

Programme at a glance

Time	Monday (Sep. 8)	Tuesday (Sep. 9)	Wednesday (Sep. 10)	Thursday (Sep. 11)
09:00				
09:20		Plavec	Polanski	Luchinat
09:40				
10:00		Hoffmann	Keser	Timári
10:20 arrivals		Andrushchenko	Varga	Csapó
10:40		coffee	coffee	coffee
11:00		Körtvélyesi	Tóth	Enyedy
11:20		Nepravishtha	Kerékgyártó	Labadi
11:40		Viglasky	Balducci	Kiss
12:00		Gyurcsik	Kosina	
12:20				
12:40 lunch				
13:00				
13:20				
13:40				
14:00				
14:20 Bertini		Noe	Manstein	
14:40				
15:00 Nyitray		Somsák	Kovács	
15:20 Pál		Szente	Luchter-Wasylewska	
15:40 Jákli		Puskás	Harmat	
16:00				departures
16:20 coffee+posters		coffee+posters	coffee+posters	
16:40				
17:00			Ahmed	
17:20 Picone		Jicsinszky	Poppe	
17:40 Süveges		Fekete	Sabelli	
18:00 Batta		Borbás	Tratar Pirc	
18:20		Yannakopoulou		
18:40 Zerbe		Vidal	Campbell	
19:00		Fügedi		
19:20 posters		posters	posters	
19:40				
20:00	Welcome reception	Bogrács party	Gala dinner	

Monday (Sep. 8)	Time	Speaker	Chemistry-related title	Biology-related title
	12:00		Lunch	
Opening lecture	14:00	Bertini Ivano	Copper homeostasis and trafficking in cells	Copper homeostasis and trafficking in cells
Proteins, peptides & folding	15:00	Nyitraj László	A hub protein: many interaction partners	DYNLL: a multifunctional protein that binds to intrinsically disordered proteins
	15:20	Pál Gábor	Combinatorial Phage-display Mutagenesis Reveals Complex Networks of Surface-Core Interactions in the Pacifast in Protease Inhibitor Family	Combinatorial Phage-display Mutagenesis Reveals Complex Networks of Surface-Core Interactions in the Pacifast in Protease Inhibitor Family
	15:40	Jákl Imre	A fast and efficient quantitative tool for protein and peptide structure determination: the CCA+	A fast and efficient quantitative tool for protein and peptide structure determination: the CCA+
	16:00		Coffee + posters	
	17:20	Picone Delia	New functions from the swapping of terminal arms: lessons from ribonucleases.	3D domain swapping of proteins: the unusual features of Bovine Ribonucleases
	17:40	Süveges Dániel	Charged single α -helix: a versatile protein structural motif	Charged single α -helix: a versatile protein structural motif
	18:00	Batta Gyula	Ambiguous disulfide bonds	Structure and dynamics of the antifungal protein PAF
	18:20	Zerbe Oliver	Folding and unfolding of peptide YY	Structural and folding studies on a small miniprotein
	19:20		Posters	
	20:00		Welcome reception	

Tuesday (Sep. 9)	Time	Speaker	Chemistry-related title	Biology-related title	
Nucleic acids	09:00	Plavec Janez	DNA G-quadruplexes and cations	Interactions of nucleic acids and proteins	
	10:00	Hoffmann Eufrozina A.	Theoretical analysis of peptide nucleic acid thermochemistry	Binding energy group contributions in PNA homoduplexes	
	10:20	Andrushchenko Valery	Quantum chemical modeling and interpretation of nucleic acid vibrational spectra	Extracting more information about nucleic acid structure by quantum chemistry computation	
	10:40		Coffee		
	11:00	Körtvélyesi Tamás	Effect of Structural Cell Proteins on the Peptide and Peptide Nucleic Acid (PNA) Binding to HSP90.	Effect of Structural Cell Proteins on the Peptide and Peptide Nucleic Acid (PNA) Binding to Heat Shock Protein 90.	
