BIO

The overarching goal of the Herschlag Lab is to understand the fundamental behavior of RNA and proteins and, in turn, how these behaviors determine and impact biology more broadly. We are particularly interested in questions of how enzymes work, how RNA folds, how proteins recognize RNA, and the roles of RNA/protein interactions in regulation and control, and the evolution of molecules and molecular interactions. The lab takes an interdisciplinary approach, spanning and integrating physics, chemistry and biology, and employing a wide range of techniques.

ACADEMIC APPOINTMENTS

• Professor, Biochemistry
• Professor (By courtesy), Chemical Engineering
• Member, Bio-X
• Faculty Fellow, Sarafan ChEM-H
• Member, Stanford Cancer Institute

ADMINISTRATIVE APPOINTMENTS

• Senior Associate Dean of Graduate Education and Postdoctoral Affairs, School of Medicine, (2011-2015)

HONORS AND AWARDS

• Member, American Academy of Arts and Sciences (2023)
• Stein and Moore Award, Protein Society (2022)
• Founders Award, Biophysical Society (2020)
• Excellence in Mentoring and Service Award, Stanford University Biosciences (2019)
• Member, National Academy of Sciences (2018)
• Student Service Faculty Award, Biochemistry, Stanford School of Medicine (2012)
• William Rose Award, ASBMB (2010)
• Fellow, AAAS (2005)
• Merit Award, NIH (2002)
• Cope Scholar Award, ACS (2000)
• Established Investigator, AHA (1998-2002)
• Pfizer Award for Enzyme Chemistry, ACS (1997)
• Fellowship in Science and Engineering, David and Lucile Packard (1995-2000)
• Scholar, Searle (1993-1996)
• Scholar in Biomedical Science, Lucille P. Markey (1990-1997)
• Postdoctoral Fellowship, Helen Hay Whitney (1989-1990; Colorado)
• Fellowship, Gillette Foundation (1986-1987; Brandeis)
• Award in Biochemistry, American Institute of Chemists (1982; SUNY)
• Award for Excellence in Biochemistry, SUNY (1982)
• Phi Beta Kappa, Michigan (1979)
• Scholar, James B. Angell (1978, 1979; Michigan)

LINKS
• Herschlag lab website: http://herschlaglab.stanford.edu

Research & Scholarship

CURRENT RESEARCH AND SCHOLARLY INTERESTS
The overarching goal of the Herschlag Lab is to understand the fundamental behavior of RNA and proteins and, in turn, how these behaviors determine and impact biology more broadly. We are particularly interested in questions of how enzymes work, how RNA folds, how proteins recognize RNA, and the roles of RNA/protein interactions in regulation and control, and the evolution of molecules and molecular interactions. The lab takes an interdisciplinary approach, spanning and integrating physics, chemistry and biology, and employing a wide range of techniques.

Teaching

COURSES

2023-24
• A Practical Guide to Success in Science: BIOS 246 (Win)
• Biochemistry Mini-Course: BIOC 202 (Aut)
• Developing an Original Research Proposal: BIOC 360 (Spr)

2022-23
• A Practical Guide to Success in Science: BIOS 246 (Win)
• Biochemistry Mini-Course: BIOC 202 (Aut)
• Developing an Original Research Proposal: BIOC 360 (Spr)
• Understanding Kinetics for Biologists and Biology: BIOS 202 (Aut)

2021-22
• Biochemistry Mini-Course: BIOC 202 (Aut)
• Chemistry for Biologists and Others: BIOC 294, BIOS 294 (Aut)

2020-21
• Becoming a Resilient Scientist: BIO 315 (Win, Spr)
• Biochemistry Mini-Course: BIOC 202 (Aut)
• Chemistry for Biologists and Others: BIOC 294, BIOS 294 (Aut)
• Connections: Life, Science, and, Community: BIOC 227 (Win, Spr)
• Understanding Kinetics for Biologists and Biology: BIOS 202 (Sum)

STANFORD ADVISEES

**Doctoral Dissertation Reader (AC)**

Nicole DelRosso

**Postdoctoral Faculty Sponsor**

Patrick Almhjell, Shawn Costello, Lauren Hagler, Albert Lee

**Doctoral Dissertation Advisor (AC)**

Siyuan Du, John Shin, Gabriel Tauber

**Doctoral Dissertation Co-Advisor (AC)**

Eliel Akinbami

GRADUATE AND FELLOWSHIP PROGRAM AFFILIATIONS

• Biochemistry (Phd Program)
• Biophysics (Phd Program)

**Publications**

**PUBLICATIONS**

• Decoupling of catalysis and transition state analog binding from mutations throughout a phosphatase revealed by high-throughput enzymology. *Proceedings of the National Academy of Sciences of the United States of America*
  Markin, C. J., Mokhtari, D. A., Du, S., Doukov, T., Sunden, F., Cook, J. A., Fordyce, P. M., Herschlag, D.  
  2023; 120 (29): e2219074120

• **Author Correction**: RNA conformational propensities determine cellular activity. *Nature*
  Ken, M. L., Roy, R., Geng, A., Ganser, L. R., Manghrani, A., Cullen, B. R., Schulze-Gahmen, U., Herschlag, D., Al-Hashimi, H. M.  
  2023

• RNA conformational propensities determine cellular activity. *Nature*
  Ken, M. L., Roy, R., Geng, A., Ganser, L. R., Manghrani, A., Cullen, B. R., Schulze-Gahmen, U., Herschlag, D., Al-Hashimi, H. M.  
  2023

• Refinement of Multiconformer Ensemble Models from Multi-temperature X-ray Diffraction Data. *bioRxiv : the preprint server for biology*
  Du, S., Wankowicz, S. A., Yabukarski, F., Doukov, T., Herschlag, D., Fraser, J. S.  
  2023

• Obtaining anomalous and ensemble information from protein crystals from 220 K up to physiological temperatures. *Acta crystallographica. Section D, Structural biology*
  Doukov, T., Herschlag, D., Yabukarski, F.  
  2023; 79 (Pt 3): 212-223

• Building a quantitative and predictive model of 5′ SS selection by human U1 snRNP using RNA-map
  White, D. S., Carrocci, T. J., Shin, J., Lin, C., Black, D. L., Greenleaf, W., Herschlag, D., Hoskins, A. A.
  CELL PRESS.2023: 219A

• Building a quantitative and predictive model of 5′SS selection by human U1 snRNP using RNA-map. *Biophysical journal*
  White, D. S., Carrocci, T. J., Shin, J., Lin, C., Black, D. L., Greenleaf, W., Herschlag, D., Hoskins, A. A.
• Refinement of multi-conformer ensemble models from multi-temperature X-ray diffraction data. *Methods in enzymology*
  Du, S., Wankowicz, S. A., Yabukarski, F., Doukov, T., Herschlag, D., Fraser, J. S.
  2023; 688: 223-254

• Ensemble-function relationships to dissect mechanisms of enzyme catalysis. *Science advances*
  Yabukarski, F., Doukov, T., Pinney, M. M., Biel, J. T., Fraser, J. S., Herschlag, D.
  2022; 8 (41): eabn7738

• A comprehensive thermodynamic model for RNA binding by the Saccharomyces cerevisiae Pumilio protein PUF4. *Nature communications*
  Sadee, C., Hagler, L. D., Becker, W. R., Jarmoskaite, I., Vaidyanathan, P. P., Denny, S. K., Greenleaf, W. J., Herschlag, D.
  2022; 13 (1): 4522

• Evaluating the impact of X-ray damage on conformational heterogeneity in room-temperature (277 K) and cryo-cooled protein crystals. *Acta crystallographica. Section D, Structural biology*
  Yabukarski, F., Doukov, T., Mokhtari, D. A., Du, S., Herschlag, D.
  2022; 78 (Pt 8): 945-963

• Ensemble-function relationships to connect structure to mechanism: application of EnsemblePDB to the serine protease reaction coordinate and its catalytic features
  Du, S., Kretsch, R. C., Parres-Gold, J., Penaherrera, D. A., Yabukarski, F., Pinney, M. M., Herschlag, D.
  CELL PRESS.2022: 441A

• Direct Measurement of Interhelical DNA Repulsion and Attraction by Quantitative Cross-Linking. *Journal of the American Chemical Society*
  Hamilton, I., Gebala, M., Herschlag, D., Russell, R.
  1800

• Systematic investigation of the link between enzyme catalysis and cold adaptation *ELIFE*
  Stark, C. D., Bautista-Leung, T., Siegfried, J., Herschlag, D.
  2022; 11

• Systematic investigation of the link between enzyme catalysis and cold adaptation. *eLife*
  Stark, C., Bautista-Leung, T., Siegfried, J., Herschlag, D.
  1800; 11

• uPIC-M: Efficient and Scalable Preparation of Clonal Single Mutant Libraries for High-Throughput Protein Biochemistry. *ACS omega*
  Appel, M. J., Longwell, S. A., Morri, M., Neff, N., Herschlag, D., Fordyce, P. M.
  2021; 6 (45): 30542-30554

• Cation enrichment in the ion atmosphere is promoted by local hydration of DNA. *Physical chemistry chemical physics : PCCP*
  Ma, C. Y., Pezzotti, S., Schwaab, G., Gebala, M., Herschlag, D., Havenith, M.
  2021

• High throughput and quantitative enzymology in the genomic era. *Current opinion in structural biology*
  Mokhtari, D. A., Appel, M. J., Fordyce, P. M., Herschlag, D.
  2021; 71: 259-273

• High-throughput dissection of the thermodynamic and conformational properties of a ubiquitous class of RNA tertiary contact motifs. *Proceedings of the National Academy of Sciences of the United States of America*
  Bonilla, S. L., Denny, S. K., Shin, J. H., Alvarez-Buylla, A., Greenleaf, W. J., Herschlag, D.
  2021; 118 (33)

• Revealing enzyme functional architecture via high-throughput microfluidic enzyme kinetics. *Science (New York, N.Y.)*
  Markin, C. J., Mokhtari, D. A., Sunden, F., Appel, M. J., Akiva, E., Longwell, S. A., Sabatti, C., Herschlag, D., Fordyce, P. M.
  2021; 373 (6553)

• Revealing enzyme functional architecture via high-throughput microfluidic enzyme kinetics *SCIENCE*
  Markin, C. J., Mokhtari, D. A., Sunden, F., Appel, M. J., Akiva, E., Longwell, S. A., Sabatti, C., Herschlag, D., Fordyce, P. M.
  2021; 373 (6553): 411+
• Parallel molecular mechanisms for enzyme temperature adaptation. *Science (New York, N.Y.)*
Pinney, M. M., Mokhtari, D. A., Akiva, E., Yabukarski, F., Sanchez, D. M., Liang, R., Doukov, T., Martinez, T. J., Babbitt, P. C., Herschlag, D.
2021; 371 (6533)

• Assessment of enzyme active site positioning and tests of catalytic mechanisms through X-ray-derived conformational ensembles. *Proceedings of the National Academy of Sciences of the United States of America*
Yabukarski, F., Biel, J. T., Pinney, M. M., Doukov, T., Powers, A. S., Fraser, J. S., Herschlag, D.
2020; 117 (52): 33204–15

• Instrumentation and experimental procedures for robust collection of X-ray diffraction data from protein crystals across physiological temperatures. *Journal of applied crystallography*
Doukov, T., Herschlag, D., Yabukarski, F.
2020; 53 (Pt 6): 1493–1501

• Rapid and accurate determination of atomistic RNA dynamic ensemble models using NMR and structure prediction. *Nature communications*
Shi, H., Rangadurai, A., Abou Assi, H., Roy, R., Case, D. A., Herschlag, D., Yesselman, J. D., Al-Hashimi, H. M.
2020; 11 (1): 5531

