

## Nucleotide Analogs and Phosphate Esters – Materials

373. A. Salehi; H-Y. Mei; and T.C. Bruice. Synthesis and DNA-Binding Studies of New Cationic Guanidine and Betaineamide Tetraphenylporphyrins. *Tet. Lett.* **1991**, 32, 3453.
385. T.C. Bruice; H.-Y. Mei; G.-X. He; and V. Lopez. Rational Design of Substituted Tri-Pyrrole Peptides Which Complex with DNA by Both Selective Minor Groove Binding and Electrostatic Interaction with Phosphate Backbone. *Proc. Natl. Acad. Sci. (USA)* **1992**, 89, 1700.
393. K.A. Browne and T.C. Bruice. Chemistry of Phosphodiester, DNA and Models. II. The Hydrolysis of Bis(8-hydroxyquinoline) Phosphate in the Absence and Presence of Metal Ions. *J. Am. Chem. Soc.* **1992**, 114, 4951.
403. G-X. He; K.A. Browne; J.C. Groppe; A. Blasko; H-Y. Mei; and T.C. Bruice. Microgonotropens and Their Interactions with DNA. I. Synthesis of the Tri-Pyrrole Peptides Dien-Microgonotropen-a, -b, and -c and Characterization of Their Interactions with dsDNA. *J. Am. Chem. Soc.* **1993**, 115, 7061.
404. K.A. Browne; G-X. He; and T.C. Bruice. Microgonotropens and Their Interactions with DNA. II. Quantitative Evaluation of Equilibrium Constants for 1:1 and 2:1 Binding of Dien-Microgonotropen-a, -b, and -c as well as Distamycin and Hoechst 33258 to d(GGCGCAAATTTGGCGG)/d(CCGCAAATTTGCGCC). *J. Am. Chem. Soc.* **1993**, 115, 7072.
405. A. Blasko; K.A. Browne; G-X. He; and T.C. Bruice. Microgonotropens and Their Interactions with DNA. III. Structural Analysis of the 1:1 Complex of d(CGCAAATTTGCG)<sub>2</sub> and Dien- Microgonotropen-c by 2D NMR Spectroscopy and Restrained Molecular Modeling. *J. Am. Chem. Soc.* **1993**, 115, 7080.
407. Ö Almarsson; T.C. Bruice; J. Kerr and R. Zuckermann. Molecular Mechanics Calculations of the Structures of Polyamide Nucleic Acid DNA Duplexes and Triple Helical Hybrids. *Proc. Natl. Acad. Sci. (USA)* **1993**, 90, 7518.
409. Ö Almarsson and T.C. Bruice. Peptide Nucleic Acid (PNA) Conformation and Polymorphism in PNA-DNA and PNA-RNA Hybrids. *Proc. Natl. Acad. Sci. (USA)* **1993**, 90, 9542.
410. A. Blaskó and T.C. Bruice. Stoichiometry and Structure of Complexes of DNA Oligomers with Microgonotropens and Distamycin by <sup>1</sup>H NMR Spectroscopy and Molecular Modeling. *Proc. Natl. Acad. Sci. (USA)* **1993**, 90, 10018.
414. H.G. Hansma, R.L. Sinsheimer, J. Groppe, T.C. Bruice, V. Elings, G. Gurley, M. Bezanilla, I.A. Mastrangelo, P.V.C. Hough, and P.K. Hansma. Recent Advances in Atomic Force Microscopy of DNA. *Scanning* **1993**, 15, 296.
417. G-X. He, K.A. Browne, A. Blaskó, and T.C. Bruice. Microgonotropens and Their Interactions with DNA. IV. Synthesis of the Tripyrrole Peptides Tren-Microgonotropen-a and -b and Characterization of Their Interactions with DsDNA. *J. Am. Chem. Soc.* **1994**, 116, 3716.

418. A. Blaskó; K.A. Browne; and T.C. Bruice. Microgonotropens and Their Interactions with DNA. V. Structural Characterization of the 1:1 complex of d(CGCAAATTTGCG)<sub>2</sub> and Tren-Microgonotropen-b by 2D NMR Spectroscopy and Restrained Molecular Modeling. *J. Am. Chem. Soc.* **1994**, *116*, 3726.