	11:20	Nepravishta Ridvan	DNA- and metal-binding of RTN1-CCT peptide: towards the function of a reticulin protein	DNA- and metal-binding of RTN1-CCT peptide: towards the function of a reticulin protein	
	11:40	Viglasky Viktor	The evaluation of G- quadruplex stability	The evaluation of G- quadruplex stability	
	12:00	Gyurcsik Béla	Metal binding chimeric peptides with nuclease activity	Artificial metallo-nucleases for gene therapy	
	12:20		Lunch		
	14:00	Noe Christian R.	Proteomic Studies on "Off Target" Effects in Nucleic Acid Therapy – An Experimental Approach towards Pharmaceutical Systems Biology	Proteomic Studies on "Off Target" Effects in Nucleic Acid Therapy – An Experimental Approach towards Pharmaceutical Systems Biology	
	15:00	Somsák László	Design, Synthesis, and Structure–Activity Relationships of Glycogen Phosphorylase Inhibitors	Glucose Derivatives against Type 2 Diabetes Mellitus	
	15:20	Szente Lajos	Cell Membrane Active Cyclodextrin Derivatives	Cyclodextrin Derivatives for Drug Delivery	
	Carbohydrates	15:40	Puskás István	Non-covalent Cyclodextrin/Protein Interactions	Biopharmaceutical Uses of Cyclodextrins
		16:00		Coffee + posters	
	17:20	Jicsinszky László	Aldoximinopyridium Cyclodextrin Derivatives	Cyclodextrin Cholinesterase Regenerators	
	17:40	Fekete Anikó	Synthesis of oligosaccharide fragments of poly- β -(1 \rightarrow 6)-N-acetyl-glucosamine	Synthesis of oligosaccharide fragments of poly- β -(1 \rightarrow 6)-N-acetyl-glucosamine	
	18:00	Borbás Anikó	Synthesis of sulfonic acid analogues of heparinoid oligosaccharides	Synthesis of sulfonic acid analogues of heparinoid oligosaccharides	
	18:20	Yannakopoulou Konstantina	Evaluation of Modified Cyclodextrins (CDs) as Inhibitors of Anthrax Toxin	Cationic Cyclic Oligosaccharides as Inhibitors of Anthrax Toxin	
	18:40	Vidal Sébastien	Synthesis of Glycoclusters by Click Chemistry : Binding Studies with Lectins	Glycoconjugates as Probes for Studying Lectin-Carbohydrate Interactions	
	19:00	Fügedi Péter	Synthesis strategy for the generation of a heparin oligosaccharide library	Towards understanding the specificity of heparin-protein interactions	
	19:20		Posters		
	20:00		Bogrács party		

Wednesday (Sep. 10)	Time	Speaker	Chemistry-related title	Biology-related title
Drug discovery	09:00	Polanski Jaroslaw	Multidimensional QSAR	Modeling ligand-protein interactions
	10:00	Keser György M.	Identification of Kinase Inhibitors: Comparative Evaluation of Theoretical and Experimental Approaches	Virtual and Experimental High Throughput Screening Against Kinase Targets
	10:20	Varga Zoltán	Affinity chromatography method in off target identification and chemistry driven drug development	Affinity chromatography method in off target identification and chemistry driven drug development
	10:40		Coffee	
Synthesis & biodegradation	11:00	Tóth Gábor	Glycopeptides – a synthetic challenge Part I.	Glycopeptides – a synthetic challenge Part I.
	11:20	Kerékgyártó János	Glycopeptides-a synthetic challenge Part II.	Glycopeptides-a synthetic challenge Part II.