• The individual and the team in collaborative science. *Proceedings of the National Academy of Sciences of the United States of America*
Herschlag, D.
2020; 117 (28): 16116

• The structural ensemble of a Holliday junction determined by X-ray scattering interference. *Nucleic acids research*
Zettl, T., Shi, X., Bonilla, S., Sedlak, S. M., Lipfert, J., Herschlag, D.
2020

• Slow Molecular Recognition by RNA
Sengupta, R., Herschlag, D.
WILEY.2020

• Biosciences Proposal Bootcamp: Structured peer and faculty feedback improves trainees' proposals and grantsmanship self-efficacy. *PloS one*
Botham, C. M., Brawn, S. n., Steele, L. n., Barrón, C. B., Kleppner, S. R., Herschlag, D. n.
2020; 15 (12): e0243973

• How to measure and evaluate binding affinities. *eLife*
Jarmoskaite, I. n., AlSadhan, I. n., Vaidyanathan, P. P., Herschlag, D. n.
2020; 9

• A Quantitative and Predictive Model for RNA Binding by Human Pumilio Proteins *MOLECULAR CELL*
Jarmoskaite, I., Denny, S. K., Vaidyanathan, P. P., Becker, W. R., Andreasson, J. L., Layton, C. J., Kappel, K., Shivashankar, V., Sreenivasan, R., Das, R., Greenleaf, W. J., Herschlag, D.
2019; 74 (5): 966–+

• Demonstration of protein cooperativity mediated by RNA structure using the human protein PUM2 *RNA*
Becker, W. R., Jarmoskaite, I., Vaidyanathan, P. P., Greenleaf, W. J., Herschlag, D.
2019; 25 (6): 702–12

• Blind tests of RNA-protein binding affinity prediction. *Proceedings of the National Academy of Sciences of the United States of America*
Kappel, K., Jarmoskaite, I., Vaidyanathan, P. P., Greenleaf, W. J., Herschlag, D., Das, R.
2019

• A Microfluidics-Based Assay for Mapping Connectivity in Highly Proficient Enzymes Reveals Functional Modularity
Markin, C. J., Mokhtari, D. A., Sunden, F., Herschlag, D., Fordyce, P. M.
CELL PRESS.2019: 66A

• Sequence-dependent RNA helix conformational preferences predictably impact tertiary structure formation. *Proceedings of the National Academy of Sciences of the United States of America*
Yesselman, J. D., Denny, S. K., Bisaria, N. n., Herschlag, D. n., Greenleaf, W. J., Das, R. n.
2019
• Quantitative Studies of an RNA Duplex Electrostatics by Ion Counting. *Biophysical journal*
  Gebala, M. n., Herschlag, D. n.
  2019

• Computational design of three-dimensional RNA structure and function. *Nature nanotechnology*
  Yesselman, J. D., Eiler, D. n., Carlson, E. D., Gotrik, M. R., d’Aquino, A. E., Ooms, A. N., Kladwang, W. n., Carlson, P. D., Shi, X. n., Costantino, D. A., Herschlag, D. n., Lucks, J. B., Jewett, et al
  2019

• Enhancement of RNA/Ligand Association Kinetics via an Electrostatic Anchor. *Biochemistry*
  Sengupta, R. N., Herschlag, D. n.
  2019

• The roles of structural dynamics in the cellular functions of RNAs. *Nature reviews. Molecular cell biology*
  Ganser, L. R., Kelly, M. L., Herschlag, D. n., Al-Hashimi, H. M.
  2019

• Ion counting demonstrates a high electrostatic field generated by the nucleosome. *eLife*
  Gebala, M. n., Johnson, S. L., Narlikar, G. J., Herschlag, D. n.
  2019; 8

• Serum electrolytes can promote hydroxyl radical-initiated biomolecular damage from inflammation. *Free radical biology & medicine*
  Komaki, Y. n., Simpson, A. M., Choe, J. K., Pinney, M. M., Herschlag, D. n., Chuang, Y. H., Mitch, W. A.
  2019; 141: 475–82

• Increasing the length of poly-pyrimidine bulges broadens RNA conformational ensembles with minimal impact on stacking energetics. *RNA*
  Merriman, D. K., Yuan, J., Shi, H., Majumdar, A., Herschlag, D., Al-Hashimi, H. M.
  2018; 24 (10): 1363–76

• The Story of RNA Folding, as Told in Epochs. *Cold Spring Harbor perspectives in biology*
  Herschlag, D., Bonilla, S., Bisaria, N.
  2018; 10 (10)

• Structural Coupling Throughout the Active Site Hydrogen Bond Networks of Ketosteroid Isomerase and Photoactive Yellow Protein *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Pinney, M. M., Natarajan, A., Yabukarski, F., Sanchez, D. M., Liu, F., Liang, R., Doukov, T., Schwans, J. P., Martinez, T. J., Herschlag, D.
  2018; 140 (31): 9827–43

• High-Throughput Investigation of Diverse Junction Elements in RNA Tertiary Folding. *Cell*
  Denny, S. K., Bisaria, N., Yesselman, J. D., Das, R., Herschlag, D., Greenleaf, W. J.
  2018

• Hydrogen Bonds: Simple after All? *BIOCHEMISTRY*
  Herschlag, D., Pinney, M. M.
  2018; 57 (24): 3338–52

• Recording and Analyzing Nucleic Acid Distance Distributions with X-Ray Scattering Interferometry (XSI). *Current protocols in nucleic acid chemistry*
  Zettl, T., Das, R., Harbury, P. A., Herschlag, D., Lipfert, J., Mathew, R. S., Shi, X.
  2018; 73 (1): e54

• Gold nanocrystal labels provide a sequence-to-3D structure map in SAXS reconstructions *SCIENCE ADVANCES*
  Zettl, T., Mathew, R. S., Shi, X., Doniach, S., Herschlag, D., Harbury, P. B., Lipfert, J.
  2018; 4 (5): eaa4418

• Hidden Structural Modules in a Cooperative RNA Folding Transition *CELL REPORTS*
  Gracia, B., Al-Hashimi, H. M., Bisaria, N., Das, R., Herschlag, D., Russell, R.
  2018; 22 (12): 3240–50

• Dissecting the Electrostatics of Nucleic Acids
  Gebala, M., Allred, B. E., Herschlag, D.
Differential catalytic promiscuity of the alkaline phosphatase superfamily bimetallo core reveals mechanistic features underlying enzyme evolution. *Journal of Biological Chemistry*

Sunden, F., AlSadhan, I., Lyubimov, A., Doukov, T., Swan, J., Herschlag, D.

2017; 292 (51): 20960–74

Slow molecular recognition by RNA. *RNA*

Gleitsman, K. R., Sengupta, R. N., Herschlag, D.

2017; 23 (12): 1745–53

Quantitative tests of a reconstitution model for RNA folding thermodynamics and kinetics. *Proceedings of the National Academy of Sciences of the United States of America*

Bisaria, N., Greenfeld, M., Limouse, C., Mabuchi, H., Herschlag, D.

2017; 114 (37): E7688–E7696

An Activator-Blocker Pair Provides a Controllable On-Off Switch for a Ketosteroid Isomerase Active Site Mutant. *Journal of the American Chemical Society*

Lamba, V., Yabukarski, F., Herschlag, D.

2017; 139 (32): 11089–95

Kemp Eliminase Activity of Ketosteroid Isomerase. *Biochemistry*

Lamba, V., Sanchez, E., Fanning, L. R., Howe, K., Alvarez, M. A., Herschlag, D., Forconi, M.

2017; 56 (4): 582-591

Pseudouridine and N-6 methyladenosine modifications weaken PUF protein/RNA interactions. *RNA (New York, N.Y.)*

Vaidyanathan, P. P., AlSadhan, I., Merriman, D. K., Al-Hashimi, H., Herschlag, D.

2017

Lessons from Enzyme Kinetics Reveal Specificity Principles for RNA-Guided Nucleases in RNA Interference and CRISPR-Based Genome Editing. *Cell systems*

Bisaria, N., Jarmoskaite, I., Herschlag, D.

2017; 4 (1): 21-29

Determination of the conformational ensemble of the TAR RNA by X-ray scattering interferometry. *Nucleic acids research*

Shi, X., Walker, P., Harbury, P. B., Herschlag, D.

2017

Single-Molecule Fluorescence Reveals Commonalities and Distinctions among Natural and in Vitro-Selected RNA Tertiary Motifs in a Multistep Folding Pathway. *Journal of the American Chemical Society*

Bonilla, S., Limouse, C., Bisaria, N., Gebala, M., Mabuchi, H., Herschlag, D.

2017: 18576-18589

Determination of Ion Atmosphere Effects on the Nucleic Acid Electrostatic Potential and Ligand Association Using AH+·C Wobble Formation in Double-Stranded DNA. *J. Am. Chem. Soc.*

Allred, B. E., Gebala, M., Herschlag, D.

2017; 22 (139): 7540-7548

Mechanistic and Evolutionary Insights from Comparative Enzymology of Phosphomonoesterases and Phosphodiesterases across the Alkaline Phosphatase Superfamily. *Journal of the American Chemical Society*

Sunden, F., AlSadhan, I., Lyubimov, A. Y., Ressl, S., Wiersma-Koch, H., Borland, J., Brown, C. L., Johnson, T. A., Singh, Z., Herschlag, D.

2016; 138 (43): 14273-14287

RNA Structural Modules Control the Rate and Pathway of RNA Folding and Assembly. *Journal of Molecular Biology*

Gracia, B., Xue, Y., Bisaria, N., Herschlag, D., Al-Hashimi, H. M., Russell, R.

2016; 428 (20): 3972-3985

Does Cation Size Affect Occupancy and Electrostatic Screening of the Nucleic Acid Ion Atmosphere? *Journal of the American Chemical Society*

Gebala, M., Bonilla, S., Bisaria, N., Herschlag, D.

