

Eamonn F. Healy – CURRICULUM VITAE

a. Professional Preparation

University College Cork, Ireland,	1976-1980	B.S. Chemistry.
University of Texas at Austin,	1980-1984	Ph.D. Chemistry.

b. Appointments

2001-	Professor of Chemistry, St. Edward's University
2010-2016	Bro. Lucian Blersch Professor of Science
1995-2001	Associate Professor of Chemistry, St. Edward's University
1990-1995	Assistant Professor of Chemistry, St. Edward's University
1986-1990	Research Scientist Associate IV, University of Texas at Austin
1984-1986	Postdoctoral Research Fellow, University of Texas at Austin

c. Honors and Professional memberships

Bro. Lucian Blersch Professor of Science
Charter F21 member, Class of 1995, Project Kaleidoscope
Member, the American Chemical Society
Member, Texas Academy of Science
Original Member, Highly Cited Researchers Database, ISI Thomson Scientific.
Piper Professor (Texas): 2001
Outstanding Teacher, St. Edward's University (1999)
Nominee, CASE Teaching Award (1999)
Outstanding Teacher, School of Natural Sciences, St. Edward's University (1992)

d. Research

The general focus of my research involves the use of molecular modeling to design structure-activity probes for the purpose of elucidating enzymatic activity. Recent targets have included HIV-1 integrase, the c-Kit and src-abl proteins associated with tumor development and certain leukemias, and the metalloproteinases associated with the shedding of chemokine CXCL16. For the latter work we have used ligand-protein docking to guide and characterize in vitro assays of CXCL16 shedding. We have also investigated the bacterial and host contributions to latent Mtb infection through the identification of the macrophage cellular responses that are modulated by the Mtb alpha-crystallin (Acr) protein. This work has allowed for an in silico characterization of the mechanism of action of Mtb Acr, that in turn has led us to a novel mechanism of action for all small Heat Shock Proteins (sHSP). More recently we have expanded this analysis to characterize mechanistic details for the heat shock response of Escherichia coli, and we have developed a model to explain the observed suppression of spinocerebellar ataxia by human alphaB-crystallin through the formation of a transient complex. A transient, non-obligate oligomer model has also been developed to explain aspects of the etiology of Amyotrophic Lateral Sclerosis or ALS.

e. Teaching

Fall/Spring:

CHEM 2323 : Organic Chemistry I
CHEM 3325 : Organic Chemistry II

CHEM 4341 : Forensic Chemistry
CHEM 3343 : Biochemistry I
CHEM 4320 : Advanced Organic

f. Publications

Eamonn F Healy, Lisa M. Goering, Charles R. Hauser, and Peter J. King “An immunomodulatory role for the Mtb Acr protein in the formation of the tuberculous granuloma” *FEBS Lett.* **2020**, submitted (FEBSL-20-0936).

Healy, E. F., & Blade, G. † “Tips and Tools for Teaching Organic Synthesis Online” *Journal of Chemical Education*, **2020**, *97*, 3163–3167.

Eamonn F Healy, Organic chemistry as representation *Foundations of Chemistry*, July **2020**
DOI: 10.1007/s10698-020-09379-z

Healy, Eamonn F., Rafael Flores†, Vincent M. Lynch, and Santiago Toledo. "Protein dynamics of [Cu-Zn] superoxide dismutase (SOD1): How protein motions at the global and local levels impact the reactivity of SOD1." *Journal of Inorganic Biochemistry* **2020**, *210*, 111161.

Eamonn F Healy, Reply to” Should Organic Chemistry be taught as Science ?,” *Journal of Chemical Education*, **2020**, *97*, 4, 1215.

Eamonn F Healy, Analise Roth-Rodriguez† and Santiago Toledo “A model for gain of function in superoxide dismutase” *Biochem. Biophys. Res.* **2020**, *21*, 100728.

