6517	4.7407×10^{-5}
0.5	D.water+TBA+HPβCD (1)	1.1299	8.2192×10^{-5}
0.5	D.water+TBA+HPβCD (2)	1.0803	7.8584×10^{-5}
0.5	D.water+TBA+HPβCD (3)	1.0976	7.9843×10^{-5}
2	D.water+TBA+HPβCD (1)	0.6696	4.8709×10^{-5}
2	D.water+TBA+HPβCD (2)	0.6442	4.6861×10^{-5}
2	D.water+TBA+HPβCD (3)	0.6612	4.8098×10^{-5}
4	D.water+TBA+HPβCD (1)	0.7386	5.3728×10^{-5}
4	D.water+TBA+HPβCD (2)	0.7722	5.6172×10^{-5}
4	D.water+TBA+HPβCD (3)	0.8096	5.8893×10^{-5}
23	D.water+TBA+HPβCD (1)	0.7348	5.3452×10^{-5}
23	D.water+TBA+HPβCD (2)	0.7302	5.3117×10^{-5}
23	D.water+TBA+HPβCD (3)	0.7096	5.1619×10^{-5}
24	D.water+TBA+HPβCD (1)	0.7825	5.6922×10^{-5}
24	D.water+TBA+HPβCD (2)	0.8069	5.8696×10^{-5}
24	D.water+TBA+HPβCD (3)	0.7595	5.5248×10^{-5}

Table C.23. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid 2-hydroxyl- propyl-β-CD (1:1 ratio) complex in phosphate buffer (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.5952	$5.7430x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5894	$5.6870x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5614	$5.4168x10^{-5}$
0.5	Phosphate Bf+TBA+HPβCD (1)	1.0679	$1.0304x10^{-4}$
0.5	Phosphate Bf+TBA+HPβCD (2)	1.1777	$1.1363x10^{-4}$
0.5	Phosphate Bf+TBA+HPβCD (3)	1.1427	$1.1026x10^{-4}$
2	Phosphate Bf+TBA+HPβCD (1)	0.7426	$7.1652x10^{-5}$
2	Phosphate Bf+TBA+HPβCD (2)	0.6859	$6.6181x10^{-5}$
2	Phosphate Bf+TBA+HPβCD (3)	0.7112	$6.8622x10^{-5}$
4	Phosphate Bf+TBA+HPβCD (1)	0.7069	$6.8207x10^{-5}$
4	Phosphate Bf+TBA+HPβCD (2)	0.7978	$7.6978x10^{-5}$
4	Phosphate Bf+TBA+HPβCD (3)	0.7884	$7.6071x10^{-5}$
23	Phosphate Bf+TBA+HPβCD (1)	0.7696	$7.4257x10^{-5}$
23	Phosphate Bf+TBA+HPβCD (2)	0.7658	$7.3890x10^{-5}$
23	Phosphate Bf+TBA+HPβCD (3)	0.7748	$7.4759x10^{-5}$
24	Phosphate Bf+TBA+HPβCD (1)	0.6396	$6.1714x10^{-5}$
24	Phosphate Bf+TBA+HPβCD (2)	0.8266	$7.9757x10^{-5}$
24	Phosphate Bf+TBA+HPβCD (3)	0.8126	$7.8406x10^{-5}$

Table C.24. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid 2-hydroxyl- propyl-β-CD (1:1 ratio) complex in phosphate buffer (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.5948	$5.7391x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5913	$5.7053x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5903	$5.6957x10^{-5}$
0.5	Phosphate Bf+TBA+HPβCD (1)	1.1448	$1.1046x10^{-4}$
0.5	Phosphate Bf+TBA+HPβCD (2)	1.1787	$1.1373x10^{-4}$
0.5	Phosphate Bf+TBA+HPβCD (3)	1.1009	$1.0622x10^{-4}$
2	Phosphate Bf+TBA+HPβCD (1)	0.6377	$6.1530x10^{-5}$
2	Phosphate Bf+TBA+HPβCD (2)	0.7566	$7.3003x10^{-5}$
2	Phosphate Bf+TBA+HPβCD (3)	0.7546	$7.2810x10^{-5}$
4	Phosphate Bf+TBA+HPβCD (1)	0.7985	$7.7046x10^{-5}$
4	Phosphate Bf+TBA+HPβCD (2)	0.7804	$7.5299x10^{-5}$
4	Phosphate Bf+TBA+HPβCD (3)	0.7301	$7.0446x10^{-5}$
23	Phosphate Bf+TBA+HPβCD (1)	0.7648	$7.3794x10^{-5}$
23	Phosphate Bf+TBA+HPβCD (2)	0.7687	$7.4170x10^{-5}$
23	Phosphate Bf+TBA+HPβCD (3)	0.7713	$7.4421x10^{-5}$
24	Phosphate Bf+TBA+HPβCD (1)	0.7089	$6.8400x10^{-5}$
24	Phosphate Bf+TBA+HPβCD (2)	0.8148	$7.8618x10^{-5}$
24	Phosphate Bf+TBA+HPβCD (3)	0.8066	$7.7827x10^{-5}$