2016; 138 (34): 10925-10934
Kinetic and thermodynamic framework for P4-P6 RNA reveals tertiary motif modularity and modulation of the folding preferred pathway. Proceedings of the National Academy of Sciences of the United States of America
Bisaria, N., Greenfeld, M., Limouse, C., Pavlichin, D. S., Mabuchi, H., Herschlag, D.
2016; 113 (34): E4956-65

Evaluation of the Catalytic Contribution from a Positioned General Base in Ketosteroid Isomerase. Journal of the American Chemical Society
Lamba, V., Yabukarski, F., Pinney, M., Herschlag, D.
2016; 138 (31): 9902-9909

Tungstate as a Transition State Analog for Catalysis by Alkaline Phosphatase JOURNAL OF MOLECULAR BIOLOGY
Peck, A., Sunden, F., Andrews, L. D., Pande, V. S., Herschlag, D.
2016; 428 (13): 2758-2768

Correction to "Evaluating the Catalytic Contribution from the Oxyanion Hole in Ketosteroid Isomerase". Journal of the American Chemical Society
Schwans, J. P., Sunden, F., Gonzalez, A., Tsai, Y., Herschlag, D.
2016; 138 (24): 7801-7802

Visualizing the formation of an RNA folding intermediate through a fast highly modular secondary structure switch NATURE COMMUNICATIONS
Xue, Y., Gracia, B., Herschlag, D., Russell, R., Al-Hashimi, H. M.
2016; 7

The solution structural ensembles of RNA kink-turn motifs and their protein complexes. Nature chemical biology
Shi, X., Huang, L., Lilley, D. M., Harbury, P. B., Herschlag, D.
2016; 12 (3): 146-152

High-throughput analysis and protein engineering using microcapillary arrays. Nature chemical biology
Chen, B., Lim, S., Kannan, A., Alford, S. C., Sunden, F., Herschlag, D., Dimov, I. K., Baer, T. M., Cochran, J. R.
2016; 12 (2): 76-81

An active site rearrangement within the Tetrahymena group I ribozyme releases nonproductive interactions and allows formation of catalytic interactions. RNA
Sengupta, R. N., Van Schie, S. N., Giambasu, G., Dai, Q., Yesselman, J. D., York, D., Piccirilli, J. A., Herschlag, D.
2016; 22 (1): 32-48

Differential Assembly of Catalytic Interactions within the Conserved Active Sites of Two Ribozymes. PloS one
Van Schie, S. N., Sengupta, R. N., Herschlag, D.
2016; 11 (8)

Cation-Anion Interactions within the Nucleic Acid Ion Atmosphere Revealed by Ion Counting. Journal of the American Chemical Society
Gebala, M., Giambasu, G. M., Lipfert, J., Bisaria, N., Bonilla, S., Li, G., York, D. M., Herschlag, D.
2015; 137 (46): 14705-14715

Evolutionary Conservation and Diversification of Puf RNA Binding Proteins and Their mRNA Targets PLOS BIOLOGY
Hogan, G. J., Brown, P. O., Herschlag, D.
2015; 13 (11)

Comment on "Extreme electric fields power catalysis in the active site of ketosteroid isomerase" SCIENCE
Natarajan, A., Yabukarski, F., Lamba, V., Schwans, J. P., Sunden, F., Herschlag, D.
2015; 349 (6251)

Determination of Hydrogen Bond Structure in Water versus Aprotic Environments To Test the Relationship Between Length and Stability JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
Sigala, P. A., Ruben, E. A., Liu, C. W., Piccoli, P. M., Hohenstein, E. G., Martinez, T. J., Schultz, A. J., Herschlag, D.
2015; 137 (17): 5730-5740

Extensive site-directed mutagenesis reveals interconnected functional units in the alkaline phosphatase active site ELIFE
Sunden, F., Peck, A., Salzman, J., Ressl, S., Herschlag, D.
2015; 4

Learning from ribozymes RNA-A PUBLICATION OF THE RNA SOCIETY
Herschlag, D.
2015; 21 (4): 527-528

- **Probing the kinetic and thermodynamic consequences of the tetraloop/tetraloop receptor monovalent ion-binding site in P4-P6 RNA by smFRET** *BIOCHEMICAL SOCIETY TRANSACTIONS*
  Bisaria, N., Herschlag, D.
  2015; 43: 172-178

- **From static to dynamic: the need for structural ensembles and a predictive model of RNA folding and function** *CURRENT OPINION IN STRUCTURAL BIOLOGY*
  Herschlag, D., Allred, B. E., Gowrishankar, S.
  2015; 30: 125-133

- **Three aSNAP and 10 ATP Molecules Are Used in SNARE Complex Disassembly by N-ethylmaleimide-sensitive Factor (NSF).** *journal of biological chemistry*
  Shah, N., Colbert, K. N., Enos, M. D., Herschlag, D., Weis, W. I.
  2015; 290 (4): 2175-2188

- **Quantifying Nucleic Acid Ensembles with X-ray Scattering Interferometry.** *Methods in enzymology*
  Shi, X., Bonilla, S., Herschlag, D., Harbury, P.
  2015; 558: 75-97

- **Single-molecule dataset (SMD): a generalized storage format for raw and processed single-molecule data.** *BMC bioinformatics*
  Greenfeld, M., van de Meent, J., Pavlitchin, D. S., Mabuchi, H., Wiggins, C. H., Gonzalez, R. L., Herschlag, D.
  2015; 16: 3-?

- **Probing the Origins of Catalytic Discrimination between Phosphate and Sulfate Monoester Hydrolysis: Comparative Analysis of Alkaline Phosphatase and Protein Tyrosine Phosphatases** *BIOCHEMISTRY*
  Andrews, L. D., Zalatan, J. G., Herschlag, D.
  2014; 53 (43): 6811-6819

- **A kinetic and thermodynamic framework for the Azoarcus group I ribozyme reaction** *RNA-A PUBLICATION OF THE RNA SOCIETY*
  Gleitsman, K. R., Herschlag, D. H.
  2014; 20 (11): 1732-1746

- **Understanding nucleic Acid-ion interactions.** *Annual review of biochemistry*
  Lipfert, J., Doniach, S., Das, R., Herschlag, D.
  2014; 83: 813-841

- **Using unnatural amino acids to probe the energetics of oxyanion hole hydrogen bonds in the ketosteroid isomerase active site.** *Journal of the American Chemical Society*
  Natarajan, A., Schwans, J. P., Herschlag, D.
  2014; 136 (21): 7643-7654

- **Assembly line polyketide synthases: mechanistic insights and unsolved problems.** *Biochemistry*
  Khosla, C., Herschlag, D., Cane, D. E., Walsh, C. T.
  2014; 53 (18): 2875-2883

- **Roles of Long-Range Tertiary Interactions in Limiting Dynamics of the Tetrahymena Group I Ribozyme** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Shi, X., Bisaria, N., Benz-Moy, T. L., Bonilla, S., Pavlitchin, D. S., Herschlag, D.
  2014; 136 (18): 6643-6648

- **Experimental and Computational Mutagenesis To Investigate the Positioning of a General Base within an Enzyme Active Site** *BIOCHEMISTRY*
  Schwans, J. P., Hanoian, P., Lengerich, B. J., Sunden, F., Gonzalez, A., Tsai, Y., Hammes-Schiffer, S., Herschlag, D.
  2014; 53 (15): 2541-2555

- **From a structural average to the conformational ensemble of a DNA bulge.** *Proceedings of the National Academy of Sciences of the United States of America*
  Shi, X., Beauchamp, K. A., Harbury, P. B., Herschlag, D.
  2014; 111 (15): E1473-80
• Ion Counting from Explicit-Solvent Simulations and 3D-RISM [BIOPHYSICAL JOURNAL]
  Giambasu, G. M., Luchko, T., Herschlag, D., York, D. M., Case, D. A.
  2014; 106 (4): 883-894

• Site-Directed Mutagenesis Maps Interactions That Enhance Cognate and Limit Promiscuous Catalysis by an Alkaline Phosphatase Superfamily Phosphodiesterase [BIOCHEMISTRY]
  Wiersma-Koch, H., Sunden, F., Herschlag, D.
  2013; 52 (51): 9167-9176

• Uncovering the Determinants of a Highly Perturbed Tyrosine pKa in the Active Site of Ketosteroid Isomerase. [Biochemistry]
  Schwans, J. P., Sunden, F., Gonzalez, A., Tsai, Y., Herschlag, D.
  2013; 52 (44): 7840-7855

• The stanford institute for chemical biology. [ACS chemical biology]
  Chen, J. K., Du Bois, J., Glenn, J., Herschlag, D., Khosla, C.
  2013; 8 (9): 1860-1861

• Use of anion-aromatic interactions to position the general base in the ketosteroid isomerase active site [PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA]
  Schwans, J. P., Sunden, F., Lassila, J. K., Gonzalez, A., Tsai, Y., Herschlag, D.
  2013; 110 (28): 11308-11313

• Quantitative dissection of hydrogen bond-mediated proton transfer in the ketosteroid isomerase active site [PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA]
  Sigala, P. A., Fafarman, A. T., Schwans, J. P., Fried, S. D., Fenn, T. D., Caaveiro, J. M., Pybus, B., Ringe, D., Petsko, G. A., Boxer, S. G., Herschlag, D.
  2013; 110 (28): E2552-E2561

• Ground State Destabilization by Anionic Nucleophiles Contributes to the Activity of Phosphoryl Transfer Enzymes [PLOS BIOLOGY]
  Andrews, L. D., Fenn, T. D., Herschlag, D.
  2013; 11 (7)

• Structural ensemble and microscopic elasticity of freely diffusing DNA by direct measurement of fluctuations. [Proceedings of the National Academy of Sciences of the United States of America]
  Shi, X., Herschlag, D., Harbury, P. A.
  2013; 110 (16): E1444-E1451

• Fundamental challenges in mechanistic enzymology: progress toward understanding the rate enhancements of enzymes. [Biochemistry]
  Herschlag, D., Natarajan, A.
  2013; 52 (12): 2050-2067

• Ground State Destabilization from a Positioned General Base in the Ketosteroid Isomerase Active Site [BIOCHEMISTRY]
  Ruben, E. A., Schwans, J. P., Sonnett, M., Natarajan, A., Gonzalez, A., Tsai, Y., Herschlag, D.
  2013; 52 (6): 1074-1081

• Nucleic Acid Conformation Ensembles Revealed by Au-SAXS Interferometry [57th Annual Meeting of the Biophysical-Society]
  Shi, X., Harbury, P., Herschlag, D.
  CELL PRESS.2013: 502A–502A

• RNA radiolabeling. [Methods in enzymology]
  Porecha, R., Herschlag, D.
  2013; 530: 255-279

• Fluorescently Labeling Synthetic RNAs. [Methods in enzymology]
  Greenfeld, M., Herschlag, D.
  2013; 530: 281-297

• Salt dependence of the radius of gyration and flexibility of single-stranded DNA in solution probed by small-angle x-ray scattering [PHYSICAL REVIEW E]
  Sim, A. Y., Lipfert, J., Herschlag, D., Doniach, S.
  2012; 86 (2)
• Metal-ion rescue revisited: Biochemical detection of site-bound metal ions important for RNA folding. *RNA-A PUBLICATION OF THE RNA SOCIETY*
  Frederiksen, J. K., Li, N., Das, R., Herschlag, D., Piccirilli, J. A.
  2012; 18 (6): 1123-1141

• Exploring purine N7 interactions via atomic mutagenesis: The group I ribozyme as a case study. *RNA-A PUBLICATION OF THE RNA SOCIETY*
  Forconi, M., Benz-Moy, T., Gleitsman, K. R., Ruben, E., Metz, C., Herschlag, D.
  2012; 18 (6): 1222-1229

• Robust design and optimization of retroalldol enzymes. *PROTEIN SCIENCE*
  Althoff, E. A., Wang, L., Jiang, L., Giger, L., Lassila, J. K., Wang, Z., Smith, M., Hari, S., Kast, P., Herschlag, D., Hilvert, D., Baker, D.
  2012; 21 (5): 717-726

• Electrostatics of Nucleic Acid Folding under Conformational Constraint. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Anthony, P. C., Sim, A. Y., Chu, V. B., Doniach, S., Block, S. M., Herschlag, D.
  2012; 134 (10): 4607-4614

• Single Molecule Analysis Research Tool (SMART): An Integrated Approach for Analyzing Single Molecule Data. *PLOS ONE*
  Greenfeld, M., Pavlichin, D. S., Mabuchi, H., Herschlag, D.
  2012; 7 (2)

• Thermodynamic evidence for negative charge stabilization by a catalytic metal ion within an RNA active site. *ACS chemical biology*
  Sengupta, R. N., Herschlag, D., Piccirilli, J. A.
  2012; 7 (2): 294-299

• Quantitative, directional measurement of electric field heterogeneity in the active site of ketosteroid isomerase. *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Fafarman, A. T., Sigala, P. A., Schwans, J. P., Fenn, T. D., Herschlag, D., Boxer, S. G.
  2012; 109 (6): E299-E308

• A Role for a Single-Stranded Junction in RNA Binding and Specificity by the Tetrahymena Group I Ribozyme. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Shi, X., Solomatin, S. V., Herschlag, D.
  2012; 134 (4): 1910-1913