	11:40	Balducci Daniele	Novel approach to the synthesis of aliphatic and aromatic keto acids	New synthesis of alpha keto acids: key intermediates in the biosynthesis and metabolism of amino acids
	12:00	Kosina Pavel	Transformation of sanguinarine to dihydrosanguinarine in vivo	Sanguinarine: Pharmacokinetics and metabolism
	12:20		Lunch	
Molecular motors, enzymes & inhibitors	14:00	Manstein Dietmar J.	Halogenated alkaloids as potent effectors of myosin function	Allosteric inhibition of myosin motor activity
	15:00	Kovács Mihály	An allosteric myosin inhibitor alters ligand-induced conformational changes	Utility of a myosin inhibitor in deciphering the structural mechanism of force generation
	15:20	Luchter-Wasylewska Ewa	L(+)-tartrate and vanadate: nonlinear competitive inhibitors of prostatic phosphatase catalytic activity	Inhibitors of allosteric human prostatic acid phosphatase
	15:40	Harmat Veronika	Crystal structure of a complement protease: towards understanding selectivity and function	Structure-function relationships of a linker enzyme between the coagulation and the innate immune systems
	16:00		Coffee + posters	
Bioprocesses	17:00	Ahmed Mehboob	Cyanobacterial indole-3-acetic acid: production and impact on plant growth	Cyanobacterial indole-3-acetic acid: production and impact on plant growth
	17:20	Poppe László	Selective biotransformations in continuous flow reactors	Selective biotransformations in continuous flow reactors
	17:40	Sabelli Renato	Allyl Thiolsulfate a natural apoptotic inducer affects the cell detoxification system	Allyl Thiolsulfate a natural apoptotic inducer affects the cell detoxification system
	18:00	Tratar Pirc Elizabeta	Molecular simulation of hyaluronates	Metal binding to hyaluronates
	18:20	Campbell Iain D.	Flexible peptides as interaction hubs	Focal adhesion assembly
	19:20		Posters	
20:00		Gala dinner		

Thursday (Sep 11.)	Time	Speaker	Chemistry-related title	Biology-related title
Metal ions	09:00	Luchinat Claudio	Revealing and characterizing interactions between proteins, metal ions, partner proteins and organic ligands	Revealing and characterizing interactions between proteins, metal ions, partner proteins and organic ligands
	10:00	Timári Sarolta	Transition metal complexes of small multihistidine peptides	Models of the active centres of some metalloenzymes
	10:20	Csapó Edit	Imidazole versus hydroxamate coordination in Cu(II) and Ni(II) complexes of histidine containing peptidehydroxamic acids	Peptidehydroxamic acids as potential metalloenzyme inhibitors
	10:40		Coffee	
	11:00	Enyedy Éva Anna	Role of serum proteins in transformation of antidiabetic zinc(II)-complexes	Interaction between antidiabetic zinc(II)-complexes and serum components
	11:20	Labádi Imre	Preparation and study of metal complexes, mimicking the SOD enzyme	Biological importance of the metal complexes, mimicking the SOD enzyme
	11:40	Kiss Tamás	Comparative studies on the biospeciation of antidiabetic vanadium and zinc compounds	What are the actual forms of antidiabetic metal compounds in the blood serum?
	12:00		Lunch	

Presenting author		Chemistry-related title	Biology-related title
Abrami	Marija	Functional tyrosine residue in the active center of human dipeptidyl peptidase III	The role of Tyr-318 in the catalytic mechanism of metallopeptidase family M49 probed with site-directed mutagenesis
Ágoston	Bianka	Structural background of the chaperone function of proteins with unstructured regions	On the chaperone function of ERD14, a LEA protein from <i>A. thaliana</i>
Ángyán	Annamária	Fast protein fold estimation based on distance restraints derived from NMR spectra	Identifying protein folds from assigned NMR spectra
Arpaci	Ozlem	Synthesis and antimicrobial activity of some novel N-[2-p-substitutedbenzyl/phenyl-5-benzoxazolyl]-2-morpholinoacetamides	Synthesis and antimicrobial activity of some novel N-[2-p-substitutedbenzyl/phenyl-5-benzoxazolyl]-2-morpholinoacetamides
Árus	Dávid	Metal ion interaction of a peptide, modelling the metal binding site of human MMP-13	A minimalist model of matrix metalloproteinases
Beke	Tamás	Structure and Stability of Collagen-like β -Peptide Nanotubes	Structure and Stability of Collagen-like β -Peptide Nanotubes
Beke	Tamás	Exploring conformational landscapes of model peptides and their complexes by matrix-isolation techniques	Structural properties of protein building units. A combined experimental and theoretical investigation of natural and non-natural dipeptides
Bodor	Andrea	Structural and dynamical characterization of an unstructured myosin fragment (M) upon binding to the dimeric dynein light chain (DLC)	Structural and dynamical characterization of an unstructured myosin fragment (M) upon binding to the dimeric dynein light chain (DLC)
Bogár	Ferenc	Folding kinetics of implicitly solvated alanine oligomers	Folding kinetics of implicitly solvated alanine oligomers
Bokor	Éva	C- and N-glucopyranosyl heterocycles as inhibitors of glycogen phosphorylase	Heterocyclic glucose derivatives as potential antidiabetics
Bucovicean	Carmen Maria	The effect of the counter ion on the nature of the Copper(II) complexes containing N,N'-bis(4-dodecyloxybenzylidene-N-propyl)-piperazine as ligand.	The effect of the counter ion on the nature of the Copper(II) complexes containing N,N'-bis(4-dodecyloxybenzylidene-N-propyl)-piperazine as ligand.