Table C.25. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid (1:1 ratio) complex in 0.1 M HCL solution (1st trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	HCL+TBA	0.4892	$1.0024x10^{-3}$
0	HCL+TBA+βCD	0.4869	$9.9773x10^{-4}$
0	HCL+TBA+βCD	0.4916	$1.0074x10^{-3}$
0.5	HCL+TBA+βCD	0.4988	$1.0221x10^{-3}$
0.5	HCL+TBA+βCD	0.4983	$1.0211x10^{-3}$
0.5	HCL+TBA+βCD	0.4939	$1.0121x10^{-3}$
2	HCL+TBA+βCD	0.5149	$1.0551x10^{-3}$
2	HCL+TBA+βCD	0.5227	$1.0711x10^{-3}$
2	HCL+TBA+βCD	0.5055	$1.0358x10^{-3}$
4	HCL+TBA+βCD	0.4961	$1.0166x10^{-3}$
4	HCL+TBA+βCD	0.5004	$1.0254x10^{-3}$
4	HCL+TBA+βCD	0.4971	$1.018x10^{-3}$
23	HCL+TBA+βCD	0.5053	$1.0354x10^{-3}$
23	HCL+TBA+βCD	0.5013	$1.0272x10^{-3}$
23	HCL+TBA+βCD	0.5037	$1.0322x10^{-3}$
24	HCL+TBA+βCD	0.5205	$1.0666x10^{-3}$
24	HCL+TBA+βCD	0.5099	$1.0449x10^{-3}$
24	HCL+TBA+βCD	0.5174	$1.0602x10^{-3}$

Table C.26. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid (1:1 ratio) complex in 0.1 M HCL solution (2nd trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	HCL+TBA	0.4894	$1.0028x10^{-3}$
0	HCL+TBA+βCD	0.4948	$1.0139x10^{-3}$
0	HCL+TBA+βCD	0.4898	$1.0037x10^{-3}$
0.5	HCL+TBA+βCD	0.4946	$1.0135x10^{-3}$
0.5	HCL+TBA+βCD	0.5034	$1.0315x10^{-3}$
0.5	HCL+TBA+βCD	0.4993	$1.0231x10^{-3}$
2	HCL+TBA+βCD	0.5139	$1.0531x10^{-3}$
2	HCL+TBA+βCD	0.5096	$1.0442x10^{-3}$
2	HCL+TBA+βCD	0.5143	$1.0539x10^{-3}$
4	HCL+TBA+βCD	0.4935	$1.0112x10^{-3}$
4	HCL+TBA+βCD	0.5028	$1.0303x10^{-3}$
4	HCL+TBA+βCD	0.5207	$1.0670x10^{-3}$
23	HCL+TBA+βCD	0.5081	$1.0412x10^{-3}$
23	HCL+TBA+βCD	0.5014	$1.0274x10^{-3}$
23	HCL+TBA+βCD	0.5017	$1.0281x10^{-3}$
24	HCL+TBA+βCD	0.5119	$1.0489x10^{-3}$
24	HCL+TBA+βCD	0.5317	$1.0895x10^{-3}$
24	HCL+TBA+βCD	0.5199	$1.0653x10^{-3}$

Table C.27. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid (1:1 ratio) complex in TEA buffer (1st trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	TEA+TBA	0.4017	1.1150×10^{-3}
0	TEA+TBA+βCD	0.3981	1.1050×10^{-3}
0	TEA+TBA+βCD	0.4071	1.1300×10^{-3}
0.5	TEA+TBA+βCD	0.4105	1.1394×10^{-3}
0.5	TEA+TBA+βCD	0.4088	1.1347×10^{-3}
0.5	TEA+TBA+βCD	0.4084	1.1336×10^{-3}
2	TEA+TBA+βCD	0.4061	1.1272×10^{-3}
2	TEA+TBA+βCD	0.3895	1.0811×10^{-3}
2	TEA+TBA+βCD	0.3910	1.0853×10^{-3}
4	TEA+TBA+βCD	0.3844	1.0669×10^{-3}
4	TEA+TBA+βCD	0.3878	1.0764×10^{-3}
4	TEA+TBA+βCD	0.4097	1.1372×10^{-3}
23	TEA+TBA+βCD	0.4004	1.1114×10^{-3}
23	TEA+TBA+βCD	0.4014	1.1141×10^{-3}
23	TEA+TBA+βCD	0.4013	1.1139×10^{-3}
24	TEA+TBA+βCD	0.4113	1.1416×10^{-3}
24	TEA+TBA+βCD	0.4163	1.1555×10^{-3}
24	TEA+TBA+βCD	0.4037	1.1205×10^{-3}

Table C.28. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid (1:1 ratio) complex in TEA buffer (2nd trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	TEA+TBA	0.4031	$1.1189x10^{-3}$
0	TEA+TBA+βCD	0.4092	$1.1358x10^{-3}$
0	TEA+TBA+βCD	0.4031	$1.1189x10^{-3}$
0.5	TEA+TBA+βCD	0.4058	$1.1263x10^{-3}$
0.5	TEA+TBA+βCD	0.4100	$1.1380x10^{-3}$
0.5	TEA+TBA+βCD	0.4192	$1.1635x10^{-3}$
2	TEA+TBA+βCD	0.4004	$1.1114x10^{-3}$
2	TEA+TBA+βCD	0.3967	$1.1011x10^{-3}$
2	TEA+TBA+βCD	0.3917	$1.0872x10^{-3}$
4	TEA+TBA+βCD	0.3929	$1.0905x10^{-3}$
4	TEA+TBA+βCD	0.3938	$1.0930x10^{-3}$
4	TEA+TBA+βCD	0.3919	$1.0878x10^{-3}$
23	TEA+TBA+βCD	0.4009	$1.1127x10^{-3}$
23	TEA+TBA+βCD	0.3987	$1.1066x10^{-3}$
23	TEA+TBA+βCD	0.3999	$1.1100x10^{-3}$
24	TEA+TBA+βCD	0.3937	$1.0928x10^{-3}$
24	TEA+TBA+βCD	0.4127	$1.1455x10^{-3}$
24	TEA+TBA+βCD	0.4115	$1.1422x10^{-3}$

