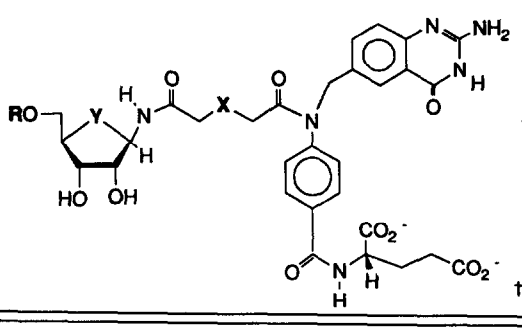
Multisubstrate Adduct Inhibitors of Glycinamide Ribonucleotide Transformylase. Synthetic$^{\Delta}$ and Enzyme Assembled$^{\#}$

Tetrahedron, **1991**, *47*, 2351

James Inglese and Stephen J. Benkovic
Department of Chemistry, Pennsylvania State University, University Park, PA 16801



	$R^{\dagger}$	Y	X	
Δ	PO_3^{2-}	O	S	β-thioacetyl glycinamide ribonucleotide 5,8-dideazafolate (β-TGDDF)
#	PO_3^{2-}	O	NH	β-glycinamide ribonucleotide acetyl 5,8-dideazafolate (GADDF)
#	PO_3^{2-}	CH_2	NH	β-carbo-glycinamide ribonucleotide acetyl 5,8-dideazafolate (CGADDF)
Δ	H	O	S	β-thioacetyl glycinamide ribonucleoside 5,8-dideazafolate

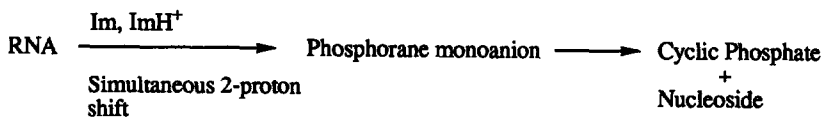
†for R = PO_3^{2-}, dissociation constants are on the order of 250 pM

Tetrahedron, **1991**, *47*, 2365

RIBONUCLEASE MIMICS

Ronald Breslow*, Eric Anslyn, and Deeng-Lih Huang
Department of Chemistry, Columbia University, New York, New York 10027

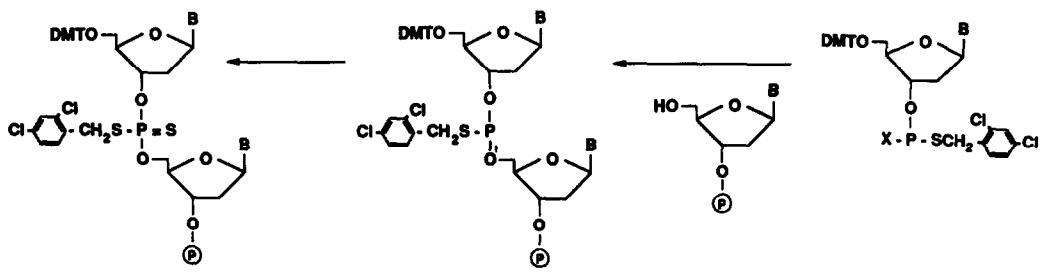
Models for the enzyme ribonuclease A imitate its catalytic action, and its detailed mechanism.



Tetrahedron, **1991**, *47*, 2377

SYNTHESIS OF OLIGONUCLEOTIDE PHOSPHORODITHIOATES

G. Beaton, W. K.-D. Brill, A. Grandas, Y.-X. Ma, J. Nielsen, E. Yau, and M. H. Caruthers* Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309-0215.



X = pyrrolidinyl; DMT, dimethoxytrityl; Ⓟ, silica support

Tetrahedron, **1991**, *47*, 2389

Site-Specific Incorporation of Non-Natural Residues into Peptides: Effects of Residue Structure on Suppression and Translation Efficiencies

*J. D. Bain, Dean A. Wacker, Eric E. Kuo, and A. Richard Chamberlin**
Department of Chemistry, University of California, Irvine, CA 92717

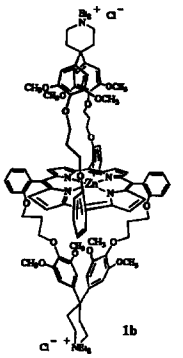
A systematic survey of the structural requirements for biosynthetic incorporation of non-natural residues into a polypeptide is presented. Relative translation efficiencies for a series of 12 semi-synthetic acylated suppressor tRNAs ranged from 0 to 91% depending on the structure of the residue incorporated.