• High-Resolution Analysis of Zn2+ Coordination in the Alkaline Phosphatase Superfamily by EXAFS and X-ray Crystallography. *JOURNAL OF MOLECULAR BIOLOGY*
  Bobyr, E., Lassila, J. K., Wiersma-Koch, H. I., Fenn, T. D., Lee, J. J., Nikolic-Hughes, I., Hodgson, K. O., Rees, D. C., Hedman, B., Herschlag, D.
  2012; 415 (1): 102-117

• Evaluating the Catalytic Contribution from the Oxyanion Hole in Ketosteroid Isomerase. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Schwans, J. P., Sunden, F., Gonzalez, A., Tsai, Y., Herschlag, D.
  2011; 133 (50): 20052-20055

• Structure-Function Analysis from the Outside In: Long-Range Tertiary Contacts in RNA Exhibit Distinct Catalytic Roles. *BIOCHEMISTRY*
  Benz-Moy, T. L., Herschlag, D.
  2011; 50 (40): 8733-8755

• 2'-Fluoro Substituents Can Mimic Native 2'-Hydroxyls within Structured RNA. *CHEMISTRY & BIOLOGY*
  Forconi, M., Schwans, J. P., Porecha, R. H., Sengupta, R. N., Piccirilli, J. A., Herschlag, D.
  2011; 18 (8): 949-954

• Isotope-Edited FTIR of Alkaline Phosphatase Resolves Paradoxical Ligand Binding Properties and Suggests a Role for Ground-State Destabilization. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Andrews, L. D., Deng, H., Herschlag, D.
  2011; 133 (30): 11621-11631

• Removal of Covalent Heterogeneity Reveals Simple Folding Behavior for P4-P6 RNA. *JOURNAL OF BIOLOGICAL CHEMISTRY*
  Greenfeld, M., Solomatin, S. V., Herschlag, D.
  2011; 286 (22): 19872-19879
• Implications of molecular heterogeneity for the cooperativity of biological macromolecules  
  Solomatin, S. V., Greenfeld, M., Herschlag, D.  
  2011; 18 (6): 732-734

• Tightening of Active Site Interactions En Route to the Transition State Revealed by Single-Atom Substitution in the Guanosine-Binding Site of the Tetrahymena Group I Ribozyme  
  Forconi, M., Porecha, R. H., Piccirilli, J. A., Herschlag, D.  
  2011; 133 (20): 7791-7800

• Identification of RNA recognition elements in the Saccharomyces cerevisiae transcriptome  
  Riordan, D. P., Herschlag, D., Brown, P. O.  
  2011; 39 (4): 1501-1509

• RNA Structure, Function, and (Thermo-) Dynamics: A SAXS and Single-Molecule Perspective  
  Lipfert, J., Herschlag, D., Doniach, S., Dekker, N. H.  
  2011; 55th Annual Meeting of the Biophysical-Society

• Biological Phosphoryl-Transfer Reactions: Understanding Mechanism and Catalysis  
  Lassila, J. K., Zalatan, J. G., Herschlag, D.  
  2011; 80: 669-702

• Hydrogen Bonding in the Active Site of Ketosteroid Isomerase: Electronic Inductive Effects and Hydrogen Bond Coupling  
  Hanoian, P., Sigala, P. A., Herschlag, D., Hammes-Schiffer, S.  
  2010; 49 (12): 10339-10348

• Decomposition of Vibrational Shifts of Nitriles into Electrostatic and Hydrogen-Bonding Effects  
  Fafarman, A. T., Sigala, P. A., Herschlag, D., Boxer, S. G.  
  2010; 132 (37): 12811-12813

• Multiple Unfolding Events during Native Folding of the Tetrahymena Group I Ribozyme  
  Wan, Y., Suh, H., Russell, R., Herschlag, D.  
  2010; 400 (5): 1067-1077

• How enzymes work  
  Herschlag, D.  
  2010; FEDERATION AMER SOC EXP BIOL

• Dissecting electrostatic screening, specific ion binding, and ligand binding in an energetic model for glycine riboswitch folding  
  Lipfert, J., Sim, A. Y., Herschlag, D., Doniach, S.  
  2010; 16 (4): 708-719

• A Rearrangement of the Guanosine-Binding Site Establishes an Extended Network of Functional Interactions in the Tetrahymena Group I Ribozyme Active Site  
  Forconi, M., Sengupta, R. N., Piccirilli, J. A., Herschlag, D.  
  2010; 49 (12): 2753-2762

• Origins of catalysis by computationally designed retroaldolase enzymes  
  Lassila, J. K., Baker, D., Herschlag, D.  
  2010; 107 (11): 4937-4942

• The Ligand-Free State of the TPP Riboswitch: A Partially Folded RNA Structure  
  Ali, M., Lipfert, J., Seifert, S., Herschlag, D., Doniach, S.  
  2010; 396 (1): 153-165

• Multiple native states reveal persistent ruggedness of an RNA folding landscape  
  Solomatin, S. V., Greenfeld, M., Chu, S., Herschlag, D.  
  2010; 463 (7281): 681-U117
• Dissecting the paradoxical effects of hydrogen bond mutations in the ketosteroid isomerase oxyanion hole. Proceedings of the National Academy of Sciences of the United States of America
Kraut, D. A., Sigala, P. A., Fenn, T. D., Herschlag, D.
2010; 107 (5): 1960-1965

• MEASURING THE ENERGETIC COUPLING OF TERTIARY CONTACTS IN RNA FOLDING USING SINGLE MOLECULE FLUORESCENCE RESONANCE ENERGY TRANSFER. Methods in Enzymology, Vol. 472: Single Molecule Tools, Pta: Fluorescence Based Approaches
Greenfeld, M., Herschlag, D.
2010; 472: 205-220

• Do conformational biases of simple helical junctions influence RNA folding stability and specificity? RNA-A Publication of the RNA Society
Chu, V. B., Lipfert, J., Bai, Y., Pande, V. S., Doniach, S., Herschlag, D.
2009; 15 (12): 2195-2205

• Concordant Regulation of Translation and mRNA Abundance for Hundreds of Targets of a Human microRNA. PLOS Biology
Hendrickson, D. G., Hogan, D. J., McCullough, H. L., Myers, J. W., Herschlag, D., Ferrell, J. E., Brown, P. O.
2009; 7 (11)

• Determining the catalytic role of remote substrate binding interactions in ketosteroid isomerase. Proceedings of the National Academy of Sciences of the United States of America
Schwans, J. P., Kraut, D. A., Herschlag, D.
2009; 106 (34): 14271-14275

• The far reaches of enzymology. Nature Chemical Biology
Zalatan, J. G., Herschlag, D.
2009; 5 (8): 516-520

• Hydrogen Bond Coupling in the Ketosteroid Isomerase Active Site. Biochemistry
Sigala, P. A., Caaveiro, J. M., Ringe, D., Petsko, G. A., Herschlag, D.
2009; 48 (29): 6932-6939

• Probing the Dynamics of the P1 Helix within the Tetrahymena Group I Intron. Journal of the American Chemical Society
Shi, X., Mollova, E. T., Pijevaljcic, G., Millar, D. P., Herschlag, D.
2009; 131 (27): 9571-9578

• Hydrogen bond dynamics in the active site of photoactive yellow protein. Proceedings of the National Academy of Sciences of the United States of America
Sigala, P. A., Tsuchida, M. A., Herschlag, D.
2009; 106 (23): 9232-9237

• Force and Form in RNA Folding
Herschlag, D.
Adenine Press. 2009: 813–13

• Evaluating the Potential for Halogen Bonding in the Oxyanion Hole of Ketosteroid Isomerase Using Unnatural Amino Acid Mutagenesis. ACS Chemical Biology
Kraut, D. A., Churchhill, M. J., Dawson, P. E., Herschlag, D.
2009; 4 (4): 269-273

• Motions of the Substrate Recognition Duplex in a Group I Intron Assessed by Site-Directed Spin Labeling. Journal of the American Chemical Society
Grant, G. P., Boyd, N., Herschlag, D., Qin, P. Z.
2009; 131 (9): 3136-?

• Coarse-grained modeling of large RNA molecules with knowledge-based potentials and structural filters. RNA-A Publication of the RNA Society
Jonikas, M. A., Radmer, R. J., Laederach, A., Das, R., Pearlman, S., Herschlag, D., Altman, R. B.
2009; 15 (2): 189-199

• Biophysical, chemical, and functional probes of RNA structure, interactions and folding: Part A. Preface. Methods in Enzymology
Herschlag, D.
THE DIVERSITY OF NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

NATO Advanced Study Institute on Biophysics and the Challenges of Emerging Threats

Liu, C. W., Alekseyev, V. Y., Allwardt, J. R., Bankovich, A. J., Cade-Menun, B. J., Davis, R. W., Du, L., Garcia, K. C., Herschlag, D., Khosla, C., Kraut, D. A., Li, Q., Null, et al.

SPRINGER. 2009: 65–81

RNA. Preface. *Methods in enzymology*

Herschlag, D.

2009; 469: xvii–?

PROBING NUCLEIC ACID-ION INTERACTIONS WITH BUFFER EXCHANGE-ATOMIC EMISSION SPECTROSCOPY

*METHODS IN ENZYMOLGY, VOL 469: BIOPHYSICAL, CHEMICAL, AND FUNCTIONAL PROBES OF RNA STRUCTURE, INTERACTIONS AND FOLDING, PT B*

Greenfeld, M., Herschlag, D.

2009; 469: 375-389

Structure and Function Converge To Identify a Hydrogen Bond in a Group I Ribozyme Active Site

*ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*

Forconi, M., Sengupta, R. N., Liu, M., Sartorelli, A. C., Piccirilli, J. A., Herschlag, D.

2009; 468: 171-1715

USE OF PHOSPHOROTHIOATES TO IDENTIFY SITES OF METAL-ION BINDING IN RNA

*METHODS IN ENZYMOLGY, VOL 468: BIOPHYSICAL, CHEMICAL, AND FUNCTIONAL PROBES OF RNA STRUCTURE, INTERACTIONS AND FOLDING, PT A*

Forconi, M., Herschlag, D.

2009; 468: 311-333

METAL ION-BASED RNA CLEAVAGE AS A STRUCTURAL PROBE

*METHODS IN ENZYMOLGY, VOL 468: BIOPHYSICAL, CHEMICAL, AND FUNCTIONAL PROBES OF RNA STRUCTURE, INTERACTIONS AND FOLDING, PT A*

Forconi, M., Herschlag, D.

2009; 468: 91-106

Riboswitch conformations revealed by small-angle X-ray scattering.

*Methods in molecular biology (Clifton, N.J.)*

Lipfert, J., Herschlag, D., Doniach, S.

2009; 540: 141-159

FLUORESCENCE POLARIZATION ANISOTROPY TO MEASURE RNA DYNAMICS

*METHODS IN ENZYMOLGY, VOL 469: BIOPHYSICAL, CHEMICAL, AND FUNCTIONAL PROBES OF RNA STRUCTURE, INTERACTIONS AND FOLDING, PT B*

Shi, X., Herschlag, D.

2009; 469: 287-302

METHODS OF SITE-SPECIFIC LABELING OF RNA WITH FLUORESCENT DYSES

*METHODS IN ENZYMOLGY, VOL 469: BIOPHYSICAL, CHEMICAL, AND FUNCTIONAL PROBES OF RNA STRUCTURE, INTERACTIONS AND FOLDING, PT B*

Solomatin, S., Herschlag, D.