APPENDIX D: 5-METHYL-1-(*O*-FLUOROPHENYL)-2-TBA (25°C)

Table D.1. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:0.25 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	1.0672	$7.7631x10^{-5}$
0	D.water+TBA (2)	0.6012	$4.3733x10^{-5}$
0	D.water+TBA (3)	0.6991	$5.0855x10^{-5}$
0.5	D.water+TBA+βCD (1)	1.1504	$8.3684x10^{-5}$
0.5	D.water+TBA+βCD (2)	1.0377	7.5486E-05
0.5	D.water+TBA+βCD (3)	1.0923	$7.9457x10^{-5}$
2	D.water+TBA+βCD (1)	1.131	$8.2272x10^{-5}$
2	D.water+TBA+βCD (2)	1.1272	8.1996E-05
2	D.water+TBA+βCD (3)	1.1839	$8.6121x10^{-5}$
4	D.water+TBA+βCD (1)	1.1818	$8.5968x10^{-5}$
4	D.water+TBA+βCD (2)	0.7806	$5.6783x10^{-5}$
4	D.water+TBA+βCD (3)	1.1996	$8.7263x10^{-5}$
23	D.water+TBA+βCD (1)	1.1796	$8.5808x10^{-5}$
23	D.water+TBA+βCD (2)	1.1702	$8.5124x10^{-5}$
23	D.water+TBA+βCD (3)	1.2013	$8.7386x10^{-5}$
24	D.water+TBA+βCD (1)	1.2118	$8.8150x10^{-5}$
24	D.water+TBA+βCD (2)	0.7806	$5.6783x10^{-5}$
24	D.water+TBA+βCD (3)	1.2196	$8.8718x10^{-5}$

Table D.2. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:0.25 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.7533	$5.4797x10^{-5}$
0	D.water+TBA (2)	0.6709	$4.8803x10^{-5}$
0	D.water+TBA (3)	0.6157	$4.4788x10^{-5}$
0.5	D.water+TBA+βCD (1)	1.0994	$7.9974x10^{-5}$
0.5	D.water+TBA+βCD (2)	1.0761	$7.8279x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.9732	$7.0794x10^{-5}$
2	D.water+TBA+βCD (1)	1.1493	$8.3604x10^{-5}$
2	D.water+TBA+βCD (2)	1.1735	$8.5364x10^{-5}$
2	D.water+TBA+βCD (3)	1.1185	$8.1363x10^{-5}$
4	D.water+TBA+βCD (1)	0.7521	$5.4710x10^{-5}$
4	D.water+TBA+βCD (2)	1.1932	$8.6797x10^{-5}$
4	D.water+TBA+βCD (3)	1.1880	$8.6419x10^{-5}$
23	D.water+TBA+βCD (1)	1.1792	$8.5779x10^{-5}$
23	D.water+TBA+βCD (2)	1.1701	$8.5117x10^{-5}$
23	D.water+TBA+βCD (3)	1.2152	$8.8397x10^{-5}$
24	D.water+TBA+βCD (1)	1.2121	$8.8172x10^{-5}$
24	D.water+TBA+βCD (2)	1.2132	$8.8252x10^{-5}$
24	D.water+TBA+βCD (3)	1.08	$7.8563x10^{-5}$

Table D.3. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:0.25 ratio) complex in phosphate buffer (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.5958	$5.7487x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5245	$5.0608x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5965	$5.7555x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (1)	0.7259	$7.0041x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (2)	0.7551	$7.2858x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (3)	0.5711	$5.5104x10^{-5}$
2	Phosphate Bf+TBA+βCD (1)	0.7859	$7.5830x10^{-5}$
2	Phosphate Bf+TBA+βCD (2)	0.7663	$7.3939x10^{-5}$
2	Phosphate Bf+TBA+βCD (3)	0.603	$5.8182x10^{-5}$
4	Phosphate Bf+TBA+βCD (1)	0.8013	$7.7316x10^{-5}$
4	Phosphate Bf+TBA+βCD (2)	0.8094	$7.8097x10^{-5}$
4	Phosphate Bf+TBA+βCD (3)	0.7564	$7.2983x10^{-5}$
23	Phosphate Bf+TBA+βCD (1)	0.7561	$7.2954x10^{-5}$
23	Phosphate Bf+TBA+βCD (2)	0.7589	$7.3225x10^{-5}$
23	Phosphate Bf+TBA+βCD (3)	0.7013	$6.7667x10^{-5}$
24	Phosphate Bf+TBA+βCD (1)	0.7824	$7.5492x10^{-5}$
24	Phosphate Bf+TBA+βCD (2)	0.8253	$7.9631x10^{-5}$
24	Phosphate Bf+TBA+βCD (3)	0.8274	$7.9834x10^{-5}$

