

Subject Index for Volume 25

A

- Acetolactate synthase
 - isozyme II, from *Escherichia coli*, inhibition by photoactivable azidosulfonylurea, 261
- 2-Acetyl-5-*N'*,*N'*-dimethylaminophenyl *N,N*-dimethylcarbamate
 - synthesis, 37
- N*-Acetyldopamine quinone
 - reactions with imidazole and *N*-acetylhistidine, in analysis of insect cuticle sclerotization, 179
- N*-Acetylhistidine
 - reactions with catecholamine quinones, in analysis of insect cuticle sclerotization, 179
- Acidic solutions
 - aqueous, natural and modified α -cyclodextrins in, chiral recognition of aliphatic amino acids, 155
- N*- β -Alanyldopamine quinone
 - reactions with imidazole and *N*-acetylhistidine, in analysis of insect cuticle sclerotization, 179
- Alcohols
 - phosphorylation by monoselenophosphate, 247
- Aliphatic amino acids
 - chiral recognition by natural and modified α -cyclodextrins in acidic aqueous solution, 155
- Alkyl ester derivatives
 - as acyl donor component in methyltrypsin-catalyzed peptide coupling, 307
- Amines
 - phosphorylation by monoselenophosphate, 247
- D-Amino acid oxidase
 - conformation, slow changes during reaction, 100
- Amino acids
 - aliphatic, chiral recognition by natural and modified α -cyclodextrins in acidic aqueous solution, 155
- 4-Amino-4,5-dihydro-2-furan carboxylic acid
 - synthesis and mechanistic studies, 43
- 4-Amino-4,5-dihydro-2-thiophene carboxylic acid
 - synthesis and mechanistic studies, 43
- 2-Aminoethanol
 - phosphorylation by monoselenophosphate, 247
- Angiotensin-converting enzyme inhibitors
 - chemical and photochemical modification, impli-

cations for development of cardiac radionuclide imaging agents, 77

- Aromatic groups
 - interactions with sulfur, computational study using dimethyl sulfide–benzene complex, 213
- Arylcarbamates
 - o*-substituted, and related compounds, synthesis, 37
- Azidosulfonylurea
 - photoactivable, inhibition of acetolactate synthase isozyme II from *Escherichia coli*, 261

B

- Benzene
 - complex with dimethyl sulfide, computational study, 213
- 2-Bromo-5-*N'*,*N'*-dimethylaminophenyl *N,N*-dimethylcarbamate
 - synthesis, 37
- 2-(4-*tert*-Butylphenoxy)propionic acid
 - esterification in organic solvent, lipase enantioselectivity for, improvement at high temperature, 88

C

- Calcium channels
 - blocking by 4-indolyl-1,4-dihydropyridines, 169
- Carbocation intermediates
 - tertiary, stepwise isomerization in water via, free energy profile, 239
- Catecholamine quinones
 - reactions with imidazole and *N*-acetylhistidine, in analysis of insect cuticle sclerotization, 179
- cdc25 phosphatase
 - inhibition by menadione, 33
- Chiral recognition
 - aliphatic amino acids by natural and modified cyclodextrins in acidic aqueous solution, 155
- 2-Chloro-5-*N'*,*N'*-dimethylaminophenyl *N,N*-dimethylcarbamate
 - synthesis, 37
- Chorismic acid
 - in vivo* synthesis and rapid purification using engineered *Escherichia coli* strain, 297

Commitment factors

- contrasting values measured from viscosity, pH, and kinetic isotope effects, analysis for D-amino acid oxidase reaction, 100

Computational studies

- dimethyl sulfide–benzene complex, 213

Conformation

- D-amino acid oxidase, slow changes during reaction, 100
- poly(ethylenimine) and derivatives, flexibility of, 221

Cuticle

- insect, sclerotization, studies using reactions of catecholamine quinones with imidazole and *N*-acetylhistidine, 179

1-Cyano-2,3,5,6-tetrafluoroarylaminoisopropyl

- synthesis and inhibition of angiotensin-converting enzyme, 77

 α -Cyclodextrin

- in acidic aqueous solution, chiral recognition of aliphatic amino acids, 155

 β -Cyclodextrin

- linking to dendrimer poly(ethylenimine)s, 63
- poly(ethylenimine) derivative containing, conformational flexibility, 221

Cysteine

- oxidation of norepinephrine and epinephrine in presence of, 130

D

Dendrimers

- poly(ethylenimine)s, linked to β -cyclodextrin, 63

 N_1 -(2,6-Dichlorobenzyl)-1,4-dihydronicotinamide

- hydride transfer reactions, primary kinetic isotope effect in, temperature dependence, 1

2,6-Dichloroindophenol

- hydride transfer reactions, primary kinetic isotope effect in, temperature dependence, 1

Dihydroorotate dehydrogenase

- human, inhibition by bioactive leflunomide metabolite, structural requirements for, 233

o,o'-Dihydroxyazobenzene

- poly(ethylenimine) derivative containing, conformational flexibility, 221

O-(3-*N'*,*N'*-Dimethylaminophenyl)-*N,N*-dimethylthiocarbamate

- synthesis, 37

S-(3-*N'*,*N'*-Dimethylaminophenyl)-*N,N*-dimethylthiocarbamate

- synthesis, 37

N'-(3-*N''*,*N''*-Dimethylaminophenyl)-*N,N*-dimethylurea

- synthesis, 37

Dimethyl sulfide

- complex with benzene, computational study, 213

Dioxetane

- identification as intermediate in dioxygen transfer from 4a-hydroperoxyflavin anion to phenolate and indole anions, 331