2009; 469: 47-68

Comparative Enzymology in the Alkaline Phosphatase Superfamily to Determine the Catalytic Role of an Active-Site Metal Ion

*JOURNAL OF MOLECULAR BIOLOGY*

Zalatan, J. G., Fenn, T. D., Herschlag, D.

2008; 384 (5): 1174-1189

Promiscuous Sulfatase Activity and Thio-Effects in a Phosphodiesterase of the Alkaline Phosphatase Superfamily

*BIOCHEMISTRY*

Lassila, J. K., Herschlag, D.

2008; 47 (48): 12853-12859

A repulsive field: advances in the electrostatics of the ion atmosphere

*CURRENT OPINION IN CHEMICAL BIOLOGY*

Chu, V. B., Bai, Y., Lipfert, J., Herschlag, D., Doniach, S.

2008; 12 (6): 619-625

Testing geometrical discrimination within an enzyme active site: Constrained hydrogen bonding in the ketosterol isomerase oxyanion hole

*JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*

Sigala, P. A., Kraut, D. A., Cauveiro, J. M., Pybus, B., Ruben, E. A., Ringe, D., Petsko, G. A., Herschlag, D.
• Diverse RNA-Binding Proteins Interact with Functionally Related Sets of RNAs, Suggesting an Extensive Regulatory System. *PLOS BIOLOGY*
Hogan, D. J., Riordan, D. P., Gerber, A. P., Herschlag, D., Brown, P. O.
2008; 6 (10): 2297-2313

• Critical assessment of nucleic acid electrostatics via experimental and computational investigation of an unfolded state ensemble. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Bai, Y., Chu, V. B., Lipfert, J., Pande, V. S., Herschlag, D., Doniach, S.
2008; 130 (37): 12334-12341

• BIOL 102-Demystifying RNA folding *236th National Meeting of the American-Chemical-Society*
Herschlag, D.
AMER CHEMICAL SOC.2008

• BIOL 100-Transition state complementarity revisited: Dissecting electrostatic and geometrical catalysis in enzyme active sites *236th National Meeting of the American-Chemical-Society*
Herschlag, D.
AMER CHEMICAL SOC.2008

• Arginine coordination in enzymatic phosphoryl transfer: Evaluation of the effect of Arg166 mutations in Escherichia coli alkaline phosphatase. *BIOCHEMISTRY*
O'Brien, P. J., Lassila, J. K., Fenn, T. D., Zalatan, J. G., Herschlag, D.
2008; 47 (29): 7663-7672

• Functional identification of ligands for a catalytic metal ion in group I introns. *BIOCHEMISTRY*
Forconi, M., Lee, J., Lee, J. K., Piccirilli, J. A., Herschlag, D.
2008; 47 (26): 6883-6894

• Coupling between ATP binding and DNA cleavage by DNA topoisomerase II - A unifying kinetic and structural mechanism. *JOURNAL OF BIOLOGICAL CHEMISTRY*
Mueller-Planitz, F., Herschlag, D.
2008; 283 (25): 17463-17476

• Unwinding RNA’s secrets: advances in the biology, physics, and modeling of complex RNAs. *CURRENT OPINION IN STRUCTURAL BIOLOGY*
Chu, V. B., Herschlag, D.
2008; 18 (3): 305-314

• Direct measurement of tertiary contact cooperativity in RNA folding. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Sattint, B. D., Zhao, W., Travers, K., Chut, S., Herschlag, D.
2008; 130 (19): 6085-?

• Systematic Identification of mRNAs Recruited to Argonaute 2 by Specific microRNAs and Corresponding Changes in Transcript Abundance. *PLOS ONE*
Hendrickson, D. G., Hogan, D. J., Herschlag, D., Ferrell, J. E., Brown, P. O.
2008; 3 (5)

• Structural inference of native and partially folded RNA by high-throughput contact mapping. *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Dast, R., Kudaravalli, M., Jonikas, M., Laederach, A., Fong, R., Schwans, J. P., Baker, D., Piccirilli, J. A., Altman, R. B., Herschlag, D.
2008; 105 (11): 4144-4149

• Semiautomated and rapid quantification of nucleic acid footprinting and structure mapping experiments. *NATURE PROTOCOLS*
Laederach, A., Das, R., Vicens, Q., Pearlman, S. M., Brenowitz, M., Herschlag, D., Altman, R. B.
2008; 3 (9): 1395-1401

• Quantitative and comprehensive decomposition of the ion atmosphere around nucleic acids. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Bai, Y., Greenfeld, M., Travers, K. J., Chu, V. B., Lipfert, J., Doniach, S., Herschlag, D.
2007; 129 (48): 14981-14988

• Evaluation of ion binding to DNA duplexes using a size-modified Poisson-Boltzmann theory. *BIOPHYSICAL JOURNAL*
Chu, V. B., Bai, Y., Lipfert, J., Herschlag, D., Doniach, S.
Do ligand binding and solvent exclusion alter the electrostatic character within the oxyanion hole of an enzymatic active site? *Journal of the American Chemical Society*
Sigala, P. A., Fafarman, A. T., Bogard, P. E., Boxer, S. G., Herschlag, D.
2007; 129 (40): 12104-?

Modulation of individual steps in group I intron catalysis by a peripheral metal ion *RNA-A Publication of the RNA Society*
Forconi, M., Piccirilli, J. A., Herschlag, D.
2007; 13 (10): 1656-1667

**PHYS 212-Traversing the RNA folding landscape**
Herschlag, D.
**AMER CHEMICAL SOC.2007**

Kinetic isotope effects for alkaline phosphatase reactions: Implications for the role of active-site metal ions in catalysis *Journal of the American Chemical Society*
Zalatan, J. G., Catrina, I., Mitchell, R., Grzyska, P. K., O'Brien, P. J., Herschlag, D., Hengge, A. C.
2007; 129 (31): 9789-9798

Low specificity of metal ion binding in the metal ion core of a folded RNA *RNA-A Publication of the RNA Society*
Travers, K. J., Boyd, N., Herschlag, D.
2007; 13 (8): 1205-1213

DNA topoisomerase II selects DNA cleavage sites based on reactivity rather than binding affinity *Nucleic Acids Research*
Mueller-Planitz, F., Herschlag, D.
2007; 35 (11): 3764-3773

Probing the origin of the compromised catalysis of E-coli Alkaline phosphatase in its promiscuous sulfatase reaction *Journal of the American Chemical Society*
Catrina, I., O'Brien, P. J., Purcell, J., Nikolic-Hughes, I., Zalatan, J. G., Hengge, A. C., Herschlag, D.
2007; 129 (17): 5760-5765

Measuring the folding transition time of single RNA molecules *Biophysical Journal*
Lee, T., Lapidus, L. J., Zhao, W., Travers, K. J., Herschlag, D., Chu, S.
2007; 92 (9): 3275-3283

Probing the role of a secondary structure element at the 5'- and 3'-splice sites in group I intron self-splicing: The Tetrahymena L-16 Scal ribozyme reveals a new role of the G center dot U pair in self-splicing *Biochemistry*
Karbstein, K., Lee, J., Herschlag, D.
2007; 46 (16): 4861-4875

Insights from global studies of eukaryotic translation *Experimental Biology 2007 Annual Meeting*
Herschlag, D.
**FEDERATION AMER SOC EXP BIOL.2007: A92–A92**

Low-resolution models for nucleic acids from small-angle X-ray scattering with applications to electrostatic modeling *13th International Conference on Small-Angle Scattering*
Lipfert, J., Chu, V. B., Bai, Y., Herschlag, D., Doniach, S.
**WILEY-BLACKWELL.2007: S229–S234**

Traversing the RNA folding landscape
Herschlag, D.
**AMER CHEMICAL SOC.2007**

Structural transitions and thermodynamics of a glycine-dependent riboswitch from Vibrio cholerae *Journal of Molecular Biology*
Lipfert, J., Das, R., Chu, V. B., Kadaravalli, M., Boyd, N., Herschlag, D., Doniach, S.
2007; 365 (5): 1393-1406

Direct measurement of the full sequence-dependent folding landscape of single nucleic acids using an optical trap *51st Annual Meeting of the Biophysical-Society*
Woodside, M. T., Ambony, P. C., Larizadeh, K., Behnke-Parks, W. M., Herschlag, D., Block, S. M.
CELL PRESS.2007: 351A–351A

- Modeling RNA low resolution structure and thermodynamics from small-angle X-ray scattering 51st Annual Meeting of the Biophysical-Society
  Lipert, J., Chu, V. B., Bai, Y., Ouellet, J., Lilley, D. M., Herschlag, D., Doniach, S.
  CELL PRESS.2007: 417A–417A

- Direct measurement of the full, sequence-dependent folding landscape of a nucleic acid SCIENCE
  Woodside, M. T., Anthony, P. C., Behnke-Parks, W. M., Larizadeh, K., Herschlag, D., Block, S. M.
  2006; 314 (5801): 1001-1004

- The paradoxical behavior of a highly structured misfolded intermediate in RNA folding JOURNAL OF MOLECULAR BIOLOGY
  Russell, R., Das, R., Suh, H., Traver, K. J., Laederach, A., Engelhardt, M. A., Herschlag, D.
  2006; 363 (2): 531-544

- The wide reach of enzymology: from bioorganic chemistry to chemical biology and beyond mechanisms - Editorial overview CURRENT OPINION IN CHEMICAL BIOLOGY
  Fierke, C. A., Herschlag, D.
  2006; 10 (5): 453-454

- Interdomain communication in DNA topoisomerase II - DNA binding and enzyme activation JOURNAL OF BIOLOGICAL CHEMISTRY
  Mueller-Planitz, F., Herschlag, D.
  2006; 281 (33): 23395-23404

- Structural and functional comparisons of nucleotide pyrophosphatase/phosphodiesterase and alkaline phosphatase: Implications for mechanism and evolution BIOCHEMISTRY
  Zalatan, J. G., Fenn, T. D., Brunger, A. T., Herschlag, D.
  2006; 45 (32): 9788-9803

- Nanomechanical measurements of the sequence-dependent folding landscapes of single nucleic acid hairpins PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA
  Woodside, M. T., Behnke-Parks, W. M., Larizadeh, K., Travers, K., Herschlag, D., Block, S. M.
  2006; 103 (16): 6190-6195

- Testing electrostatic complementarity in enzyme catalysis: Hydrogen bonding in the ketosteroid isomerase oxyanion hole PLOS BIOLOGY
  Kraut, D. A., Sigala, P. A., Pybus, B., Liu, C. W., Ringe, D., Petsko, G. A., Herschlag, D.
  2006; 4 (4): 501-519

- Genome-wide identification of mRNAs associated with the translational regulator PUMILIO in Drosophila melanogaster PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA
  Gerber, A. P., Luschnig, S., Krasnow, M. A., Brown, P. O., Herschlag, D.
  2006; 103 (12): 4487-4492

- Alkaline phosphatase mono- and diesterase reactions: Comparative transition state analysis JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
  Zalatan, J. G., Herschlag, D.
  2006; 128 (4): 1293-1303

- Functional identification of catalytic metal ion binding sites within RNA PLOS BIOLOGY
  Houglund, J. L., Kravchuk, A. V., Herschlag, D., Piccirilli, J. A.
  2005; 3 (9): 1536-1548

- Structural specificity conferred by a group I RNA peripheral element PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA
  Johnson, T. H., Tijerina, P., Chadee, A. B., Herschlag, D., Russell, R.
  2005; 102 (29): 10176-10181

- Alkaline phosphatase catalysis is ultrasensitive to charge sequestered between the active site zinc ions JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
  Nikolic-Hughes, I., O'Brien, P. J., Herschlag, D.
  2005; 127 (26): 9314-9315
• Determining the Mg2+ stoichiometry for folding an RNA metal ion core *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Das, R., Travers, K. J., Bai, Y., Herschlag, D.
  2005; 127 (23): 8272-8273