Table D.4. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid -β-CD (1:0.25 ratio) complex in phosphate buffer (2nd trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	Phosphate Buffer+TBA (1)	0.5055	$4.8775x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5996	$5.7854x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5995	$5.7844x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (1)	0.7259	$7.0041x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (2)	0.6135	$5.9195x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (3)	0.7675	$7.4054x10^{-5}$
2	Phosphate Bf+TBA+βCD (1)	0.6307	$6.0855x10^{-5}$
2	Phosphate Bf+TBA+βCD (2)	0.7656	$7.3871x10^{-5}$
2	Phosphate Bf+TBA+βCD (3)	0.7881	$7.6042x10^{-5}$
4	Phosphate Bf+TBA+βCD (1)	0.8014	$7.7325x10^{-5}$
4	Phosphate Bf+TBA+βCD (2)	0.8102	$7.8174x10^{-5}$
4	Phosphate Bf+TBA+βCD (3)	0.7798	$7.5241x10^{-5}$
23	Phosphate Bf+TBA+βCD (1)	0.7601	$7.3340x10^{-5}$
23	Phosphate Bf+TBA+βCD (2)	0.7577	$7.3109x10^{-5}$
23	Phosphate Bf+TBA+βCD (3)	0.7002	$6.7561x10^{-5}$
24	Phosphate Bf+TBA+βCD (1)	0.7657	$7.3881x10^{-5}$
24	Phosphate Bf+TBA+βCD (2)	0.8245	$7.9554x10^{-5}$
24	Phosphate Bf+TBA+βCD (3)	0.8217	$7.9284x10^{-5}$

Table D.5. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:0.5 ratio) complex distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	1.1372	$8.2724x10^{-5}$
0	D.water+TBA (2)	0.6063	$4.4104x10^{-5}$
0	D.water+TBA (3)	0.6828	$4.9669x10^{-5}$
0.5	D.water+TBA+βCD (1)	1.1745	$8.5437x10^{-5}$
0.5	D.water+TBA+βCD (2)	0.9874	$7.1827x10^{-5}$
0.5	D.water+TBA+βCD (3)	1.1932	$8.6797x10^{-5}$
2	D.water+TBA+βCD (1)	1.2599	$9.1649x10^{-5}$
2	D.water+TBA+βCD (2)	0.9885	$7.1907x10^{-5}$
2	D.water+TBA+βCD (3)	1.2440	$9.0492x10^{-5}$
4	D.water+TBA+βCD (1)	1.2763	$9.2842x10^{-5}$
4	D.water+TBA+βCD (2)	1.2965	$9.4311x10^{-5}$
4	D.water+TBA+βCD (3)	1.065	$7.7471x10^{-5}$
23	D.water+TBA+βCD (1)	1.2613	$9.1751x10^{-5}$
23	D.water+TBA+βCD (2)	1.2691	$9.2318x10^{-5}$
23	D.water+TBA+βCD (3)	1.2148	$8.8368x10^{-5}$
24	D.water+TBA+βCD (1)	0.8463	$6.1563x10^{-5}$
24	D.water+TBA+βCD (2)	1.3165	$9.5766x10^{-5}$
24	D.water+TBA+βCD (3)	1.3065	$9.5039x10^{-5}$

Table D.6. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:0.5 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	1.0755	$7.8235x10^{-5}$
0	D.water+TBA (2)	0.6596	$4.7981x10^{-5}$
0	D.water+TBA (3)	0.693	$5.0411x10^{-5}$
0.5	D.water+TBA+βCD (1)	1.1633	$8.4622x10^{-5}$
0.5	D.water+TBA+βCD (2)	1.0109	$7.3536x10^{-5}$
0.5	D.water+TBA+βCD (3)	1.1877	$8.6397x10^{-5}$
2	D.water+TBA+βCD (1)	1.0301	$7.4933x10^{-5}$
2	D.water+TBA+βCD (2)	1.2494	$9.0885x10^{-5}$
2	D.water+TBA+βCD (3)	1.2466	$9.0682x10^{-5}$
4	D.water+TBA+βCD (1)	1.2999	$9.4559x10^{-5}$
4	D.water+TBA+βCD (2)	1.2732	$9.2617x10^{-5}$
4	D.water+TBA+βCD (3)	1.1714	$8.5211x10^{-5}$
23	D.water+TBA+βCD (1)	1.2702	$9.2398x10^{-5}$
23	D.water+TBA+βCD (2)	1.2699	$9.2377x10^{-5}$
23	D.water+TBA+βCD (3)	1.2158	$8.8441x10^{-5}$
24	D.water+TBA+βCD (1)	0.9699	$7.0554x10^{-5}$
24	D.water+TBA+βCD (2)	1.3032	$9.4799x10^{-5}$
24	D.water+TBA+βCD (3)	1.3014	$9.4668x10^{-5}$

Table D.7. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:0.5 ratio) complex in phosphate buffer (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.5856	$5.6503x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5454	$5.2624x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5839	$5.6339x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (1)	0.5942	$5.7333x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (2)	0.8543	$8.2430x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (3)	0.8578	$8.2767x10^{-5}$
2	Phosphate Bf+TBA+βCD (1)	0.7207	$6.9539x10^{-5}$
2	Phosphate Bf+TBA+βCD (2)	0.8405	$8.1098x10^{-5}$
2	Phosphate Bf+TBA+βCD (3)	0.8602	$8.2999x10^{-5}$
4	Phosphate Bf+TBA+βCD (1)	0.8896	$8.5836x10^{-5}$
4	Phosphate Bf+TBA+βCD (2)	0.8758	$8.4504x10^{-5}$
4	Phosphate Bf+TBA+βCD (3)	0.7759	$7.4865x10^{-5}$
23	Phosphate Bf+TBA+βCD (1)	0.8591	$8.2893x10^{-5}$
23	Phosphate Bf+TBA+βCD (2)	0.8572	$8.2709x10^{-5}$
23	Phosphate Bf+TBA+βCD (3)	0.8017	$7.7354x10^{-5}$
24	Phosphate Bf+TBA+βCD (1)	0.7772	$7.4990x10^{-5}$
24	Phosphate Bf+TBA+βCD (2)	0.9039	$8.7215x10^{-5}$
24	Phosphate Bf+TBA+βCD (3)	0.9092	$8.7727x10^{-5}$