Tetrahedron, **1991**, *47*, 2401

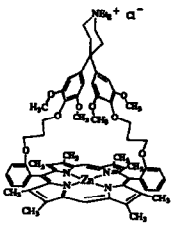
Porphyrin-Cyclophanes: Inclusion Complexation and X-Ray Crystal Structure of a Zinc Octamethyl-diphenylporphyrin

David R. Benson, Robert Valentekovich, Carolyn B. Knobler, and François Diederich*

Department of Chemistry and Biochemistry
University of California
Los Angeles, California 90024-1569, U.S.A.



1b

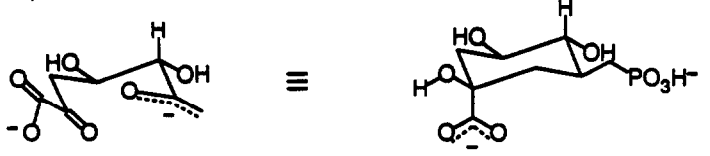


2b

Tetrahedron, **1991**, *47*, 2423

PREDICTING INHIBITION OF DEHYDROQUINATE SYNTHASE

L. T. Piehler, J. -L. Montchamp, J. W. Frost* and Charles J. Manly*
Department of Chemistry, Purdue University, West Lafayette, IN 47907
DowElanco, Greenfield, IN 46140

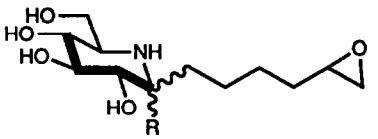


Tetrahedron, **1991**, *47*, 2433

EFFECT OF 1-EPOXYALKYL-1-DEOXY-NOJIRIMYCINS ON EXOGLUCOSIDASES

Louis J. Liotta, Jeehiun Lee and Bruce Ganem*
Department of Chemistry, Baker Laboratory, Cornell University, Ithaca, New York 14853 USA

Two novel nojirimycin derivatives were synthesized which inhibit or inactivate glucosidases



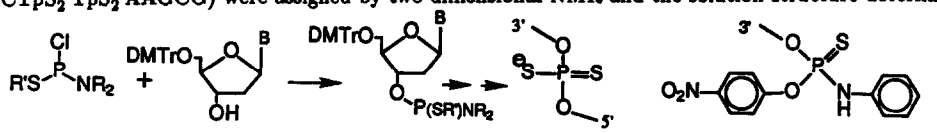
15 R= α–H
33 R= β–H

Tetrahedron, **1991**, *47*, 2449

SYNTHESIS, NMR AND STRUCTURE OF OLIGONUCLEOTIDE PHOSPHORODITHIOATES

Martial E. Piotto, Jill Nelson Granger, Yesun Cho, Nasser Farschtschi and David G. Gorenstein*
Department of Chemistry, Purdue University, West Lafayette, Indiana 47907

Thiophosphoramidite as well as thiophosphoramidate chemistry has been used to prepare dithiophosphate analog of oligonucleotides. The ^{1}H and ^{31}P resonances of the 3'-thymidine phosphorodithioate decamer d(CGCTpS$_2^-$TpS$_2^-$AAGCG) were assigned by two-dimensional NMR and the solution structure determined.

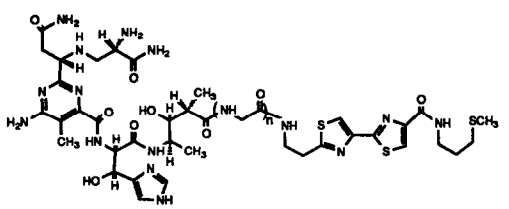


Tetrahedron, **1991**, *47*, 2463

POLYNUCLEOTIDE RECOGNITION AND STRAND SCISSION BY FE·BLEOMYCIN

Barbara J. Carter, Kalakota S. Reddy, and Sidney M. Hecht*
Departments of Chemistry and Biology, University of Virginia, Charlottesville, VA 22901 USA

Four bleomycin analogs are used to determine the structural features in BLM responsible for sequence selectivity of DNA damage. The sequence selective damage of RNA is also reported.