419. R.O. Dempcy and T.C. Bruice. The Negative Charge of Alkyl Phosphate Diesters and the Slow-gated Hydrolysis of RNA and DNA. Catalysis of RNA Hydrolysis through Metal Ion Ligation to the Ester >PO<sub>2</sub>- Moiety. *J. Am. Chem. Soc.* **1994**, *116*, 4511.
421. R. O. Dempcy; Ö. Almarsson; and T. C. Bruice. The Design and Synthesis of DNG: A Polycation Analogue of DNA. *Proc. Natl. Acad. Sci. (USA)* **1994**, *91*, 7864.
422. H. G. Hansma; K. A. Browne; M. Bezanilla; and T. C. Bruice. Bending and Straightening of DNA Induced by the Same Ligand: Characterization with the Atomic Force Microscope. *Biochemistry* **1994**, *33*, 8436.
424. A. Tsubouchi; T. C. Bruice. A Remarkable (~10<sup>13</sup>) Rate Enhancement in Phosphonate Ester Hydrolysis Catalyzed by Two Metal Ions. *J. Am. Chem. Soc.* **1994**, *116*, 11614.
425. T. Xue; K. A. Browne; T. C. Bruice. A Novel Minor Groove Binding Reagent Designed to Serve as a "Truck" to Carry DNA Modifying Moieties into the Major Groove. *Bioconjugate Chem.* **1995**, *6*, 82.
426. T. C. Bruice; A. Blaskó'; R. D. Arasasingham; J-S. Kim; M. Petyak. Hydrolysis of a Phosphate Diester by Simultaneous Carboxylate and Carboxyl Group Participation in a Rigid System with Kinetically Unfavorable Rotamers Frozen Out. *J. Am. Chem. Soc.* **1995**, *117*, 3639.
429. R. O. Dempcy; K. A. Browne and T. C. Bruice. Synthesis of the Polycation Thymidyl DNG, It's Fidelity in Binding Polyanionic DNA/RNA, and the Stability and Nature of the Hybrid Complexes. *J. Am. Chem. Soc.* **1995**, *117*, 6140.
430. R. O. Dempcy; K. A. Browne; T. C. Bruice. Synthesis of a Thymidyl Pentamer of DNG and Binding Studies with DNA Homopolyoligonucleotides. *Proc. Natl. Acad. Sci (USA)* **1995**, *92*, 6097.
431. K. A. Browne; R. O. Dempcy; T. C. Bruice. Binding Studies of Cationic DNG to RNA Homopolynucleotides. *Proc. Natl. Acad. Sci(USA)* **1995**, *92*, 7051.
432. A. Blasko; K. A. Browne; T. C. Bruice. NMR Structure of d(CGCA3T3GCG)<sub>2</sub>:Tren-Microgonotropen-b:Zn(II) Complex and Solution Studies of Metal Ion Complexes of Tren- Microgonotropen-b Interacting with DNA. *Bioorganic and Medicinal Chemistry* **1995**, *3*, 631.
434. A. Tsubouchi; T. C. Bruice. Phosphonate Ester Hydrolysis Catalyzed by Two Lanthanum Ions. Intramolecular Nucleophilic Attack of Coordinated Hydroxide and Lewis Acid Activation. *J. Am. Chem. Soc.* **1995**, *117*, 7399.
435. Thomas C. Bruice; Andrei Blaskó; and Mark E. Petyak. Participation of two Carboxyl Groups in Phosphodiester Hydrolysis. I. The Hydrolysis of Bis-(2-carboxyphenyl) Phosphate. *J. Am. Chem. Soc.* **1995**, *117*, 12064.

436. Thomas C. Bruice; Andrei Blaskó; Ramesh D. Arasasingham; and Jang- Seob Kim. Participation of two Carboxyl Groups in Phosphodiester Hydrolysis. II A Kinetic, Isotopic and  $^{31}\text{P}$  NMR Study of the Hydrolysis of a Phosphodiester with Carboxyl Groups Fixed in an Attack Conformation. *J. Am. Chem. Soc.* **1995**, *117*, 12070.