Table D.8. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid -β-CD (1:0.5 ratio) complex in phosphate buffer (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.5914	5.7063×10^{-5}
0	Phosphate Buffer+TBA (2)	0.6322	6.1000×10^{-5}
0	Phosphate Buffer+TBA (3)	0.5987	5.7767×10^{-5}
0.5	Phosphate Bf+TBA+βCD (1)	0.8728	8.4215×10^{-5}
0.5	Phosphate Bf+TBA+βCD (2)	0.8459	8.1619×10^{-5}
0.5	Phosphate Bf+TBA+βCD (3)	0.7227	6.9732×10^{-5}
2	Phosphate Bf+TBA+βCD (1)	0.8674	8.3694×10^{-5}
2	Phosphate Bf+TBA+βCD (2)	0.8661	8.3568×10^{-5}
2	Phosphate Bf+TBA+βCD (3)	0.7635	7.3668×10^{-5}
4	Phosphate Bf+TBA+βCD (1)	0.8814	8.5044×10^{-5}
4	Phosphate Bf+TBA+βCD (2)	0.8794	8.4851×10^{-5}
4	Phosphate Bf+TBA+βCD (3)	0.7996	7.7152×10^{-5}
23	Phosphate Bf+TBA+βCD (1)	0.8562	8.2613×10^{-5}
23	Phosphate Bf+TBA+βCD (2)	0.8598	8.2960×10^{-5}
23	Phosphate Bf+TBA+βCD (3)	0.8013	7.7316×10^{-5}
24	Phosphate Bf+TBA+βCD (1)	0.7142	6.8912×10^{-5}
24	Phosphate Bf+TBA+βCD (2)	0.9007	8.6907×10^{-5}
24	Phosphate Bf+TBA+βCD (3)	0.9041	8.7235×10^{-5}

Table D.9. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.6199	$4.5093x10^{-5}$
0	D.water+TBA (2)	0.6337	$4.6097x10^{-5}$
0	D.water+TBA (3)	0.6857	$4.9880x10^{-5}$
0.5	D.water+TBA+βCD (1)	1.2057	$8.7706x10^{-5}$
0.5	D.water+TBA+βCD (2)	1.2236	$8.9009x10^{-5}$
0.5	D.water+TBA+βCD (3)	0.7277	$5.2935x10^{-5}$
2	D.water+TBA+βCD (1)	0.8307	$6.0428x10^{-5}$
2	D.water+TBA+βCD (2)	1.2757	$9.2798x10^{-5}$
2	D.water+TBA+βCD (3)	1.2872	$9.3635x10^{-5}$
4	D.water+TBA+βCD (1)	1.2996	$9.4537x10^{-5}$
4	D.water+TBA+βCD (2)	1.2981	$9.4428x10^{-5}$
4	D.water+TBA+βCD (3)	1.2289	$8.9394x10^{-5}$
23	D.water+TBA+βCD (1)	1.2607	$9.1707x10^{-5}$
23	D.water+TBA+βCD (2)	1.2696	$9.2355x10^{-5}$
23	D.water+TBA+βCD (3)	1.2003	$8.7314x10^{-5}$
24	D.water+TBA+βCD (1)	1.3296	$9.6719x10^{-5}$
24	D.water+TBA+βCD (2)	1.3781	$1.0025x10^{-4}$
24	D.water+TBA+βCD (3)	1.3289	$9.6668x10^{-5}$

Table D.10. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in distilled water (2nd trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	D.water+TBA (1)	0.6506	4.7327×10^{-5}
0	D.water+TBA (2)	0.5839	4.2475×10^{-5}
0	D.water+TBA (3)	0.6827	4.9662×10^{-5}
0.5	D.water+TBA+βCD (1)	1.2471	9.0718×10^{-5}
0.5	D.water+TBA+βCD (2)	0.9475	6.8924×10^{-5}
0.5	D.water+TBA+βCD (3)	1.2257	8.9161×10^{-5}
2	D.water+TBA+βCD (1)	1.1511	8.3735×10^{-5}
2	D.water+TBA+βCD (2)	1.2745	9.2711×10^{-5}
2	D.water+TBA+βCD (3)	1.2839	9.3395×10^{-5}
4	D.water+TBA+βCD (1)	1.1485	8.3546×10^{-5}
4	D.water+TBA+βCD (2)	1.2973	9.4370×10^{-5}
4	D.water+TBA+βCD (3)	1.2938	9.4115×10^{-5}
23	D.water+TBA+βCD (1)	1.2648	9.2006×10^{-5}
23	D.water+TBA+βCD (2)	1.2652	9.2035×10^{-5}
23	D.water+TBA+βCD (3)	1.2013	8.7386×10^{-5}
24	D.water+TBA+βCD (1)	1.1485	8.3546×10^{-5}
24	D.water+TBA+βCD (2)	1.3273	9.6552×10^{-5}
24	D.water+TBA+βCD (3)	1.3238	9.6297×10^{-5}