Bucovicean	Carmen Maria	Comparative study regarding the absorption and fluorescence spectra of Zn(II) complexes of tetrapyrrolylporphyrine and tetra(3-hydroxyphenyl)porphyrine	Comparative study regarding the absorption and fluorescence spectra of Zn(II) complexes of tetrapyrrolylporphyrine and tetra(3-hydroxyphenyl)porphyrine
Calinescu	Mirela	Synthesis, characterization and antimicrobial activity of some Zn(II) and Ag(I) complexes with chlorhexidine	Synthesis, characterization and antimicrobial activity of some Zn(II) and Ag(I) complexes with chlorhexidine
Cevcec	Mirko	RNA hairpin molecule studied by NMR	Structure of the miRNA:mRNA complex
Cogliati	Clelia	Effect of the introduction of a disulphide bridge on protein dynamic and interaction properties of Chicken Liver Bile Acid Binding Protein	Determinants of binding and dynamics properties of bile acid binding proteins by a mutagenesis and NMR approach
Cretu	Daniela Carmen	New Copper(II) complexes of the polidentate ligand with C10 alkyloxy chain. The study concerning the influence of the anion on the nature of the complexes compound.	New Copper(II) complexes of the polidentate ligand with C10 alkyloxy chain. The study concerning the influence of the anion on the nature of the complexes compound.
Cretu	Daniela Carmen	Syntheses and Monitoring of Manganese Porphyrins. UV-vis, FT-IR and Fluorescence Comparative Characterization	Syntheses and Monitoring of Manganese Porphyrins. UV-vis, FT-IR and Fluorescence Comparative Characterization
Csiki	Zsuzsanna	Synthesis of azadisaccharides as heparanase inhibitors	Targeted selective inhibition of glycosidase enzymes
Csizmók	Veronika	Structural and dynamic characterization of intrinsically disordered human securin by NMR	Structural and dynamic characterization of intrinsically disordered human securin by NMR
Daragics	Katalin	Synthesis of Heparin Tetrasaccharides Based On Orthogonal Protecting Group Strategy	Oligosaccharide Library for the Study of Carbohydrate-Protein Interactions
Deleanu	Alia-Cristina	β -D-Glucopyranosyl-modified thiosemicarbazones as inhibitors of glycogen phosphorylase	β -D-Glucopyranosyl-modified thiosemicarbazones as inhibitors of glycogen phosphorylase

Presenting author		Chemistry-related title	Biology-related title
Dundar	Oya	Synthesis and antimicrobial activity of some new triazolo-thiazoly-thiazolidine-2,4-diones	Synthesis and antimicrobial activity of some new triazolo-thiazoly-thiazolidine-2,4-diones
Enyedy	Éva Anna	Potential MMPs inhibitor γ -hydroxamate derivatives of folic acid and their binding properties towards Zinc(II) and human serum albumin	Binding of hydroxamate-folate MMPs inhibitors to Zinc(II) and to albumin
Gáspári	Zoltán	Generation and evaluation of realistic protein structural ensembles	What do dynamic protein structural ensembles tell us?