• Promiscuous catalysis by the Tetrahymena group I ribozyme *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Forconi, M., Herschlag, D.
  2005; 127 (17): 6160-6161

• SAFA: Semi-automated footprinting analysis software for high-throughput quantification of nucleic acid footprinting experiments *RNA-A PUBLICATION OF THE RNA SOCIETY*
  Das, R., Laederach, A., Pearlman, S. M., Herschlag, D., Altman, R. B.
  2005; 11 (3): 344-354

• Probing counterion modulated repulsion and attraction between nucleic acid duplexes in solution *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Bai, Y., Das, R., Millett, I. S., Herschlag, D., Doniach, S.
  2005; 102 (4): 1035-1040

• Dissecting eukaryotic translation and its control by ribosome density mapping *NUCLEIC ACIDS RESEARCH*
  Arava, Y., Boas, F. E., Brown, P. O., Herschlag, D.
  2005; 33 (8): 2421-2432

• Spatial distribution of competing ions around DNA in solution *PHYSICAL REVIEW LETTERS*
  Andresen, K., Das, R., Park, H. Y., Smith, H., Kwok, L. W., Lamb, J. S., Kirkland, E. J., Herschlag, D., Finkelstein, K. D., Pollack, L.
  2004; 93 (24)

• Principles of RNA compaction: Insights from the equilibrium folding pathway of the P4-P6 RNA domain in monovalent cations *JOURNAL OF MOLECULAR BIOLOGY*
  Takamoto, K., Das, R., He, Q., Doniach, S., Brenowitz, M., Herschlag, D., Chance, M. R.
  2004; 343 (5): 1195-1206

• A base triple in the Tetrahymena group I core affects the reaction equilibrium via a threshold effect *RNA-A PUBLICATION OF THE RNA SOCIETY*
  Karbstein, K., Tang, K. H., Herschlag, D.
  2004; 10 (11): 1730-1739

• Do electrostatic interactions with positively charged active site groups tighten the transition state for enzymatic phosphoryl transfer? *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Nikolic-Hughes, L., Rees, D. C., Herschlag, D.
  2004; 126 (38): 11814-11819

• Extensive association of functionally and cytotopically related mRNAs with Puf family RNA-binding proteins in yeast *PLOS BIOLOGY*
  Gerber, A. P., Herschlag, D., Brown, P. O.
  2004; 2 (3): 342-354

• Adenosine 5’-O-(3-thio)triphosphate (ATP-gamma S) is a substrate for the nucleotide hydrolysis and RNA unwinding activities of eukaryotic translation initiation factor eIF4A *RNA-A PUBLICATION OF THE RNA SOCIETY*
  Peck, M. L., Herschlag, D.
  2003; 9 (10): 1180-1187

• Widespread cytoplasmic mRNA transport in yeast: Identification of 22 bud-localized transcripts using DNA microarray analysis *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Shepard, K. A., Gerber, A. P., Jambhekar, A., Takizawa, P. A., Brown, P. O., Herschlag, D., DeRisi, J. L., Vale, R. D.
  2003; 100 (20): 11429-11434

• The fastest global events in RNA folding: Electrostatic relaxation and tertiary collapse of the tetrahymena ribozyme *JOURNAL OF MOLECULAR BIOLOGY*
  Das, R., Kwok, L. W., Millett, I. S., Bai, Y., Mills, T. T., JACOB, J., Maskel, G. S., Seifert, S., Mochrie, S. G., Thiagarajan, P., Doniach, S., Pollack, L., Herschlag, et al
  2003; 332 (2): 311-319
• Exploration of the transition state for tertiary structure formation between an RNA helix and a large structured RNA *JOURNAL OF MOLECULAR BIOLOGY*
  Bartley, L. E., Zhuang, X. W., Das, R., Chu, S., Herschlag, D.
  2003; 328 (5): 1011-1026

• Counterion distribution around DNA probed by solution X-ray scattering *PHYSICAL REVIEW LETTERS*
  Das, R., Mills, T. T., Kwok, L. W., Maskel, G. S., Millett, I. S., Doniach, S., Finkelstein, K. D., Herschlag, D., Pollack, L.
  2003; 90 (18)

• Genome-wide analysis of mRNA translation profiles in *Saccharomyces cerevisiae* *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Arava, Y., Wang, Y. L., Storey, J. D., Liu, C. L., Brown, P. O., Herschlag, D.
  2003; 100 (7): 3889-3894

• Extraordinarily slow binding of guanosine to the Tetrahymena group I ribozyme: Implications for RNA preorganization and function *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Karbstein, K., Herschlag, D.
  2003; 100 (5): 2300-2305

• Challenges in enzyme mechanism and energetics *ANNUAL REVIEW OF BIOCHEMISTRY*
  Kraut, D. A., Carroll, K. S., Herschlag, D.
  2003; 72: 517-571

• Environmental effects on phosphoryl group bonding probed by vibrational spectroscopy: Implications for understanding phosphoryl transfer and enzymatic catalysis *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Cheng, H., Nikolic-Hughes, I., Wang, J. H., Deng, H., O'Brien, P. J., Wu, L., Zhang, Z. Y., Herschlag, D., Callender, R.
  2002; 124 (38): 11295-11306

• Probing the Tetrahymena group I ribozyme reaction in both directions *BIOCHEMISTRY*
  Karbstein, K., Carroll, K. S., Herschlag, D.
  2002; 41 (37): 11171-11183

• Dissection of a metal-ion-mediated conformational change in Tetrahymena ribozyme catalysis *RNA-A PUBLICATION OF THE RNA SOCIETY*
  Shan, S. O., Herschlag, D.
  2002; 8 (7): 861-872

• Precision and functional specificity in mRNA decay *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Wang, Y. L., Liu, C. L., Storey, J. D., Tibshirani, R. J., Herschlag, D., Brown, P. O.
  2002; 99 (9): 5860-5865

• RNA simulations: Probing hairpin unfolding and the dynamics of a GNRA tetraloop *JOURNAL OF MOLECULAR BIOLOGY*
  Sorin, E. J., Engelhardt, M. A., Herschlag, D., Pande, V. S.
  2002; 317 (4): 493-506

• Rapid compaction during RNA folding *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Russell, R., Millett, I. S., Tate, M. W., Kwok, L. W., Nakatani, B., Gruner, S. M., Mochrie, S. G., Pande, V., Doniach, S., Herschlag, D., Pollack, L.
  2002; 99 (7): 4266-4271

• Alkaline phosphatase revisited: Hydrolysis of alkyl phosphates *BIOCHEMISTRY*
  O'Brien, P. J., Herschlag, D.
  2002; 41 (9): 3207-3225

• Exploring the folding landscape of a structured RNA *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Russell, R., Zhuang, X. W., Babcock, H. P., Millett, I. S., Doniach, S., Chu, S., Herschlag, D.
  2002; 99 (1): 155-160

• Role of SRP RNA in the GTPase cycles of ffh and FtsY *BIOCHEMISTRY*
  Peluso, P., Shan, S. O., Nock, S., Herschlag, D., Walter, P.
Identifying ligands within the Tetrahymena ribozyme that bind and position the catalytic metal ions.
Piccirilli, J., Hougland, J. L., Kravchuk, A. V., Herschlag, D.
AMER CHEMICAL SOC. 2001: U145–U145

Channels in the RNA folding landscape.
Herschlag, D.
AMER CHEMICAL SOC. 2001: U136–U136

Channels in the RNA folding landscape.
Herschlag, D.
AMER CHEMICAL SOC. 2001: 8635–35

Identifying ligands within the Tetrahymena ribozyme that bind and position the catalytic metal ions.
Hougland, J. L., Kravchuk, A. V., Herschlag, D., Piccirilli, J.
AMER CHEMICAL SOC. 2001: 8647–48

Probing the folding landscape of the Tetrahymena ribozyme: Commitment to form the native conformation is late in the folding pathway JOURNAL OF MOLECULAR BIOLOGY
Russell, R., Herschlag, D.
2001; 308 (5): 839-851

Functional interrelationships in the alkaline phosphatase superfamily: phosphodiesterase activity of Escherichia coli alkaline phosphatase BIOCHEMISTRY
O'Brien, P. J., Herschlag, D.
2001; 40 (19): 5691-5699

Defining the catalytic metal ion interactions in the Tetrahymena ribozyme reaction BIOCHEMISTRY
Shan, S., Kravchuk, A. V., Piccirilli, J. A., Herschlag, D.
2001; 40 (17): 5161-5171

Comparison of the hammerhead cleavage reactions stimulated by monovalent and divalent cations RNA-A PUBLICATION OF THE RNA SOCIETY
O'Rear, J. L., Wang, S. L., Feig, A. L., Beigelman, L., Uhlenbeck, O. C., Herschlag, D.
2001; 7 (4): 537-545

Chemical rescue of phosphoryl transfer in a cavity mutant: a cautionary tale for site-directed mutagenesis BIOCHEMISTRY
Admiraal, S. J., Meyer, P., Schneider, B., Deville-Bonne, D., Janin, J., Herschlag, D.
2001; 40 (2): 403-413

A single molecule study of the folding dynamics of a large RNA enzyme
Babcock, H., Zhuang, X. W., Russell, R., Bartley, L., Herschlag, D., Chu, S.
CELL PRESS. 2001: 201A–201A

Exploring the RNA folding landscape, one molecule at a time.
Herschlag, D., Russell, R., Zhuang, X. W., Bartley, L., Babcock, H. P., Miller, I. S., Doniach, S., Chu, S.
AMER CHEMICAL SOC. 2000: U82–U82

A single-molecule study of RNA catalysis and folding SCIENCE
Zhuang, X. W., Bartley, L. E., Babcock, H. P., Russell, R., Ha, T. J., Herschlag, D., Chu, S.
2000; 288 (5473): 2048–?