Table D.11. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer (1st trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	Phosphate Buffer+TBA (1)	0.9607	$9.2696x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5907	$5.6995x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5929	$5.7208x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (1)	0.9934	$9.5851x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (2)	1.0528	1.0158E-04
0.5	Phosphate Bf+TBA+βCD (3)	1.0948	$1.0563x10^{-4}$
2	Phosphate Bf+TBA+βCD (1)	1.2411	$1.1975x10^{-4}$
2	Phosphate Bf+TBA+βCD (2)	1.1888	$1.1470x10^{-4}$
2	Phosphate Bf+TBA+βCD (3)	1.2341	$1.1908x10^{-4}$
4	Phosphate Bf+TBA+βCD (1)	1.2016	$1.1594x10^{-4}$
4	Phosphate Bf+TBA+βCD (2)	1.2104	$1.1679x10^{-4}$
4	Phosphate Bf+TBA+βCD (3)	1.2094	$1.1669x10^{-4}$
23	Phosphate Bf+TBA+βCD (1)	1.1796	$1.1382x10^{-4}$
23	Phosphate Bf+TBA+βCD (2)	1.1758	$1.1345x10^{-4}$
23	Phosphate Bf+TBA+βCD (3)	1.1148	$1.0756x10^{-4}$
24	Phosphate Bf+TBA+βCD (1)	1.182	$1.1405x10^{-4}$
24	Phosphate Bf+TBA+βCD (2)	1.1009	$1.0622x10^{-4}$
24	Phosphate Bf+TBA+βCD (3)	1.2255	$1.1825x10^{-4}$

Table D.12. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:1 ratio) complex in phosphate buffer (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	Phosphate Buffer+TBA (1)	0.5939	5.7304×10^{-5}
0	Phosphate Buffer+TBA (2)	0.9232	8.9078×10^{-5}
0	Phosphate Buffer+TBA (3)	0.5951	5.7420×10^{-5}
0.5	Phosphate Bf+TBA+βCD (1)	1.1599	1.1192×10^{-4}
0.5	Phosphate Bf+TBA+βCD (2)	1.0546	1.0176×10^{-4}
0.5	Phosphate Bf+TBA+βCD (3)	1.0985	1.0599×10^{-4}
2	Phosphate Bf+TBA+βCD (1)	1.1533	1.1128×10^{-4}
2	Phosphate Bf+TBA+βCD (2)	1.1996	1.1575×10^{-4}
2	Phosphate Bf+TBA+βCD (3)	1.1008	1.0621×10^{-4}
4	Phosphate Bf+TBA+βCD (1)	1.2004	1.1582×10^{-4}
4	Phosphate Bf+TBA+βCD (2)	1.2118	1.1692×10^{-4}
4	Phosphate Bf+TBA+βCD (3)	1.2072	1.1648×10^{-4}
23	Phosphate Bf+TBA+βCD (1)	1.1760	1.1347×10^{-4}
23	Phosphate Bf+TBA+βCD (2)	1.1782	1.1368×10^{-4}
23	Phosphate Bf+TBA+βCD (3)	1.1352	1.0953×10^{-4}
24	Phosphate Bf+TBA+βCD (1)	1.2179	1.1751×10^{-4}
24	Phosphate Bf+TBA+βCD (2)	1.2372	1.1937×10^{-4}
24	Phosphate Bf+TBA+βCD (3)	0.7466	7.2038×10^{-5}

Table D.13. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.6891	$5.0127x10^{-5}$
0	D.water+TBA (2)	0.6212	$4.5188x10^{-5}$
0	D.water+TBA (3)	0.7513	$5.4652x10^{-5}$
0.5	D.water+TBA+βCD (1)	1.2854	$9.3504x10^{-5}$
0.5	D.water+TBA+βCD (2)	1.3103	$9.5315x10^{-5}$
0.5	D.water+TBA+βCD (3)	1.2712	$9.2471x10^{-5}$
2	D.water+TBA+βCD (1)	1.1523	$8.3822x10^{-5}$
2	D.water+TBA+βCD (2)	1.3188	$9.5934x10^{-5}$
2	D.water+TBA+βCD (3)	1.3293	$9.6697x10^{-5}$
4	D.water+TBA+βCD (1)	1.3499	$9.8196x10^{-5}$
4	D.water+TBA+βCD (2)	1.3491	$9.8138x10^{-5}$
4	D.water+TBA+βCD (3)	1.3776	$1.0021x10^{-4}$
23	D.water+TBA+βCD (1)	1.3013	$9.4661x10^{-5}$
23	D.water+TBA+βCD (2)	1.3058	$9.4988x10^{-5}$
23	D.water+TBA+βCD (3)	1.2857	$9.3526x10^{-5}$
24	D.water+TBA+βCD (1)	1.3689	$9.9578x10^{-5}$
24	D.water+TBA+βCD (2)	1.3727	$9.9855x10^{-5}$
24	D.water+TBA+βCD (3)	1.3652	$9.9309x10^{-5}$

Table D.14. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.6713	4.8832×10^{-5}
0	D.water+TBA (2)	0.6152	4.4752×10^{-5}
0	D.water+TBA (3)	0.7913	5.7562×10^{-5}
0.5	D.water+TBA+βCD (1)	1.3565	9.8676×10^{-5}
0.5	D.water+TBA+βCD (2)	1.2864	9.3577×10^{-5}
0.5	D.water+TBA+βCD (3)	1.2835	9.3366×10^{-5}
2	D.water+TBA+βCD (1)	0.7447	5.4172×10^{-5}
2	D.water+TBA+βCD (2)	1.3107	9.5344×10^{-5}
2	D.water+TBA+βCD (3)	1.3249	9.6377×10^{-5}
4	D.water+TBA+βCD (1)	1.3482	9.8072×10^{-5}
4	D.water+TBA+βCD (2)	1.3491	9.8138×10^{-5}
4	D.water+TBA+βCD (3)	1.3879	1.0096×10^{-4}
23	D.water+TBA+βCD (1)	1.3049	9.4923×10^{-5}
23	D.water+TBA+βCD (2)	1.3017	9.4690×10^{-5}
23	D.water+TBA+βCD (3)	1.2359	8.9903×10^{-5}
24	D.water+TBA+βCD (1)	1.3605	9.8967×10^{-5}
24	D.water+TBA+βCD (2)	1.3671	9.9447×10^{-5}
24	D.water+TBA+βCD (3)	1.3172	9.5817×10^{-5}