437. R. A. Torres and T. C. Bruice. Interresidue Hydrogen Bonding in a PNA.RNA Heteroduplex. *Proc. Natl. Acad. Sci (USA)* **1996**, *93*, 649.
440. Dempcy, Robert O.; Bruice, Thomas C. The synthesis and DNA/RNA hybridization properties of DNG, a putative antisense agent with an attractive polycationic guanidinium backbone. *NATO ASI Series, Series C: Mathematical and Physical Sciences* **1996**, *479*(DNA and RNA Cleavers and Chemotherapy of Cancer and Viral Diseases), 143-162.
441. D. Sengupta; A. Blasko; T. C. Bruice. A Microgonotropin Pentaaza Pentabutylamine and its Interactions with DNA. *Bioorganic and Med. Chem.* **1996**, *4*, 803.
442. R.O. Dempcy; Jia Luo and T.C. Bruice. Design and Synthesis of Ribonucleic Guanidine: A polycationic analog of RNA. *Proc. Natl. Acad. Sci (USA)* **1996**, *93*, 4326.
443. R. A. Torres; Ö. Almarsson and T. C. Bruice. Molecular Mechanics Calculations of the Riboacetal Internucleotide Linkage in Double and Triple Helices. *Proc. Natl. Acad. Sci (USA)* **1996**, *93*, 6875.
446. A. Blasko; R. O. Dempcy; E. E. Minyat & T. C. Bruice. Association of Short Strand DNA Oligomers with Guanidinium Linked Nucleosides (DNG). A Kinetic and Thermodynamic Study. *J. Am. Chem. Soc.* **1996**, *118*, 7892.
447. T. C. Bruice; A. Tsubouchi; R. O. Dempcy and L. P. Olson. One and Two Metal Ion Catalysis of the Hydrolysis of Adenosine-3'-(alkyl)phosphate esters. Models for One and Two Metal Ion Catalysis of RNA Hydrolysis. *J. Am. Chem. Soc.* **1996**, *118*, 9867.
448. T. C. Bruice; D. Sengupta; A. Blasko; S-Y. Chiang; & T. A. Beerman. A Microgonotropin Branched Decaaza Decabutylamine and its Interactions with DNA & DNA/Transcription Factor Interactions. *Bioorganic and Med. Chem.* **1997**, *5*, 685.
449. S.-Y. Chiang; T. C. Bruice; J. C. Azizkhan; L. Gawron & T. Beerman. Targeting E2F1/DNA Complexes with Microgonotropin DNA Binding Agents. *Proc. Natl. Acad. Sci. (USA)* **1997**, *94*, 2811.
452. A. Blasko; E. E. Minyat; R. O. Dempcy & T. C. Bruice. Fidelity of Binding of the Guanidinium Nucleic Acid (DNG) d(Tg)<sub>4</sub>-T-azido with Short Strand DNA Oligomers {A5G3A5, GA4G3A4G, G2A3G3A3G2, G2A2G5A2G2} with a Guanidinium Linked (DNG) Nucleoside. A Kinetic and Thermodynamic Study. *Biochemistry* **1997**, *36*, 7821.
456. T. C. Bruice; Y-C. Yip; A. Blasko; M. E. Petyak; K. A. Browne & F. C. Lightstone. Design, Synthesis, Characterization of a Novel Hexa-azacyclophane and Interactions with d(CGCA3T3GCG), ctDNA and T4DNA. *Tetrahedron* **1997**, *53*, 8105.

468. D. P. Arya & T. C. Bruice. Replacement of the Negative Phosphodiester Linkages of DNA by Positive S-Methyl Thiourea Linkers: A Novel Approach to Putative Antisense Agents. *J. Am. Chem. Soc.* **1998**, *120*, 6619.
465. B. Linkletter & T. C. Bruice. Solid Phase Synthesis of Oligomeric Deoxynucleic Guanidine (DNG): A Polycationic Analogue of DNA. *Bioorganic & Med. Lett.* **1998**, *8*, 1285.