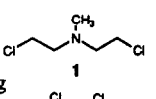
gly$_0$-BLM n = 0
gly$_1$-BLM n = 1
gly$_2$-BLM n = 2
gly$_4$-BLM n = 4

Tetrahedron, **1991**, *47*, 2475

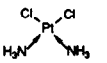
Sequence Preferences of DNA Interstrand Cross-Linking Agents: Importance of Minimal DNA Structural Reorganization in the Cross-Linking Reactions of Mechlorethamine, Cisplatin, and Mitomycin C

Paul B. Hopkins*, Julie T. Millard, Jinsuk Woo, Margaret F Weidner, James J. Kirchner, Snorri Th. Sigurdsson, and Stanley Raucher
Department of Chemistry, University of Washington, Seattle, Washington 98195

The DNA interstrand cross-linking reactions of **1-4** were studied using synthetic DNA fragments. It is suggested that the conversion of monoadducts to cross-linked molecules is a critical reaction in determining the nucleotide sequence preference of these reactions.



1



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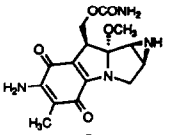

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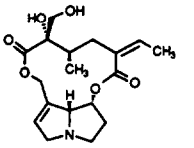


4

Tetrahedron, **1991**, *47*, 2491

Monte Carlo Simulations Yield Absolute Free Energies of Binding for Guanine–Cytosine and Adenine–Uracil Base Pairs in Chloroform

Julianto Pranata and William L. Jorgensen*
Department of Chemistry, Yale University, New Haven, Connecticut 06511

Monte Carlo simulations with statistical perturbation theory and the OPLS potential functions were employed to calculate the absolute free energies of binding between 9-methyladenine (A) and 1-methyluracil (U) and between 9-methylguanine (G) and 1-methylcytosine (C) in chloroform at 25 °C.

$$A + U \rightarrow A\text{–}U \qquad \Delta G = -3.6 \text{ kcal/mol}$$
$$G + C \rightarrow G\text{–}C \qquad \Delta G = -7.9 \text{ kcal/mol}$$

Tetrahedron, **1991**, *47*, 2503

SUBSTRATE ATTENUATION: AN APPROACH TO IMPROVE ANTIBODY CATALYSIS.

Kim D. Janda,*[a] Stephen J. Benkovic,[b] Donald A. McLeod,[a] Diane M Schloeder[a] and Richard A. Lerner,*[a] [a]*Departments of Molecular Biology and Chemistry, Research Institute of Scripps Clinic, La Jolla, California 92037, USA*, and [b]*Department of Chemistry, Pennsylvania State University, University Park, PA 16802, USA.*

Abstract: Antibodies raised to quinaldine phosphonamide **1a** showed no ability to hydrolyze its most homologous substrates amide and ester **2** and **3**, respectively. However, within this same set of antibodies some thirteen showed a great propensity to hydrolyse a structurally similar naphthyl ester. In addition to heteroatom discrimination one of the antibodies examined in detail displayed an increase in catalytic efficiency presumably via weak apparent binding (K_m) when phenylesters were employed as substrates. These findings suggest abzyme catalysis may be improved via substrate attenuation.

Tetrahedron, **1991**, *47*, 2507

CONVERGENT FUNCTIONAL GROUPS XI.

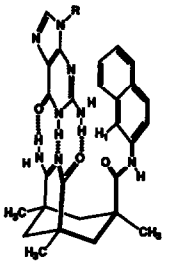
SELECTIVE BINDING OF GUANOSINE DERIVATIVES.

Tae Kyo Park, Joseph Schroeder and Julius Rebek, Jr.*

Department of Chemistry, Massachusetts Institute of Technology,

Cambridge, Massachusetts 02139

New synthetic receptors for guanosines are introduced and evaluated using solubility titration methods. Base-pairing and some aromatic stacking effects are observed in $CDCl_3$.