Eamonn F Healy, Should Organic Chemistry be taught as Science ?, *Journal of Chemical Education*, **2019** , *96*, *10*, 2069-2071

Eamonn F Healy, Luis Cervantes†, Barret Nabona†, Jacob Williams† , *Biochemical and Biophysical Research Communications*, **2018**, *497*, 1123-1128.

E.F. Healy, “Visualizing the molecular wave function in σ -coordinated complexes”, *Computational and Theoretical Chemistry*, **2018**, *1125*, 128-132

Eamonn F. Healy “A prion-like mechanism for the propagated misfolding of SOD1 ”, *PLoS ONE* **2017**, *12* (5), e0177284.

Eamonn F. Healy “A mechanism for propagated SOD1 misfolding from frustration analysis of a G85R mutant protein assembly”, *Biochem. Biophys. Res. Commun.* **2016**, *478*, 1634-1639.

Eamonn F. Healy and Luis Cervantes† “An in silico study of the effect of SOD1 electrostatic loop dynamics on amyloid-like filament formation ”, *Euro. Biophys. J.* **2016**, *Aug.5* [Epub ahead of print].

Eamonn F. Healy “A role for non-obligate oligomer formation in protein aggregation”, *Biochem. Biophys. Res. Commun.* **2015**, *465* , 523-527.

Eamonn F. Healy, Carley Little† and Peter J. King “A model for small heat shock protein inhibition of polyglutamine aggregation" *Cell Biochemistry and Biophysics* **2014**, *69*, 275-281.

Eamonn F. Healy “Michael J. S. Dewar: A Model Iconoclast” In *Pioneers of Quantum Chemistry*, E. Thomas Strom, Angela K. Wilson , Eds. , ACS Symposium Series, Vol. 1122; American Chemical Society: Washington, DC, **2013** pp 139–153.

Eamonn F. Healy " A model for heterooligomer formation in the heat shock response of *E. coli*", *Biochem. Biophys. Res. Commun.*, **2012**, 420, 639-643.

Eamonn F. Healy, and Peter J. King "A Mechanism of Action for Small Heat Shock Proteins", *Biochem. Biophys. Res. Commun.*, **2012**, 417, 268–273.

E.F. Healy, "Heisenberg's Chemical Legacy: Resonance and the Chemical Bond", *Foundations of Chemistry*, **2011**, 13, 39-49.

E.F. Healy, "The effect of desolvation on nucleophilic halogenase activity", *Computational and Theoretical Chemistry*, **2011**, 964, 91-93.

Eamonn F. Healy, Pablo Romano[†], Moises Mejia[†] and Gunnar Lindfors III[†], Acetylenic Inhibitors of ADAM10 and ADAM17: In silico analysis of potency and selectivity *J. Mol. Graph. Model*, **2010**, 29, 436-442.

Eamonn F. Healy, Samuel Manzer, Jeffrey Gorman, Alicia Jones[†] and Nicholas Cristea[†] "A dramatic heavy atom effect in the quenching of dichlorosubstituted lucigenin fluorescence", *Chem. Phys. Lett.*, **2010**, 485, 258-261.

E.F. Healy "In Defense of a Heuristic Interpretation of Quantum Mechanics", *J. Chem. Educ.*, **2010**, 87, 559-563.

Eamonn F. Healy, Skylar Johnson[†], Charles Hauser, and Peter King "Tyrosine kinase inhibition: Ligand binding and conformational change in c-Kit and c-Abl." *FEBS Lett.* **2009**, 583, 2899-2906..

Eamonn F. Healy, Jonathan Sanders[†], Peter J. King and W. Edward Robinson, Jr "A Docking Study of L-Chicoric Acid with HIV-1 Integrase" *J Mol. Graph. Model.* **2009**, 27, 14.

E.F. Healy "Quantitative Determination of DNA-Ligand Binding Using Fluorescence Spectroscopy", *J. Chem. Educ.*, **2007**, 84, 1304.

E.F. Healy "Huckel Calculations using Mathematica", *J. Chem. Educ.*, **1995**, 72, A120.