466. D. A. Barawkar; B. Linkletter & T. C. Bruice. Synthesis of Protected Guanidinium Linked Dinucleoside for Incorporable into an Oligonucleotide Using Solid Phase DNA Methodology. *Bioorganic & Med. Lett.* **1998**, *8*, 1517.
471. D. A. Barawkar & T. C. Bruice. Synthesis, biological properties and nuclease resistance properties of mixed backbone oligodeoxynucleotides containing cationic internucleoside guanidinium linkages: DNG/DNA chimeras. *Proc. Natl. Acad. Sci. (USA)* **1998**, *95*, 11047.
476. D. P. Arya & T. C. Bruice. Positively Charged DeoxyNucleic MethylThioureas (DNmt): Synthesis and Binding Properties of Pentameric Thymidyl S-Methyl thiourea. *J. Am. Chem. Soc.* **1998**, *120*, 12419.
460. J. Luo & T. C. Bruice. Nanosecond Molecular Dynamics of Hybrid Triplex and Duplex of Polycation Deoxyribonucleic Guanidine (DNG) Strands with a Complimentary DNA Strand. *J. Am. Chem. Soc.* **1998**, *120*, 1115.
479. Linkletter, B. A.; Szabo, I. E.; Bruice, T. C. Solid-phase synthesis of deoxynucleic guanidine (DNG) oligomers and melting point and circular dichroism analysis of binding fidelity of octameric thymidyl oligomers with DNA oligomers. *J. Am. Chem. Soc.* **1999**, *121*, 3888–3896.
480. Arya, D. P.; Bruice, T. C. Triple-helix formation of DNA oligomers with methylthiourea-linked nucleosides (DNmt): A kinetic and thermodynamic analysis. *Proc. Natl. Acad. Sci. (USA)* **1999**, *96*, 4384–4389.
481. Blaskó, A.; Bruice, T. C. Recent studies of nucleophilic, general-acid, and metal ion catalysis of phosphate diester hydrolysis. *Acc. Chem. Res.* **1999**, *32*, 475–484.
486. Barawkar, D. A.; Bruice, T. C. Deoxynucleic guanidines/PNA (DNG/PNA) chimeras: oligonucleoside analogues containing cationic guanidinium and neutral amide linkages. *J. Am. Chem. Soc.* **1999**, *121*, 10418–10419.
487. Arya, D. P.; Bruice, T. C. Fidelity of deoxynucleic S–methylthiourea (DNmt) binding to DNA oligomers: influence of C mismatches. *J. Am. Chem. Soc.* **1999**, *121*, 10680–10684.
489. Satz, A. L.; Bruice, T. C. Synthesis of fluorescent microgonotropen (FMGT–1) and its interactions with the dodecamer d(CCGGAATTCCGG). *Bioorg. Med. Chem. Lett.* **1999**, *9*, 3261–3266.
491. Kojima, N.; Bruice, T. C. Replacement of the phosphodiester linkages of RNA with guanidinium linkages: The solid-phase synthesis of ribonucleic guanidine. *Org. Lett.* **2000**, *2*, 81–84.

496. Arya, D. P.; Bruice, T. C. Solid-phase synthesis of oligomeric deoxynucleic-thiourea (DNT) and deoxynucleic S-methylthiourea (DNmt): a neutral/polycationic analogue of DNA. *Bioorg. Med. Chem. Lett.* **2000**, *10*, 691-693.
498. Linkletter, B. A.; Bruice, T. C. Solid-phase synthesis of positively charged deoxynucleic guanidine (DNG) modified oligonucleotides containing neutral urea linkages: effect of charge deletions on binding and fidelity. *Bioorg. Med. Chem.* **2000**, *8*, 1893-1901.
499. Barakar, D. A.; Kwok, Y.; Bruice, T. W. and Bruice, T. C. Deoxynucleic Guanidine/Peptide Nucleic Acid Chimeras: Synthesis, Binding and Invasion Studies with DNA. *J. Am. Chem Soc.* **2000**, *122*, 5244.
502. Satz, A. L. & Bruice, T. C. Synthesis of Fluorescent Microgonotropens (FMGTs) and Their Interactions with dsDNA. *Bioorg. Med. Chem.* **2000**, *8*, 1871-1880.