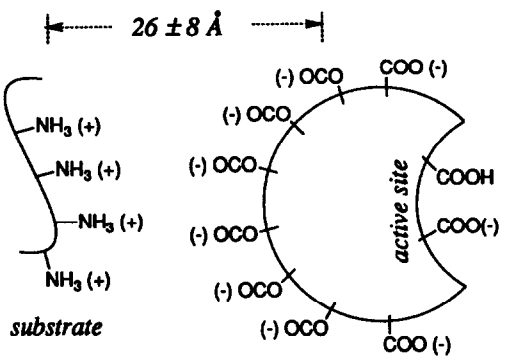


Tetrahedron, **1991**, *47*, 2519

LONG RANGE ELECTROSTATIC EFFECTS IN PEPSIN CATALYSIS

Petr Kuzmič, Chong-Qing Sun, Zhi-Cheng Zhao, and Daniel H. Rich

Binding of polycationic substrates and inhibitors to pepsin is a stepwise process. Fast nonspecific association, governed by long range electrostatic forces, is followed by slow surface diffusion into the active site.

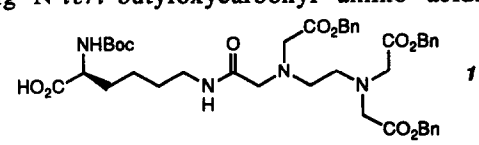


Tetrahedron, **1991**, *47*, 2535

SYNTHESIS OF N-α-BOC-N-ε-TRIBENZYL EDTA-L-LYSINE. AN AMINO ACID ANALOGUE SUITABLE FOR SOLID PHASE PEPTIDE SYNTHESIS

Bernard Cuenoud and Alanna Schepartz, Department of Chemistry, Yale University, New Haven, Connecticut 06511 USA*

The synthesis of an amino acid analogue suitable for appending ethylenediaminetetraacetic acid to unique internal amino acid residues of a synthetic peptide prepared using N-*tert*-butyloxycarbonyl amino acids is described.

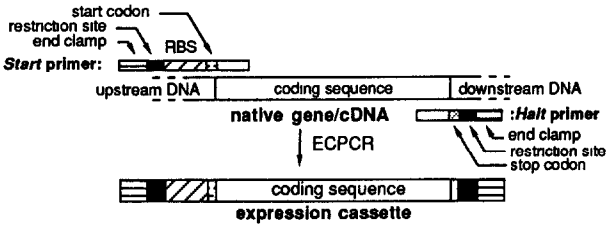


1

Tetrahedron, **1991**, *47*, 2543

PROTEIN OVERPRODUCTION FOR ORGANIC CHEMISTS

STUART L. SCHREIBER* AND GREGORY L. VERDINE*
DEPARTMENT OF CHEMISTRY, HARVARD UNIVERSITY, 12 OXFORD ST., CAMBRIDGE, MA, 02138



The theory and practice of constructing protein-overproducing bacterial strains are reviewed. Our recently developed chemical/enzymatic technique for gene refabrication — the Expression-Cassette Polymerase Chain Reaction (ECPCR) — which greatly reduces the need for training in molecular biology, is discussed.

Tetrahedron, **1991**, *47*, 2563

MONOCLONAL ANTIBODIES WITH SEQUENCE SPECIFIC AFFINITY FOR A STEM - LOOP STRUCTURE IN DNA.

Jean Chmielewski and Peter Schultz*, *Department of Chemistry, University of California, Berkeley, CA 94720*

Abstract: Monoclonal antibodies have been raised against an oligonucleotide with a stem-loop structure (**1**). Antibody 41H7 binds hapten **1** with a dissociation constant of 2.0×10^{-6} M and with sequence specificity.

$$\begin{array}{l} \text{ACCGGCCAATTCCGGCC}\,{}^{\text{T}}_{\text{T}}\,\text{C}\,{}^{\text{C}}_{\text{C}}\,\text{G} \\ \text{TGGCCGGTTAAGGCCGG} \end{array} \qquad (1)$$

Tetrahedron, **1991**, *47*, 2573

CHORISMATE MUTASE/PREPHENATE DEHYDRATASE FROM ESCHERICHIA COLI: SUBCLONING, OVERPRODUCTION AND PURIFICATION

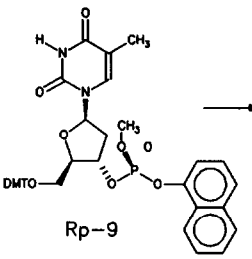
Jon Stewart,* David B. Wilson and Bruce Ganem
Department of Chemistry; Section of Biochemistry, Cell and Molecular Biology
Cornell University, Ithaca, New York 14853 USA

CM/PD has been overexpressed as 20% of soluble protein using recombinant DNA techniques. This efficient source of pure mutase should facilitate mechanistic and physical studies.