Dioxygen

- transfer from 4a-hydroperoxyflavin anion to phenolate and indole anions, intermediate in, identification, 331

DNA polymerase β

- conformational changes induced by consecutive binding of nucleotide and Mg^{2+} , 43

E

Editorial

- Bioorganic Chemistry at a Crossroads, 275

Enantioselectivity

- lipase for esterifications of 2-phenoxypropionic acids in organic solvent, improvement at high temperature, 88

Enzyme structure

- in nonaqueous solvents, 43

Epinephrine

- oxidation in presence of cysteine, 130

Escherichia coli

- acetolactate synthase isozyme II from, inhibition by photoactivable azidosulfonylurea, 261
- chorismic acid synthesis by engineered chorismate mutase-deficient strain, 297

Esterification

- 2-phenoxypropionic acids in organic solvent, lipase enantioselectivity for, improvement at high temperature, 88

Ethanol

- reaction with oxyphosphoranes, kinetics, 23

Ethanolamine ammonia-lyase

- radical enzymology, 43

Ethylene diamine

- phosphorylation by monoselenophosphate, 247

Ethylene glycol

- phosphorylation by monoselenophosphate, 247
- reaction with oxyphosphoranes, kinetics, 23

2-(4-Ethylphenoxy)propionic acid

- esterification in organic solvent, lipase enantioselectivity for, improvement at high temperature, 88

F

Fermentation

- natural abundance isotopic fractionation in, effect of fermentation medium, 117

Flash chromatography
 chorismic acid synthesized *in vivo* by engineered
Escherichia coli strain, 297

Fluorescein 5-thiosemicarbazide
 glycoprotein labeled with, detection on SDS–
 polyacrylamide gel, 163

Free energy
 guanidinium acetate and methylammonium ace-
 tate ion pairs in water, 11
 stepwise isomerization in water via tertiary car-
 bocation intermediate, 239

Fumarase C
 structure, 43

G

Gel electrophoresis
 glycoproteins labeled with fluorescein 5-thio-
 semicarbazide, detection on SDS–poly-
 acrylamide, 163

Glucosamine 6-phosphate synthase
 nitrogen transfer in, mechanistic study with tran-
 sition state analogs, 283

Glutamic acid
 γ -phosphono- and γ -sulfonic analogs, synthesis
 for mechanistic study of nitrogen transfer
 in glucosamine 6-phosphate synthase, 283

Glutamine
 γ -phosphono- and γ -sulfonic analogs, synthesis
 for mechanistic study of nitrogen transfer
 in glucosamine 6-phosphate synthase, 283

Glycerol
 phosphorylation by monoselenophosphate, 247
 reaction with oxyphosphoranes, kinetics, 23

Glycoproteins
 fluorescein 5-thiosemicarbazide-labeled, detec-
 tion on SDS–polyacrylamide gel, 163

Glycyl-proline backbone
 chiral peptide nucleic acids with, for hybridiza-
 tion studies, 321

Guanidinium acetate
 and methylammonium acetate, ion pairs in wa-
 ter, Monte Carlo simulations, 11

Guanidinophenyl ester derivatives
 as acyl donor component in methyltrypsin-cata-
 lyzed peptide coupling, 307

H

Heart
 imaging, development of radionuclide agents
 for, implications of modification of angio-
 tensin-converting enzyme inhibitors, 77

Human immunodeficiency virus type 1
 reverse transcriptase, inhibitor characteriza-
 tion, 43

Hybridization studies
 with chiral peptide nucleic acids, 321

Hydride transfer reactions
 with NAD^+ and NADH models, primary kinetic
 isotope effect in, temperature dependence, 1

Hydrolysis
 monoselenophosphate, ^{31}P NMR study, 247

4a-Hydroperoxyflavin anion
 dioxygen transfer from, to phenolate and indole
 anions, intermediate identification, 331

I

Imaging agents
 radionuclide, development for heart, implica-
 tions of modification of angiotensin-con-
 verting enzyme inhibitors, 77

Imidazole
 reactions with catecholamine quinones, in analy-
 sis of insect cuticle sclerotization, 179

Indole anion
 dioxygen transfer from 4a-hydroperoxyflavin
 anion to, intermediate in, identification, 331

4-Indolyl-1,4-dihydropyridines
 synthesis and calcium channel blocking activ-
 ity, 169

Interaction energy
 in sulfur–aromatic interactions, computational
 study using dimethyl sulfide–benzene com-
 plex, 213

2-Iodo-5-*N'*,*N'*-dimethylaminophenyl *N*,*N*-dimeth-
 ylcarbamate
 synthesis, 37

Isocyclosporin A
 prepared in organic solvent and in aqueous solu-
 tion, ^1H NMR, 110

Isomerization
 stepwise, in water via tertiary carbocation inter-
 mediate, free energy profile, 239

Isopentenyl pyrophosphate isomerase
 reaction catalyzed by, mechanistic imperatives,
 239

Isotope effects
 kinetic, *see* Kinetic isotope effect

Isotopic fractionation
 in fermentation reaction, effect of fermentation
 medium, 117

K

Kinetic isotope effect
 and pH and viscosity, commitment factor values