Role of 4.5S RNA in assembly of the bacterial signal recognition particle with its receptor SCIENCE
Peluso, P., Herschlag, D., Nock, S., Freymann, D. M., Johnson, A. E., Walter, P.
2000; 288 (5471): 1640-1643

An unconventional origin of metal-ion rescue and inhibition in the Tetrahymena group I ribozyme reaction RNA-A PUBLICATION OF THE RNA SOCIETY
Shan, S. O., Herschlag, D.
2000; 6 (6): 795-813

Use of duplex rigidity for stability and specificity in RNA tertiary structure BIOCHEMISTRY
Narlikar, G. J., Bartley, L. E., Herschlag, D.  
2000; 39 (20): 6183-6189

- **Enzymatic activity and folding of single RNA molecules**  
  Zhuang, X., Bartley, L., Babcock, H., Russell, R., Ha, T., Herschlag, D., Chu, S.  
  FEDERATION AMER SOC EXP BIOL. 2000: A1587–A1587

- **Small angle X-ray scattering reveals a compact intermediate in RNA folding**  
  *Nature Structural Biology*  
  Russell, R., Millett, I. S., Doniach, S., Herschlag, D.  
  2000; 7 (5): 367-370

- **The substrate-assisted general base catalysis model for phosphate monoester hydrolysis: Evaluation using reactivity comparisons**  
  *Journal of the American Chemical Society*  
  Admiraal, S. J., Herschlag, D.  
  2000; 122 (10): 2145-2148

- **The P5abc peripheral element facilitates preorganization of the Tetrahymena group I ribozyme for catalysis**  
  *Biochemistry*  
  Engelhardt, M. A., Doherty, E. A., Knitt, D. S., Doudna, J. A., Herschlag, D.  
  2000; 39 (10): 2639-2651

- **The role of the cleavage site 2'-hydroxyl in the Tetrahymena group I ribozyme reaction**  
  *Chemistry & Biology*  
  Yoshida, A., Shan, S., Herschlag, D., Piccirilli, J. A.  
  2000; 7 (2): 85-96

- **Does the active site arginine change the nature of the transition state for alkaline phosphatase-catalyzed phosphoryl transfer?**  
  *Journal of the American Chemical Society*  
  O'Brien, P. J., Herschlag, D.  
  1999; 121 (47): 11022-11023

- **Kinetic dissection of fundamental processes of eukaryotic translation initiation in vitro**  
  *EMBO Journal*  
  Lorsch, J. R., Herschlag, D.  
  1999; 18 (23): 6705-6717

- **Stereospecificity of reactions catalyzed by HIV-1 integrase**  
  *Journal of Biological Chemistry*  
  Gerlon, J. L., Herschlag, D., Brown, P. O.  
  1999; 274 (47): 33480-33487

- **Characterization of a local folding event of the Tetrahymena group I ribozyme: Effects of oligonucleotide substrate length pH, and temperature on the two substrate binding steps**  
  *Biochemistry*  
  Narlikar, G. J., Bartley, L. E., Khosla, M., Herschlag, D.  
  1999; 38 (43): 14192-14204

- **Identification of the hammerhead ribozyme metal ion binding site responsible for rescue of the deleterious effect of a cleavage site phosphorothioate**  
  *Biochemistry*  
  Wang, S. L., Karbstein, K., Peracchi, A., Beigelman, L., Herschlag, D.  
  1999; 38 (43): 14363-14378

- **Three metal ions at the active site of the Tetrahymena group I ribozyme**  
  *Proceedings of the National Academy of Sciences of the United States of America*  
  Shan, S. O., Yoshida, A., Sun, S. G., Piccirilli, J. A., Herschlag, D.  
  1999; 96 (22): 12299-12304

- **Impaired transition state complementarity in the hydrolysis of O-arylphosphorothioates by protein-tyrosine phosphatases**  
  *Biochemistry*  
  Zhang, Y. L., Hollfelder, F., Gordon, S. J., Chen, L., Keng, Y. F., Wu, L., Herschlag, D., Zhang, Z. Y.  
  1999; 38 (37): 12111-12123

- **New pathways in folding of the Tetrahymena group I RNA enzyme**  
  *Journal of Molecular Biology*  
  Russell, R., Herschlag, D.  
  1999; 291 (5): 1155-1167
• Effects of oligonucleotide length and atomic composition on stimulation of the ATPase activity of translation initiation factor eIF4A. RNA-A PUBLICATION OF THE RNA SOCIETY
Peck, M. L., Herschlag, D.
1999; 5 (9): 1210-1221

• Protonated 2'-aminoguanosine as a probe of the electrostatic environment of the active site of the Tetrahymena group I ribozyme. BIOCHEMISTRY
Shan, S. O., Narlikar, G. J., Herschlag, D.
1999; 38 (34): 10976-10988

• Probing the role of metal ions in RNA catalysis: Kinetic and thermodynamic characterization of a metal ion interaction with the 2'-moiety of the guanosine nucleophile in the Tetrahymena group I ribozyme. BIOCHEMISTRY
Shan, S. O., Herschlag, D.
1999; 38 (34): 10958-10975

• Catalysis of phosphoryl transfer from ATP by amine nucleophiles. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
Admiraal, S. J., Herschlag, D.
1999; 121 (25): 5837-5845

• Phosphoryl transfer: Transition states, catalysis and evolution of enzyme diversity. FEDERATION AMER SOC EXP BIOL. 1999: A1424–A1424
Herschlag, D.

• Nucleophilic activation by positioning in phosphoryl transfer catalyzed by nucleoside diphosphate kinase. BIOCHEMISTRY
Admiraal, S. J., Schneider, B., Meyer, P., Janin, J., Veron, M., Deville-Bonne, D., Herschlag, D.
1999; 38 (15): 4701-4711

• Catalytic promiscuity and the evolution of new enzymatic activities. CHEMISTRY & BIOLOGY
O’Brien, P. J., Herschlag, D.
1999; 6 (4): R91-R105

• Assembly of an exceptionally stable RNA tertiary interface in a group I ribozyme. BIOCHEMISTRY
Doherty, E. A., Herschlag, D., Doudna, J. A.
1999; 38 (10): 2982-2990

• Specificity from steric restrictions in the guanosine binding pocket of a group I ribozyme. RNA-A PUBLICATION OF THE RNA SOCIETY
Russell, R., Herschlag, D.
1999; 5 (2): 158-166

• A new heat shock protein that binds nucleic acids. JOURNAL OF BIOLOGICAL CHEMISTRY
Korber, P., Zander, T., Herschlag, D., Bardwell, J. C.
1999; 274 (1): 249-256

• Hydrogen bonding in enzymatic catalysis: Analysis of energetic contributions. ENZYME KINETICS AND MECHANISM, PT E
Shan, S. O., Herschlag, D.
1999; 308: 246-276

• Sulfatase activity of E-coli alkaline phosphatase demonstrates a functional link to arylsulfatases, an evolutionarily related enzyme family. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
O’Brien, P. J., Herschlag, D.
1998; 120 (47): 12369-12370

• Structure-function relationships in the hammerhead ribozyme probed by base rescue. RNA-A PUBLICATION OF THE RNA SOCIETY
Peracchi, A., Matulic-Adamic, J., Wang, S. L., Beigelman, L., Herschlag, D.
1998; 4 (11): 1332-1346

• A core folding model for catalysis by the hammerhead ribozyme accounts for its extraordinary sensitivity to abasic mutations. BIOCHEMISTRY
Peracchi, A., Karpeisky, A., Maloney, L., Beigelman, L., Herschlag, D.
1998; 37 (42): 14765-14775

• RNA structure - Ribozyme crevices and catalysis. NATURE
Herschlag, D.
1998; 395 (6702): 548-549

- Direct demonstration of the catalytic role of binding interactions in an enzymatic reaction. *Biochemistry*
  Narlikar, G. J., Herschlag, D.
  1998; 37 (28): 9902-9911

- The DEAD box protein eIF4A. 2. A cycle of nucleotide and RNA-dependent conformational changes. *Biochemistry*
  Lorsch, J. R., Herschlag, D.
  1998; 37 (8): 2194-2206

- The DEAD box protein eIF4A. 1. A minimal kinetic and thermodynamic framework reveals coupled binding of RNA and nucleotide.*Biochemistry*
  Lorsch, J. R., Herschlag, D.
  1998; 37 (8): 2180-2193

- Involvement of a specific metal ion in the transition of the hammerhead ribozyme to its catalytic conformation. *Journal of Biological Chemistry*
  Peracchi, A., Beigelman, L., Scott, E. C., Uhlenbeck, O. C., Herschlag, D.
  1997; 272 (43): 26822-26826

- Use of intrinsic binding energy for catalysis by an RNA enzyme. *Proceedings of the National Academy of Sciences of the United States of America*
  Hertel, K. J., Peracchi, A., Uhlenbeck, O. C., Herschlag, D.
  1997; 94 (16): 8497-8502

- Biological catalysis: Lessons from the comparison of RNA and protein enzymes.
  Herschlag, D., Narlikar, G. J., Peracchi, A., Shan, S.
  Federation Amer Soc Exp Biol. 1997: A852–A852

- Phosphoryl transfer to nitrogen nucleophiles: Enzymatic and model studies.
  Admiraal, S., Herschlag, D.
  Federation Amer Soc Exp Biol. 1997: A1317–A1317

- Catalytic proficiency of E.coli alkaline phosphatase.
  O'Brien, P., Herschlag, D.
  Federation Amer Soc Exp Biol. 1997: A1318–A1318

- Effects of divalent metal ions on individual steps of the Tetrahymena ribozyme reaction. *Biochemistry*
  McConnell, T. S., Herschlag, D., Cech, T. R.
  1997; 36 (27): 8293-8303

- Quantitating tertiary binding energies of 2' OH groups on the P1 duplex of the Tetrahymena ribozyme: Intrinsic binding energy in an RNA enzyme. *Biochemistry*
  Narlikar, G. J., Khosla, M., Usman, N., Herschlag, D.
  1997; 36 (9): 2465-2477

- Mechanistic aspects of enzymatic catalysis: Lessons from comparison of RNA and protein enzymes. *Annual Review of Biochemistry*
  Narlikar, G. J., Herschlag, D.
  1997; 66: 19-59

- The change in hydrogen bond strength accompanying charge rearrangement: Implications for enzymatic catalysis. *Proceedings of the National Academy of Sciences of the United States of America*
  Shan, S. O., Herschlag, D.
  1996; 93 (25): 14474-14479

- Rescue of abasic hammerhead ribozymes by exogenous addition of specific bases. *Proceedings of the National Academy of Sciences of the United States of America*
  Peracchi, A., Beigelman, L., Usman, N., Herschlag, D.
  1996; 93 (21): 11522-11527

- Biological catalysis: From ribozymes to ras.
  Herschlag, D.
• Ras-catalyzed hydrolysis of GTP: A new perspective from model studies. *Proceedings of the National Academy of Sciences of the United States of America*
  Maegley, K. A., Admiraal, S. J., Herschlag, D.
  1996; 93 (16): 8160-8166

• Isolation of a local tertiary folding transition in the context of a globally folded RNA. *Nature Structural Biology*
  Narlikar, G. J., Herschlag, D.
  1996; 3 (8): 701-710

• Biological catalysis: From ribozymes to Ras. *American Chemical Society*
  Herschlag, D.
  1996; 3–3

• Specificity of hammerhead ribozyme cleavage. *EMBO Journal*
  Hertel, K. J., Herschlag, D., Uhlenbeck, O. C.
  1996; 15 (14): 3751-3757

• Energetic effects of multiple hydrogen bonds. Implications for enzymatic catalysis. *Journal of the American Chemical Society*
  Shan, S. O., Herschlag, D.
  1996; 118 (24): 5515-5518

• Mechanistic investigations of a ribozyme derived from the Tetrahymena group I intron: Insights into catalysis and the second step of self-splicing. *Biochemistry*
  Mei, R., Herschlag, D.
  1996; 35 (18): 5796-5809

• The energetics of hydrogen bonds in model systems: Implications for enzymatic catalysis. *Science*
  Shan, S. O., Loh, S., Herschlag, D.
  1996; 272 (5258): 97-101

• pH dependencies of the Tetrahymena ribozyme reveal an unconventional origin of an apparent pK(a). *Biochemistry*
  Knitt, D. S., Herschlag, D.
  1996; 35 (5): 1560-1570

• Mapping the transition-state for ATP hydrolysis - Implications for enzymatic catalysis. *Chemistry & Biology*
  Admiraal, S. J., Herschlag, D.
  1995; 2 (11): 729-739

• The nature of the transition-state for enzyme-catalyzed phosphoryl transfer - Hydrolysis of O-arly phosphorothioates by alkaline-phosphatase. *Biochemistry*
  Hollfelder, F., Herschlag, D.
  1995; 34 (38): 12255-12264

• RNA chaperones and the RNA folding problem. *Journal of Biological Chemistry*
  Herschlag, D.
  1995; 270 (36): 20871-20874

• Use of binding-energy by an RNA enzyme for catalysis by positioning and substrate destabilization. *Proceedings of the National Academy of Sciences of the United States of America*
  Narlikar, G. J., Gopalakrishnan, V., McConnell, T. S., Usman, N., Herschlag, D.
  1995; 92 (9): 3668-3672