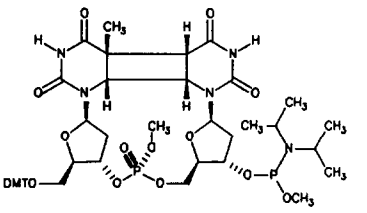
Tetrahedron, **1991**, *47*, 2579

UNRAVELING THE ORIGIN OF THE MAJOR MUTATION INDUCED BY ULTRAVIOLET LIGHT, THE C→T TRANSITION AT dTpdC SITES. A DNA SYNTHESIS BUILDING BLOCK FOR THE CIS-SYN CYCLOBUTANE DIMER OF dTpdU.

John-Stephen Taylor*
and Sourena Nadji
Department of Chemistry
Washington University
1 Brookings Drive
St. Louis, MO 63130



Rp−9



Rp−14

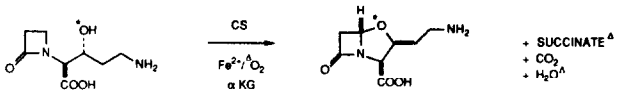
The preparation of *Rp*-**9** and its conversion to the dTpdU cis-syn dimer building block *Rp*-**14** is described.

Tetrahedron, **1991**, *47*, 2591

EXPERIMENTS AND SPECULATIONS ON THE ROLE OF OXIDATIVE CYCLIZATION CHEMISTRY IN NATURAL PRODUCT BIOSYNTHESIS

Craig A. Townsend* and Amit Basak
Department of Chemistry, The Johns Hopkins University, Baltimore, Maryland 21218

Isotopically-labeled samples of proclavaminic acid (**8**) have been prepared and converted to clavaminic acid (**9**) by the enzyme clavaminate synthase (CS). Results of these experiments point to a subset of oxygenase chemistry involving cyclization/desaturation reactions that may play a role in the biosynthesis of other natural product groups, *e.g.* polyethers as monensin and brevetoxin A.

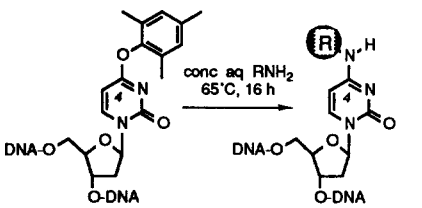


8 **9**

Tetrahedron, **1991**, *47*, 2603

ENGINEERING TETHERED DNA MOLECULES BY THE CONVERTIBLE NUCLEOSIDE APPROACH

ANDREW M. MACMILLAN AND GREGORY L. VERDINE*
DEPARTMENT OF CHEMISTRY, HARVARD UNIVERSITY, 12 OXFORD ST., CAMBRIDGE, MA, 02138



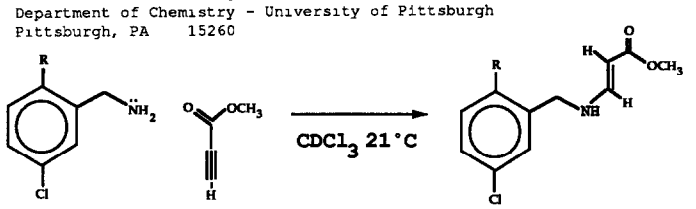
TMP-dU residue, **2** N^4-alkyl-dC residue, **4**

Oligonucleotides containing the convertible nucleoside O^4-trimethylphenyl-2'-deoxyuridine (TMP-dU, **2**) react with a variety of aqueous amines, resulting in the site-specific generation of N^4-alkyl-dC residues (**2**). This *convertible nucleoside strategy* represents a novel, convergent synthesis of functionally tethered oligonucleotides.