Table D.15. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer (1st trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	Phosphate Buffer+TBA (1)	0.5904	$5.6966x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5923	$5.7150x10^{-4}$
0	Phosphate Buffer+TBA (3)	0.5377	$5.1882x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (1)	0.7909	$7.6312x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (2)	1.1534	$1.1129x10^{-4}$
0.5	Phosphate Bf+TBA+βCD (3)	1.1889	$1.1471x10^{-4}$
2	Phosphate Bf+TBA+βCD (1)	0.8282	$7.9911x10^{-5}$
2	Phosphate Bf+TBA+βCD (2)	1.2034	$1.1611x10^{-4}$
2	Phosphate Bf+TBA+βCD (3)	1.2182	$1.1754x10^{-4}$
4	Phosphate Bf+TBA+βCD (1)	1.2705	$1.2259x10^{-4}$
4	Phosphate Bf+TBA+βCD (2)	1.2731	$1.2284x10^{-4}$
4	Phosphate Bf+TBA+βCD (3)	1.1835	$1.1419x10^{-4}$
23	Phosphate Bf+TBA+βCD (1)	1.2684	$1.2239x10^{-4}$
23	Phosphate Bf+TBA+βCD (2)	1.2634	$1.2190x10^{-4}$
23	Phosphate Bf+TBA+βCD (3)	1.2014	$1.1592x10^{-4}$
24	Phosphate Bf+TBA+βCD (1)	1.2925	$1.2471x10^{-4}$
24	Phosphate Bf+TBA+βCD (2)	1.2997	$1.2541x10^{-4}$
24	Phosphate Bf+TBA+βCD (3)	1.2228	$1.1799x10^{-4}$

Table D.16. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:2 ratio) complex in phosphate buffer (2nd trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	Phosphate Buffer+TBA (1)	0.5948	5.7391×10^{-5}
0	Phosphate Buffer+TBA (2)	0.5899	5.6918×10^{-5}
0	Phosphate Buffer+TBA (3)	0.5146	4.9653×10^{-5}
0.5	Phosphate Bf+TBA+βCD (1)	1.9994	1.9292×10^{-4}
0.5	Phosphate Bf+TBA+βCD (2)	1.1679	1.1269×10^{-4}
0.5	Phosphate Bf+TBA+βCD (3)	0.8976	8.6607×10^{-5}
2	Phosphate Bf+TBA+βCD (1)	0.8619	8.3163×10^{-5}
2	Phosphate Bf+TBA+βCD (2)	1.2151	1.1724×10^{-4}
2	Phosphate Bf+TBA+βCD (3)	1.2094	1.1669×10^{-4}
4	Phosphate Bf+TBA+βCD (1)	1.1805	1.1390×10^{-4}
4	Phosphate Bf+TBA+βCD (2)	1.2731	1.2284×10^{-4}
4	Phosphate Bf+TBA+βCD (3)	1.2835	1.2384×10^{-4}
23	Phosphate Bf+TBA+βCD (1)	1.2674	1.2229×10^{-4}
23	Phosphate Bf+TBA+βCD (2)	1.2652	1.2208×10^{-4}
23	Phosphate Bf+TBA+βCD (3)	1.2021	1.1599×10^{-4}
24	Phosphate Bf+TBA+βCD (1)	1.2986	1.2530×10^{-4}
24	Phosphate Bf+TBA+βCD (2)	1.2871	1.2419×10^{-4}
24	Phosphate Bf+TBA+βCD (3)	1.2307	1.1875×10^{-4}

Table D.17. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water (1st trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.6696	4.8709×10^{-5}
0	D.water+TBA (2)	0.6513	4.7378×10^{-5}
0	D.water+TBA (3)	0.7517	5.4681×10^{-5}
0.5	D.water+TBA+βCD (1)	1.3339	9.7032×10^{-5}
0.5	D.water+TBA+βCD (2)	1.3214	9.6123×10^{-5}
0.5	D.water+TBA+βCD (3)	0.7036	5.1182×10^{-5}
2	D.water+TBA+βCD (1)	0.6006	4.3690×10^{-5}
2	D.water+TBA+βCD (2)	1.3648	9.9280×10^{-5}
2	D.water+TBA+βCD (3)	1.3732	9.9891×10^{-5}
4	D.water+TBA+βCD (1)	1.3494	9.8160×10^{-5}
4	D.water+TBA+βCD (2)	1.3806	1.0043×10^{-4}
4	D.water+TBA+βCD (3)	1.3871	1.0090×10^{-4}
23	D.water+TBA+βCD (1)	1.3433	9.7716×10^{-5}
23	D.water+TBA+βCD (2)	1.3452	9.7854×10^{-5}
23	D.water+TBA+βCD (3)	1.3013	9.4661×10^{-5}
24	D.water+TBA+βCD (1)	1.4009	1.0191×10^{-4}
24	D.water+TBA+βCD (2)	1.4091	1.0250×10^{-4}
24	D.water+TBA+βCD (3)	1.4429	1.0496×10^{-4}