E.F. Healy; J. D. Lewis; A. B. Minnear[†] "A Study of the Aluminum Hydride Reduction of Unsaturated Cyclic Epoxides", *Tetrahedron Lett.*, **1994**, 35, 6647.

E.F. Healy; A.J. Holder, "An Evaluation of AM1 Vibrational Frequencies", *J. Mol. Struct. (Theochem)*; **1993**, 281, 141.

E. F. Healy, C. G. Wall[†], M.A. Fox, "Peptide Conformational Analysis using the TRIPOS Force Field", *Intl. J. Quant. Chem.*, **1992**, 44, 543

E.F. Healy, M.J.S. Dewar, A.J. Holder, D.R. Kuhn, "AM1 Calculations for compounds containing Tin", *Organometallics*, **1991**, 10, 431.

M.J.S. Dewar, E.F. Healy, A.J. Holder, Y-C Yuan, "Comments on a comparison of AM1 with the Recently Developed PM3 Method", *J. Comput. Chem.*, **1990**, 11, 541.

M.J.S. Dewar, A.J. Holder, E.F. Healy, S. Olivella, "Comparison of Single Point ab initio Energies calculated using 3-21G and AM1 Geometries", *J. Chem. Soc., Chem. Comm.*, **1989**, 1452.

M.J.S. Dewar, D.A. Liotard, E.F. Healy, J.M. Ruiz, *QCPE Bulletin*, "AMPAC: A General Molecular Orbital Package", **1989**, 9, QCPE # 506.

M.J.S. Dewar, E.F. Healy, J.R. Ruiz, "Mechanism of the 1,5-Sigmatropic Shift in 1,3-Pentadiene", *J. Am. Chem. Soc.*, **1988**, 110, 2666

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- M.J.S. Dewar, E.F. Healy, J. Ruiz, "A High Level *ab initio* Study of Corner-Protonated Cyclopropane", *J. Chem. Soc. Chem. Comm.*, **1987**, 943.
- M.J.S. Dewar, G.L. Grady, E.F. Healy, "MNDO Calculations for Compounds Containing Germanium", *Organometallics*, **1987**, 6, 186.
- M.J.S. Dewar, G.L. Grady, J. Friedheim, E.F. Healy, J.J.P. Stewart "Revised MNDO Parameters for Silicon", *Organometallics*, **1986**, 5, 375.
- M.J.S. Dewar, E.F. Healy, J. Ruiz, "Cruciaromaticity in organometallic compounds", *Pure & Appl. Chem.*, **1986**, 58, 67.
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- M.J.S. Dewar, E.F. Healy, "MNDO Study of the Claisen Rearrangement", *J. Am. Chem. Soc.*, **1985**, 107, 3902.
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- M.J.S. Dewar, , E.F. Healy, "MNDO Calculations for Compounds Containing Bromine", *J. Comput. Chem.*, **1983**, 4, 542.
- W. S. Murphy, E.F. Healy[†], S. Wattansin, "Synthesis of 1-Arylnaphthalenes from Cyclopropyl Ketones", *Proc. R. Ir. Acad.*, **1983**, 83, 13.
- M.J.S. Dewar, , E.F. Healy, "Why Life Exists", *Organometallics*, **1982**, 1, 1705.
- P. Brint, E.F. Healy[†], T. Spalding, T. Whelan, "Bonding in Clusters. Protonation of *nido*- Pentaborane, *nido*-Hexaborane and *closo*- Hexaborane", *J. Chem. Soc. Dalton* , **1981**, 2515.

† student author

g. Recent Professional Presentations

12th EBSA 10th ICBP-IUPAP Congress in Madrid, Spain, in July 2019. Short-listed as primary speaker, but in neither case was I chosen due to the competitive nature of the process (in both instances the keynote for my putative session was a Nobel laureate). Nevertheless the organizers wished for me to send on my work so that they could publish in the book of abstracts. Without a speaking engagement I chose to not attend either in person due to the costs involved Abstract published as: Healy, E., **2019**, July. A mechanism for coupled gain of structure and loss of function in amyotrophic lateral sclerosis. In EUROPEAN BIOPHYSICS JOURNAL WITH BIOPHYSICS LETTERS (Vol. 48, pp. S143-S143). 233 SPRING ST, NEW YORK, NY 10013 USA: SPRINGER.