• Dissection of the role of the conserved G-center-dot-U pair in group-I RNA self-spooling. *Biochemistry*
  Knitt, D. S., Narlikar, G. J., Herschlag, D.
  1994; 33 (46): 13864-13879

• Escherichia coli proteins, including ribosomal-protein S12, facilitate in-vitro splicing of phage-T4 introns by acting as RNA chaperones. *Genes & Development*
  Coetzee, T., Herschlag, D., Belfort, M.
• AN RNA CHAPERONE ACTIVITY OF NONSPECIFIC RNA-BINDING PROTEINS IN HAMMERHEAD RIBOZYME CATALYSIS. *EMBO JOURNAL*
Herschlag, D., Khosla, M., Tsuihishi, Z., Karpel, R. L.
1994; 13 (12): 2913-2924

• COMPARISON OF pH DEPENDENCIES OF THE TETRAHYMENA RIBOZYME REACTIONS WITH RNA 2'-SUBSTITUTED AND PHOSPHOROTHIOATE SUBSTRATES REVEALS A RATE-LIMITING CONFORMATIONAL STEP. *BIOCHEMISTRY*
Herschlag, D., Khosla, M.
1994; 33 (17): 5291-5297

• A KINETIC AND THERMODYNAMIC FRAMEWORK FOR THE HAMMERHEAD RIBOZYME REACTION. *BIOCHEMISTRY*
Hertel, K. J., Herschlag, D., Uhlenbeck, O. C.
1994; 33 (11): 3374-3385

• PROTEIN ENHANCEMENT OF HAMMERHEAD RIBOZYME CATALYSIS. *SCIENCE*
Tsuihishi, Z., Khosla, M., Herschlag, D.
1993; 262 (5130): 99-102

• GUANOSINE BINDING TO THE TETRAHYMENA RIBOZYME - THERMODYNAMIC COUPLING WITH OLIGONUCLEOTIDE BINDING. *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
McConnell, T. S., Cech, T. R., Herschlag, D.
1993; 90 (18): 8362-8366

• CATALYSIS OF THE HYDROLYSIS OF PHOSPHORYLATED PYRIDINES BY ALKALINE-PHOSPHATASE HAS LITTLE OR NO DEPENDENCE ON THE PK(A) OF THE LEAVING GROUP. *BIOCHEMISTRY*
Labow, B. I., Herschlag, D., Jencks, W. P.
1993; 32 (34): 8737-8741

• THE IMPORTANCE OF BEING RIBOSE AT THE CLEAVAGE SITE IN THE TETRAHYMENA RIBOZYME REACTION. *BIOCHEMISTRY*
Herschlag, D., Eckenstein, F., Cech, T. R.
1993; 32 (32): 8312-8321

• CONTRIBUTIONS OF 2'-HYDROXYL GROUPS OF THE RNA SUBSTRATE TO BINDING AND CATALYSIS BY THE TETRAHYMENA RIBOZYME - AN ENERGETIC PICTURE OF AN ACTIVE-SITE COMPOSED OF RNA. *BIOCHEMISTRY*
Herschlag, D., Eckenstein, F., Cech, T. R.
1993; 32 (32): 8299-8311

• SYNERGISM IN TRANSCRIPTIONAL ACTIVATION - A KINETIC VIEW. *GENES & DEVELOPMENT*
Herschlag, D., Johnson, F. B.
1993; 7 (2): 173-179

• MUTATIONS AT THE GUANOSINE-BINDING SITE OF THE TETRAHYMENA RIBOZYME ALSO AFFECT SITE-SPECIFIC HYDROLYSIS. *NUCLEIC ACIDS RESEARCH*
Legault, P., Herschlag, D., Celander, D. W., Cech, T. R.
1992; 20 (24): 6613-6619

• RNA CATALYSIS BY A GROUP-I RIBOZYME - DEVELOPING A MODEL FOR TRANSITION-STATE STABILIZATION. *JOURNAL OF BIOLOGICAL CHEMISTRY*
Cech, T. R., Herschlag, D., Piccirilli, J. A., Pyle, A. M.
1992; 267 (25): 17479-17482

• EVIDENCE FOR PROCESSIVITY AND 2-STEP BINDING OF THE RNA SUBSTRATE FROM STUDIES OF J1/2 MUTANTS OF THE TETRAHYMENA RIBOZYME. *BIOCHEMISTRY*
Herschlag, D.
1992; 31 (5): 1386-1399

• MUTATIONS IN A NONCONSERVED SEQUENCE OF THE TETRAHYMENA RIBOZYME INCREASE ACTIVITY AND SPECIFICITY. *CELL*
Young, B., Herschlag, D., Cech, T. R.
1991; 67 (5): 1007-1019
• IMPLICATIONS OF RIBOZYME KINETICS FOR TARGETING THE CLEAVAGE OF SPECIFIC RNA MOLECULES INVIVO - MORE ISNT ALWAYS BETTER. *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Herschlag, D.
1991; 88 (16): 6921-6925

• RIBOZYME-CATALYZED AND NONENZYMATIC REACTIONS OF PHOSPHATE DIESTERS - RATE EFFECTS UPON SUBSTITUTION OF SULFUR FOR A NONBRIDGING PHOSPHORYL OXYGEN ATOM. *BIOCHEMISTRY*
Herschlag, D., Piccirilli, J. A., Cech, T. R.
1991; 30 (20): 4844-4854

• CATALYSIS OF RNA CLEAVAGE BY THE TETRAHYMENA-THERMOPHILA RIBOZYME .1. KINETIC DESCRIPTION OF THE REACTION OF AN RNA SUBSTRATE COMPLEMENTARY TO THE ACTIVE-SITE. *BIOCHEMISTRY*
Herschlag, D., Cech, T. R.
1990; 29 (44): 10159-10171

• CATALYSIS OF RNA CLEAVAGE BY THE TETRAHYMENA-THERMOPHILA RIBOZYME .2. KINETIC DESCRIPTION OF THE REACTION OF AN RNA SUBSTRATE THAT FORMS A MISMATCH AT THE ACTIVE-SITE. *BIOCHEMISTRY*
Herschlag, D., Cech, T. R.
1990; 29 (44): 10172-10180

• CATALYSIS OF THE HYDROLYSIS OF PHOSPHORYLATED PYRIDINES BY Mg(OH)+ - A POSSIBLE MODEL FOR ENZYMATIC PHOSPHORYL TRANSFER. *BIOCHEMISTRY*
Herschlag, D., Jencks, W. P.
1990; 29 (21): 5172-5179

• DNA CLEAVAGE CATALYZED BY THE RIBOZYME FROM TETRAHYMENA. *NATURE*
Herschlag, D., Cech, T. R.
1990; 344 (6265): 405-409

• NUCLEOPHILES OF HIGH REACTIVITY IN PHOSPHORYL TRANSFER-REACTIONS - ALPHA-EFFECT COMPOUNDS AND FLUORIDE-ION. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Herschlag, D., Jencks, W. P.
1990; 112 (5): 1951-1956

• THE EFFECTS OF Mg2+, HYDROGEN-BONDING, AND STERIC FACTORS ON RATE AND EQUILIBRIUM-CONSTANTS FOR PHOSPHORYL TRANSFER BETWEEN CARBOXYLATE IONS AND PYRIDINES. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Herschlag, D., Jencks, W. P.
1990; 112 (5): 1942-1950

• Nucelophiles of High Reactivity in Phosphoryl Transfer Reactions: &alpha;-Effect Compounds and Fluoride Ion. *J. Am. Chem. Soc.*
Herschlag, D., Jencks, W.P.
1990; 112: 1951-1956

• The Effect of Mg2+, Hydrogen Bonding and Steric Factors on Rate and Equilibrium Constants for Phosphoryl Transfer between Carboxylate Ions and Pyridines. *J. Am. Chem. Soc.*
Herschlag, D., Jencks, W.P.
1990; 112: 1942-1950

• PHOSPHORYL TRANSFER TO ANIONIC OXYGEN NUCLEOPHILES - NATURE OF THE TRANSITION-STATE AND ELECTROSTATIC REPULSION. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Herschlag, D., Jencks, W. P.
1989; 111 (19): 7587-7596

• EVIDENCE THAT META-PHOSPHATE MONOANION IS NOT AN INTERMEDIATE IN SOLVOLYSIS REACTIONS IN AQUEOUS-SOLUTION. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Herschlag, D., Jencks, W. P.
1989; 111 (19): 7579-7586

• Phosphoryl Transfer to Oxyanions: The Nature of the Transition State and Electrostatic Repulsion. *J. Am. Chem. Soc.*
Herschlag, D., Jencks, W.P.
1989; 111: 7587-7596
Evidence That Metaphosphate is Not an Intermediate in Solvolysis Reactions in Aqueous Solution. *J. Am. Chem. Soc.*
Herschlag, D., Jencks, W.P.
1989; 111: 7579-7586

The Role of Induced Fit and Conformational Changes of Enzymes in Specificity and Catalysis. *Bioorganic Chemistry*
Herschlag, D.
1988; 16: 62-96

**THE EFFECT OF DIVALENT METAL-IONS ON THE RATE AND TRANSITION-STATE STRUCTURE OF PHOSPHORYL-TRANSFER REACTIONS** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Herschlag, D., JENCKS, W. P.
1987; 109 (15): 4665-4674

The Effect of Divalent Metal Ions on the Rate and Transition State Structure of Phosphoryl Transfer Reactions. *J. Am. Chem. Soc.*
Herschlag, D., Jencks, W.P.
1987; 109: 4665-4674

**PYROPHOSPHATE FORMATION FROM ACETYL PHOSPHATE AND ORTHO-PHOSPHATE ANIONS IN CONCENTRATED AQUEOUS SALT-SOLUTIONS DOES NOT PROVIDE EVIDENCE FOR A META-PHOSPHATE INTERMEDIATE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Herschlag, D., JENCKS, W. P.
1986; 108 (25): 7938-7946

Additions and Corrections: Decreasing Reactivity with Increasing Nucleophile Basicity. The Effect of Solvation on (nuc) for Phosphoryl Transfer to Amines. *Journal of the American Chemical Society*
JENCKS, W. P., Haber, M. T., Herschlag, D., NAZARETIAN, K. L.
1986; 108 (19): 6100-7

**DECREASING REACTIVITY WITH INCREASING NUCLEOPHILE BASICITY - THE EFFECT OF SOLVATION ON BETA-NUC FOR PHOSPHORYL TRANSFER TO AMINES** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
JENCKS, W. P., Haber, M. T., Herschlag, D., NAZARETIAN, K. L.
1986; 108 (3): 479-483

Pyrophosphate Formation from Acetyl Phosphate and Orthophosphate Anions in Concentrated Aqueous Salt Solutions Does Not Provide Evidence for a Metaphosphate Intermediate. *J. Am. Chem. Soc.*
Herschlag, D., Jencks, W.P.
1986; 108: 7938

Decreasing Reactivity with Increasing Nucleophile Basicity. The Effect of Solvation on βnuc for Phosphoryl Transfer to Amines *J. Am. Chem. Soc.*
Jencks, W.P., Haber, M.T., Herschlag, D., Nazaretian, K.L.
1986; 108: 479

**GALACTOFURANOSYL-CONTAINING GLYCOPEPTIDE OF PENICILLIUM-CHARLESII - VACUUM ULTRAVIOLET CIRCULAR-DICHROISM** *INTERNATIONAL JOURNAL OF PEPTIDE AND PROTEIN RESEARCH*
Herschlag, D., Stevens, E. S., Gander, J. E.
1983; 22 (1): 16-20