Table D.18. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in distilled water (2nd trial)

Time (h)	Type of solution	ABS	C (mol/L)
0	D.water+TBA (1)	0.6618	1.8141×10^{-5}
0	D.water+TBA (2)	0.6572	4.7807×10^{-5}
0	D.water+TBA (3)	0.7819	5.6878×10^{-5}
0.5	D.water+TBA+βCD (1)	1.3427	9.7672×10^{-5}
0.5	D.water+TBA+βCD (2)	1.3338	9.7025×10^{-5}
0.5	D.water+TBA+βCD (3)	1.0907	7.9341×10^{-5}
2	D.water+TBA+βCD (1)	1.3778	1.0023×10^{-4}
2	D.water+TBA+βCD (2)	1.3033	9.4806×10^{-5}
2	D.water+TBA+βCD (3)	1.3602	9.8945×10^{-5}
4	D.water+TBA+βCD (1)	1.3018	9.4697×10^{-5}
4	D.water+TBA+βCD (2)	1.3813	1.0048×10^{-4}
4	D.water+TBA+βCD (3)	1.3861	1.0083×10^{-4}
23	D.water+TBA+βCD (1)	1.3449	9.7832×10^{-5}
23	D.water+TBA+βCD (2)	1.3460	9.7912×10^{-5}
23	D.water+TBA+βCD (3)	1.3062	9.5017×10^{-5}
24	D.water+TBA+βCD (1)	1.4041	1.0214×10^{-4}
24	D.water+TBA+βCD (2)	1.4073	1.0237×10^{-4}
24	D.water+TBA+βCD (3)	1.4209	1.0336×10^{-4}

Table D.19. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer (1st trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	Phosphate Buffer+TBA (1)	0.5957	$5.7478x10^{-5}$
0	Phosphate Buffer+TBA (2)	0.5961	$5.7516x10^{-5}$
0	Phosphate Buffer+TBA (3)	0.5317	$5.1303x10^{-5}$
0.5	Phosphate Bf+TBA+βCD (1)	1.2925	$1.2471x10^{-4}$
0.5	Phosphate Bf+TBA+βCD (2)	1.2979	$1.2523x10^{-4}$
0.5	Phosphate Bf+TBA+βCD (3)	1.3589	$1.3112x10^{-4}$
2	Phosphate Bf+TBA+βCD (1)	1.2482	$1.2044x10^{-4}$
2	Phosphate Bf+TBA+βCD (2)	0.8511	$8.2121x10^{-5}$
2	Phosphate Bf+TBA+βCD (3)	1.2471	$1.2033x10^{-4}$
4	Phosphate Bf+TBA+βCD (1)	1.1073	$1.0684x10^{-4}$
4	Phosphate Bf+TBA+βCD (2)	1.2918	$1.2464x10^{-4}$
4	Phosphate Bf+TBA+βCD (3)	1.3072	$1.2613x10^{-4}$
23	Phosphate Bf+TBA+βCD (1)	1.2678	$1.2233x10^{-4}$
23	Phosphate Bf+TBA+βCD (2)	1.2642	$1.2198x10^{-4}$
23	Phosphate Bf+TBA+βCD (3)	1.2118	$1.1692x10^{-4}$
24	Phosphate Bf+TBA+βCD (1)	1.3151	$1.2689x10^{-4}$
24	Phosphate Bf+TBA+βCD (2)	1.3144	$1.2682x10^{-4}$
24	Phosphate Bf+TBA+βCD (3)	1.3736	$1.3254x10^{-4}$

Table D.20. Absorbance & concentration results of 5-methyl-1-(*o*-fluorophenyl)-2-thiobarbituric acid-β-CD (1:4 ratio) complex in phosphate buffer (2nd trial)

Time (h)	**Type of solution**	**ABS**	**C (mol/L)**
0	Phosphate Buffer+TBA (1)	0.5917	5.7092×10^{-5}
0	Phosphate Buffer+TBA (2)	0.6001	5.7902×10^{-5}
0	Phosphate Buffer+TBA (3)	0.5211	5.0280×10^{-5}
0.5	Phosphate Bf+TBA+βCD (1)	1.2969	1.2514×10^{-4}
0.5	Phosphate Bf+TBA+βCD (2)	1.3271	1.2805×10^{-4}
0.5	Phosphate Bf+TBA+βCD (3)	1.2919	1.2465×10^{-4}
2	Phosphate Bf+TBA+βCD (1)	1.2566	1.2125×10^{-4}
2	Phosphate Bf+TBA+βCD (2)	1.2404	1.1968×10^{-4}
2	Phosphate Bf+TBA+βCD (3)	1.2922	1.2468×10^{-4}
4	Phosphate Bf+TBA+βCD (1)	1.3617	1.3139×10^{-4}
4	Phosphate Bf+TBA+βCD (2)	1.2913	1.2459×10^{-4}
4	Phosphate Bf+TBA+βCD (3)	1.2997	1.2541×10^{-4}
23	Phosphate Bf+TBA+βCD (1)	1.2658	1.2213×10^{-4}
23	Phosphate Bf+TBA+βCD (2)	1.2680	1.2235×10^{-4}
23	Phosphate Bf+TBA+βCD (3)	1.2196	1.1768×10^{-4}
24	Phosphate Bf+TBA+βCD (1)	1.3195	1.2732×10^{-4}
24	Phosphate Bf+TBA+βCD (2)	1.3121	1.2660×10^{-4}
24	Phosphate Bf+TBA+βCD (3)	1.3497	1.3023×10^{-4}