507. Satz, A. L. & Bruice, T. C. Recognition of nine base pairs in the minor groove of dsDNA by a Tripyrrole Peptide-Hoechst Conjugate. *J. Am. Chem. Soc.* **2001**, *123*, 2469-2477.
508. Linkletter, B.; Szabo, I. E. and Bruice, T. C. Solid phase synthesis of oligopurine deoxynucleic guanidine (DNG) and analysis of binding with DNA oligomers. *Nucleic Acid Res.* **2001**, *29*, 2370-2376.
509. Satz, L. S.; White, C. M.; Beerman, T. A. & Bruice, T. C. Double -stranded DNA binding characteristics and subcellular distribution of a minor groove binding diphenylether bisbenzimidazole. *Biochemistry* **2001**, *40*, 6465-6467.
511. White, C. M.; Satz, A. L.; Bruice, T. C. & Beerman, T. A. Inhibition of transcription factor-DNA complexes and gene expression by a novel microgonotropen. *Proc. Natl. Acad. (USA)* **2001**, *98*, 10590-10595.
512. Challa, H. & Bruice, T. C. Incorporation of positively charged deoxynucleic S-methylthiourea linkages into oligonucleotides: Synthesis and characterization of DNmt/DNA chimera. *Bioorg. Med. Chem. Lett.* **2001**, *11*, 2423-2427.
515. White, C. M.; Satz, A. L.; Gawron, L. S.; Bruice, T. C. & Beerman, T. A. Inhibiting transcription factor/DNA complexes using fluorescent microgonotropens. *Biochemica et Biophysica Acta gene expression.* **2001**, *1574*, 100-108.
516. Satz, L. S. & Bruice, T. C. Recognition of nine base pair sequence in the minor groove of DNA at subpicomolar concentrations by a novel microgonotropen. *Bioorg. & Med. Chem.* **2002**, *10*, 241-262.
517. Kojima, N.; Szabo, I. E. & Bruice, T. C. Synthesis of ribonucleic guanidine: Replacement of the negative phosphodiester linkages of RNA with positive guanidinium linkages. *Tetrahedron* **2002**, *58*, 867-879.
518. Satz, L. S. & Bruice, T. C. Recognition in the Minor Groove of double-stranded DNA by microgonotropens. *Acc. Chem. Res.* **2002**, *35*, 86-95.
532. Reddy, P. M. & Bruice, T. C. Solid phase synthesis of positively charged deoxynucleic guanidine (DNG) oligonucleotide mixed sequences. *Bioorg. & Med. Chem. Lett.* **2003**, 1281-1285.

536. Reddy, P. M., Jindra, P., Satz, L. S. & Bruice, T. C.. Sequence selective recognition in the minor groove of dsDNA by pyrrole, imidazole-Hochst conjugates. *J. Am. Chem. Soc.*, **2003**, *125*, 7843-7848.
544. Challa, H. & Bruice, T. C., Deoxynucleic Guanidine: Synthesis and incorporation of purine nucleosides into positively charged DNG oligonucleotides. *Bioorganic & Med. Chem. Lett.*, **2004**, *12*, 1475-1481.
548. Reddy, P.M. and Bruice, T.C., Solid-Phase Synthesis of Positively Charged Deoxynucleic Guanidine (DNG) Tethering a Hoechst 33258 Analogue: Triplex and Duplex Stabilization by Simultaneous Minor Groove Binding. *J. Am. Chem. Soc.* **2004**, *126*, 3736-3747.
550. Szabo, I. & Bruice, T. C., DNG Cytidine: Synthesis and binding properties of octomeric guanidinium-linked deoxycytidine oligomer. *Bioorganic & Med. Chem.*, **2004**, *12*, 4233-4244.
551. Reddy, M. P., Dexter, R. & Bruice, T.C., DNA sequence recognition in the minor groove by hairpin pyrrole polyamide-Hochst 33258 analog conjugate. *Bioorganic & Med. Chem. Lett.*, **2004**, *14*, 3803-3807.