Gáspári	Zoltán	A biochemical system for site-specific incorporation of isoforms for all 20 proteinogenic amino acids	A vision of a genetic code for NMR
Göker	Hakan	Synthesis and Potent antistaphylococcus activity of some novel -1 <i>H</i> -benzimidazole-5-carboxamidines	Synthesis and Potent antistaphylococcus activity of some novel -1 <i>H</i> -benzimidazole-5-carboxamidines
Herczeg	Mihály	Synthesis of 6-methylenesulfonic acid containing analogues of heparin	Synthesis of 6-methylenesulfonic acid containing analogues of heparin
Hóbor	Fruzsina	Structure – function relationship of a myosin alpha-helical coiled-coil region	Possible structural basis of different regulation of myosin II isoforms
Hoffmann	Eufrozina	Linear scaling semiempirical molecular orbital calculations on the complexation of zinc ions by the Alzheimer's β -amyloid peptide	Theoretical study on zinc-A β metallopeptides
Horváth	László	Interaction of the carrier ligands of insulin mimetic metal complexes with human serum albumin	What happens to the antidiabetic metal complexes after absorption
Jabło ska-Wawrzycka	Agnieszka	Synthesis and physical properties of the new Ca(II) and Cd(II) model complexes with N, O-chelating ligands in the light of investigations of osteoporosis problems	Model complexes of Ca(II) and Cd(II) with small molecule of ligands: investigation of osteoporosis problems
Jaj anin Jozi	Nina	Human dipeptidyl peptidase III acts like a postproline-cleaving enzyme on endomorphins	Degradation of opioid tetrapeptide endomorphin -1 by dipeptidyl peptidase III
Jakab	Zsolt Krisztián	Synthesis of sulfonic acid containing oligosaccharide mimetics of sialyl Lewis A	Synthesis of sulfonic acid containing oligosaccharide mimetics of sialyl Lewis A
Jancsó	Attila	Metal binding of peptides from the His- rich region of histidine-rich glycoprotein	Oligopeptides as probes for the metal binding of histidine-rich glycoprotein
Jeli	Ratomir	Equilibria studies of the reactions between $[\text{Pt}(\text{H}_2\text{O})_2(\text{dach})]^{2+}$ complex and some sulphur and nitrogen donor biomolecules	Studies of interactions between some sulfur and nitrogen containing biomolecules and metal complexes
Keckesova	Simona	Synthesis and physicochemical properties of novel potential ultrashort acting beta-adrenergic blockers	Synthesis and physicochemical properties of novel potential ultrashort acting beta-adrenergic blockers
Kiss	Róbert	Calcium-induced tripartite binding of intrinsically disordered calpastatin to calpain	Calcium-induced tripartite binding of intrinsically disordered calpastatin to calpain
Kolozsi	András	Metal ion interaction with the N-terminal part of endostatine, a protein with antitumor activity	Metal ion interaction with the N-terminal part of endostatine, a protein with antitumor activity
Körtvélyesi	Tamás	On the Structure and Stability of PNA.DNA and PNA.PNA Duplexes: A Theoretical Study	On the Structure and Stability of PNA.DNA and PNA.PNA Duplexes: A Theoretical Study.
Körtvélyesi	Tamás	Effect of Metal Ions on the Stability of PNA, PNA.DNA and PNA.PNA Duplexes.	Effect of Metal Ions on the Stability of PNA, PNA.DNA and PNA.PNA Duplexes.
Kozłowski	Michał	Hydrolysis of RNA by lanthanide complexes	Lanthanide complexes as artificial ribonucleases
Kraszewski	Adam	Dinucleoside phosphonate-phosphates and nucleoside α -hydroxyphosphonates as a potential anti-HIV-1 pronucleotides	Our recent studies on anti-HIV-1 pronucleotides
Labádi	Imre	Preparation and study of metal complexes of antipyrene derivatives.	Biological importance of the metal complexes of the antipyrene derivatives
Labádi	Imre	Preparation and study of transition and lantanoida metal complexes of the polyamino-polyphosphonic acids.	Biological importance of the transition and lantanoida metal complexes of the polyamino-polyphosphonic acids.
Láng	András	Effect of pH on tandem protein modules	Complement control module stabilization by protonation
Lazzari	Sandra	Merging disulphide bonds for drug design	Interfering with a cancer key protein
Lengyel	László	Deuteration using continuous flow devices	Deuterated biologically relevant molecules for structure determination, in mechanistic studies

Presenting author		Chemistry-related title	Biology-related title
Lescic Asler Ivana		How promiscuous are SGNH-hydrolases?	Activity profile of some bacterial SGNH-hydrolases
Leszczynska Grazyna		Chemical synthesis of tRNA ^{Arg} 3 (s2C32, mmm5U34, t6A37) E.coli anticodon stem-loop sequence (ASL ^{Arg} 3)	Model studies on amplification/restriction of tRNAs decoding capacity: synthesis of native tRNA ^{Arg} 3 (E.coli) anticodon stem-loop sequence.