19th International Union of Pure and Applied Biophysics (IUPAB) and 11th European Biophysical Societies' Association (EBSA) Congress in Edinburgh, Scotland, in July 2017. Short-listed as primary speaker, but in neither

case was I chosen due to the competitive nature of the process (in both instances the keynote for my putative session was a Nobel laureate). Nevertheless the organizers wished for me to send on my work so that they could publish in the book of abstracts. Without a speaking engagement I chose to not attend either in person due to the costs involved Abstract published as: Healy, E.F., **2017**, July. A Prion-like mechanism in Amyotrophic Lateral Sclerosis. In EUROPEAN BIOPHYSICS JOURNAL WITH BIOPHYSICS LETTERS (Vol. 46, pp. S217-S217). 233 SPRING ST, NEW YORK, NY 10013 USA: SPRINGER.SPRINGER.

Cervantes, L.*, & Healy, E. (**2017**, April). Protein dynamics in Superoxide Dismutase (SOD1). In ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY (Vol. 253). 1155 16TH ST, NW, WASHINGTON, DC 20036 USA: AMER CHEMICAL SOC.

"Structural Ontology and Chemical Epistemology: The case of the pi-complex" Eamonn F Healy, presented at the International Society for the Philosophy of Chemistry - Summer Symposium , Boca Raton, **2016**.

Paper HIST 22 , "Between two stools: Pauling, Mulliken, and Michael J. S. Dewar" Eamonn F Healy, presented at the 251st ACS National Meeting & Exposition, San Diego, Spring, **2016**.

Cienega, L.*, & Healy, E. F. (**2014**, March). Rational design for matrix metalloproteinase (MMP-1). In ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY (Vol. 247). 1155 16TH ST, NW, WASHINGTON, DC 20036 USA: AMER CHEMICAL SOC.

Bui, A.*, & Healy, E. F. (**2014**, March). Modeling the conformational flexibility of resveratrol. In ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY (Vol. 247). 1155 16TH ST, NW, WASHINGTON, DC 20036 USA: AMER CHEMICAL SOC.

Little, C.*, & Healy, E. (**2013**, April). Model for small heat shock protein inhibition of polyglutamine aggregation. In ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY (Vol. 245). 1155 16TH ST, NW, WASHINGTON, DC 20036 USA: AMER CHEMICAL SOC.

Petty, C. N.*, Healy, E. F., & King, P. (**2013**, April). Resveratrol and resveratrol derivatives as class IA PI3K inhibitors. In ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY (Vol. 245). 1155 16TH ST, NW, WASHINGTON, DC 20036 USA: AMER CHEMICAL SOC.

Paper COMP 193 "Tyrosine kinase inhibition: Ligand binding and conformational change in c-Kit and c-Abl", Eamonn F Healy, presented at the 244th National Meeting of the American Chemical Society in Philadelphia, Fall **2012**.

Paper CHED 360 "Acetylenic inhibitors of ADAM10 and ADAM17: In silico analysis of potency and selectivity", Pablo G Romano*, Moises Mejia*, Eamonn F Healy, presented at the 243rd National Meeting of the American Chemical Society in San Diego, Spring **2012**.

Paper CHED 206 "Resveratrol effects on PGHS-1 using molecular modeling: Applications in biochemistry", Brenna Sura*, Eamonn F Healy, presented at the 243rd National Meeting of the American Chemical Society in San Diego, Spring **2012**.

"A role for Heat Shock Proteins in the formation of the tuberculous granuloma", Eamonn F. Healy, 2011 Lucian Symposium, Global Health and Infectious Disease: Tuberculosis, October **2011**.