Tetrahedron, **1991**, *47*, 2617

THE CHEMISTRY OF FUNCTIONAL GROUP ARRAYS. ELECTROSTATIC CATALYSIS AND THE "INTRAMOLECULAR SALT EFFECT".

Paul A. Smith and Craig S. Wilcox*
Department of Chemistry - University of Pittsburgh
Pittsburgh, PA 15260



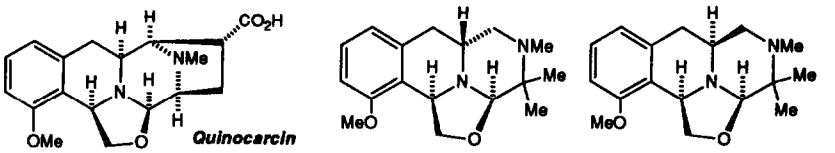
-R = -H	$k = 3 \times 10^{-5}$	$l \cdot mol^{-1} \cdot sec^{-1}$
$-R = -SO_3^- NBu_4^+$	$k = 1.5 \times 10^{-2}$	$l \cdot mol^{-1} \cdot sec^{-1}$

Tetrahedron, **1991**, *47*, 2629

SYNTHESIS CONFORMATION, CRYSTAL STRUCTURES AND DNA CLEAVAGE ABILITIES OF TETRACYCLIC ANALOGS OF QUINOCARCIN

Robert M. Williams*, Tomasz Glinka, Renee Gallegos, Paul P. Ehrlich, Mark E. Flanagan, Hazel Coffman and Gyoosoon Park
Department of Chemistry, Colorado State University, Fort Collins, Colorado 80523

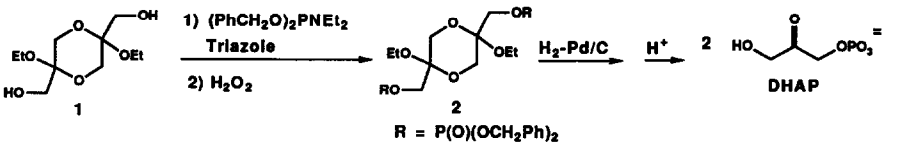
Two totally synthetic, racemic analogs of quinocarcin have been designed and their crystal structures determined. Both substances effect the modest cleavage of plasmid DNA.



Tetrahedron, **1991**, *47*, 2643

AN IMPROVED SYNTHESIS OF DIHYDROXYACETONE PHOSPHATE

Richard L. Pederson, John Esker and Chi-Huey Wong*
Department of Chemistry, The Research Institute of Scripps Clinic, La Jolla, CA 92037

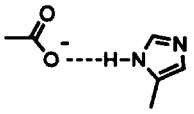


R = P(O)(OCH$_2$Ph)$_2$

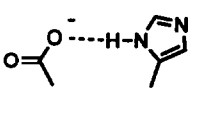
Tetrahedron, **1991**, *47*, 2649

Syn and Anti-Oriented Imidazole Carboxylates as Models for the Histidine-Aspartate Couple in Serine Proteases and Other Enzymes

Steven C. Zimmerman,* Jean S. Korthals, and Katherine D. Cramer
Department of Chemistry, University of Illinois, Urbana, Illinois 61801



syn



anti

Tetrahedron, **1991**, *47*, 2661

AN ALTERNATIVE AND CONVENIENT STRATEGY FOR GENERATION OF SUBSTANTIAL QUANTITIES OF SINGLY 5′-^{32}P-END-LABELED DOUBLE-STRANDED DNA FOR BINDING STUDIES: DEVELOPMENT OF A PROTOCOL FOR EXAMINATION OF FUNCTIONAL FEATURES OF (+)-CC-1065 AND THE DUOCARMYCINS THAT CONTRIBUTE TO THEIR SEQUENCE-SELECTIVE DNA ALKYLATION PROPERTIES.

Dale L. Boger,* Stephen A. Munk, Hamideh Zarrinmayeh, Takayoshi Ishizaki, Joan Haught, and M. Bina,* *Department of Chemistry, Purdue University, West Lafayette, Indiana 47907, USA*

Abstract: The comparative DNA alkylation properties of (+)-CC-1065 and a series of structural (CI) analogs are detailed in efforts to further define the structural origin of the DNA alkylation sequence selectivity.