Loch Joanna		High pressure crystal structure of insulin	Pressure as a tool to study insulin folding
Mot Corina		Synthesis and properties of some heteronuclear complexes containing oxalate as ligand in the system: Cu(II)-VO(IV)	Synthesis and properties of some heteronuclear complexes containing oxalate as ligand in the system: Cu(II)-VO(IV)
Mótyán János		Subsite mapping of α -amylase enzymes with molecular modeling	Examination of the substrate binding sites of α -amylase enzymes with molecular modeling
Náray-Szabó Gábor		Four spatial points that define enzyme families	Four spatial points that define enzyme families
Niculescu Violeta		New high performance liquid chromatographic method for determination of 5-hydroxy-1,4-naphthoquinone (juglone)	Juglone's natural biosynthesis highlight in fresh leaves from black walnut tree
Oleksyn Barbara J		Small bioactive molecule interactions in crystalline environment	Inhibitor – enzyme interactions inferred from crystal structures: a comparative study
Pál Ildikó		Monte Carlo analysis of an enzyme kinetic network	Viability tests on eukaryotic cell cycle models
Paragi Gábor		Computational investigation of the interactions of 3- and 5-methyl-6-aminouracils with natural nucleobases	In silico investigation of the interaction of new artificial nucleobases with the natural ones
Paun Nadia		An efficient HPLC method for determination of lawsone from <i>Impatiens balsamina</i>	An efficient HPLC method for determination of lawsone from <i>Impatiens balsamina</i>
Petrovi Biljana		Reactivity of some biomolecules toward novel monofunctional platinum(II) complex	Reactivity of some DNA constituents and amino acids toward novel metal complexes
Picone Delia		Stability-activity relationships in BS-RNase	Anti-tumor activity and structural properties of BS-RNase
Pohl Gábor		Preparation of uniformly labeled point mutants of Tc5b miniprotein for NMR dynamic studies	Application of the ubiquitin fusion expression system: bacterial expression of uniformly labeled point mutants of Tc5b
Porrogi Pálma		Crystal structure of human trypsin 4 complexed with tripeptide aldehyde serine protease inhibitors	A chemical approach to explore the biological function of a Primate-specific serine protease, human trypsin 4
Praly Jean-Pierre		Synthesis of <i>c</i> -glycosyl derivatives of hydroquinone, chromanol and tocopherol as enzyme inhibitors or anti-oxidants	Synthesis of <i>c</i> -glycosyl derivatives of hydroquinone, chromanol and tocopherol as enzyme inhibitors or anti-oxidants
Rapali Péter		Mechanism of DLC binding to multiple protein partners	Mechanism of DLC binding to multiple protein partners
Seff Amalia-Laura		Computational investigation of a bacterial histidine ammonia-lyase (HAL) model with a completely closed active center	Computational investigation of a bacterial histidine ammonia-lyase (HAL) model with a completely closed active center
Seregélyes Csaba		Genetically modified flagellin as a potential tool for display-based target molecule identification	Stable flagellar filaments from flagellin subunits deprived of the variable D3 domain
Sille Julius		Receptor-Based 3D-QSAR Study on Matrix Metalloproteinase Inhibition by Sulfonlated Amino Acid Hydroxamates	Combination of 3D-QSAR and Docking in Inhibition Activity Prediction on Matrix Metalloproteinase Enzymes
Sket Primoz		NMR studies of DNA G-quadruplexes	G-quadruplexes and cation movement
Somsák László		Glucopyranosylidene-spiro-heterocycles as inhibitors of glycogen phosphorylase	Spiro-bicyclic glucose derivatives as potential antidiabetics
Stefu Monica		Generation of nanostructures by map operations	Modeling of hypermolecules
Stráner Pál		Backbone mobility of Trp-cage mutants	Skeletal motion of miniproteins
Szappanos Balázs		Wrapped or unfolded? On the reliability of predictions of special peptide structural features	Critical evaluation of coiled-coil and disorder predictions
Szurmai Zoltán		Preparation of neoglycoproteins by reductive amination	Preparation of artificial carbohydrate antigens
Tóth-Petróczy Ágnes		Disordered Tails of Homeodomains: Effect on Folding and Binding	Disordered Tails in Transcriptional Regulation
Tratar Pirc Elizabeta		Binding modes of metal ions to hyaluronate	Binding modes of metal ions to hyaluronate
Yildiz Ilkay		Molecular Modelling Studies on Some Benzazoles as Eukaryotic DNA Topoisomerase II Inhibitors	Molecular Modelling Studies on Some Benzazoles as Eukaryotic DNA Topoisomerase II Inhibitors