"This House Fears the rise of Artificial Intelligence," Eamonn F. Healy, University Philosophical Society in Trinity College Dublin (debate) December **2011**.

"The Role of Desolvation in Ligand Binding and Protein Aggregation," Eamonn F. Healy, Departments of Biochemistry and Immunology, Trinity College, Dublin, Ireland, December **2011**.

Paper CHED 401 “Rational design of Mtb enoyl acyl carrier protein reductase inhibitors”, Mina C Nakhla*, Eamonn F Healy, presented at the 241st National Meeting of the American Chemical Society in Anaheim, Spring **2011**.

Paper CHED 402 “ Acetylenic inhibitors of ADAM10 and ADAM17: In silico analysis of potency and selectivity “, Moises Mejia*, Eamonn F Healy, presented at the 241st National Meeting of the American Chemical Society in Anaheim, Spring **2011**.

“Life After Darwin”, Eamonn F. Healy, invited presentation at VIBes in Biosciences 2010, University of Leuven, Belgium, October **2010**

“HIV–1 Integrase: Rational Drug Design and Drug Resistance”, Eamonn F. Healy, 2010 Lucian Symposium, HIV/AIDS: Global Health and Infectious Diseases, October **2010**.

Paper CHED 351 “Inhibition of tyrosine kinases: The influence of protein flexibility on ligand design “, April Fields*, Alden Clemments*, and Eamonn F. Healy, presented at the 237th ACS National Meeting, Salt Lake City, UT, March 22-26, **2009**.

“HIV Integrase and c-Kit : Ligand Design and Drug Resistance” Eamonn F. Healy, Jonathan Sanders*, Skylar Johnson*, Peter J. King, Charles R. Hauser and W. Edward Robinson, Jr, Keystone Symposium on Computer-Aided Drug Design, Steamboat Springs, CO, March 29-April 3, **2008**.

Paper CHED 544 "Mechanism of Lucigenin Fluorescence Quenching by Chloride Ions," Chelsea Ragland*, N. Cristea*, J. Kugler*, Eamonn Healy, and Jeff Gorman, presented at the 235rd National Meeting of the American Chemical Society in New Orleans April 5-8, **2008**.

Paper CHED 1300 "HIV Integrase and c-Kit: Ligand Design and Docking Protocols, Skylar Johnson*, Jon Sanders*, and Eamonn Healy, presented at the 235rd National Meeting of the American Chemical Society in New Orleans April 5-8, **2008**.

Presenters are underlined; undergraduate student authors are noted by asterisks.

h. Collaborators and Other Affiliates

(i) Collaborators:

King, Peter, St. Edward’s University, Austin, Tx.

Hauser, Charles, St. Edward’s University, Austin, Tx.

Fernandez, Ariel Morgridge Institute for Research

Quinn, Frederick D., College of Veterinary Medicine, University of Georgia

Robinson, W. Edward Jr., University of California at Irvine, Irvine, Ca.

Merz, Kenneth M. Jr., Quantum Theory Project and the University of Florida Gainesville, Fl.

Holder, Andrew, University of Missouri at Kansas City, Kansas City, Ks.

Fox, Marye Anne University of California at San Diego, San Diego Ca.

(ii) Graduate and postdoctoral Advisors:

Dewar, Michael J.S., University of Texas at Austin

i. Ongoing and Recently Completed Research Support

07/15/2013 – 06/30/2019

National Institute of General Medical Sciences (NIGMS), “IRACDA Postdoctoral Program: Collaborative Opportunities for Research” .

7/01/2010-6/31/2015

The National Science Foundation (NSF), “Community for Achievement in Science, Academics, and Research (CASAR), Healy (CO-PI).

7/01/2007-6/31/2010

W.M. Keck Foundation Research and Undergraduate Programs Grant. “Interdisciplinary Undergraduate Research on HIV-1 Drug Resistance”, Healy (PI).

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