Sameh Abdelwahed
Prairie View A&M University, Prairie View, TX 77446 P.O. Box 519, MS 2215
Phone: 936-261-3192 FAX: 936-261-3117
shabdelwahed@pvamu.edu

Appointment and Positions: -

2018 – present: Assistant Professor, Prairie View A&M University, Prairie View, Prairie View, Texas

Professional Preparation

Previous Organization (s) & Location (s)	Degree	Receipt Date	Field of study
Cairo University (Cairo, Egypt)	BS MS	05/1995	General Chemistry
Cairo University (Cairo, Egypt)	PHD	11/1999	Organic Chemistry
Marquette University (Wisconsin, USA)	Postdoctoral	05/2006	Supramolecular Chem.
Marquette University (Wisconsin, USA)	Postdoctoral	06/2008	Supramolecular Chem.
Cornell University (Ithaca, USA)	Postdoctoral	07/2009	Organic Synthesis
Texas A&M University (Texas, USA)		09/2018	Organic synthesis

Personal Statement:

Dedicated to the pursuit of excellence in education, mentorship, and cutting-edge research, I am an accomplished professional with a proven track record in the field of Organic Chemistry. My academic journey, spanning from a master's degree in Medicinal Chemistry at Cairo University to my current role as a faculty member at Texas A&M University, reflects my unwavering commitment to advancing scientific knowledge and fostering the development of students at all levels.

1- Undergraduate and Graduate Advising:

I have successfully mentored both graduate and undergraduate students, guiding them in field studies and research projects, particularly in the realm of Organic Chemistry. My commitment extends beyond the classroom, as evidenced by the seamless transition of numerous students into prestigious graduate programs. Notably, this year alone, I have proudly guided three master's degree graduates into the TAMU PhD program.

2- Editorial Contributions and NSF CHE MRI Spectroscopy and Microscopy Panelist Review:

Serving as a reviewer for esteemed journals like Molecules, Bioorganic Chemistry, and Frontiers in Chemistry, I actively contribute to the scholarly peer-review process. Additionally, my involvement in the NSF CHE MRI competition underscores my dedication to advancing research initiatives and supporting the scientific community's growth.

3- Teaching Development:

As the Chair of the Seminar Committee, I take a leadership role in curating seminar topics and selecting speakers. Collaborating with colleagues and students, I foster interdisciplinary learning, creating an environment that enhances our academic community's knowledge and engagement.

4- Community Involvements and Outreach:

My commitment to community outreach is exemplified through educational field trips organized for chemistry majors. These experiences provide valuable insights at the Texas A&M Department of Chemistry, inspiring students and encouraging their pursuit of advanced education. Additionally, my role as a Faculty Senate member within the Faculty Research and Development Committee underscores my dedication to shaping research and development programs for faculty.

5- Workshop Development:

I have successfully managed and organized workshops tailored for both graduate and undergraduate students, focusing on crucial aspects such as instrument operation, including NMR and ultraviolet-visible near-infrared spectrophotometry equipment.

My diverse academic background, from designing and synthesizing heterocyclic organic compounds during my master's to groundbreaking research on charge delocalization mechanisms published in the Journal of the American Chemical Society, showcases my multifaceted expertise. Furthermore, my postdoctoral research at Cornell University and subsequent contributions at Texas A&M University underscore my commitment to pioneering research at the intersection of chemistry and biology.

With 34 peer-reviewed publications in top-tier journals, including Science, Nature Communications, Journal of American Chemical Society, Organic Letters, Biochemistry, and Angewandte Chemie Int. Ed., I am proud of my substantial contributions to the scientific community, with over 400 citations attesting to the impact of my work.

As I continue my academic journey, my overarching goal remains rooted in the relentless pursuit of high-quality education, impactful mentorship, and active participation in groundbreaking research. I am poised to contribute meaningfully to the advancement of knowledge, the development of future scientists, and the collective pursuit of scientific excellence.

Skilled and Experience with General Laboratory instrumentation.

Lab Equipment: Proficient in operating advanced laboratory equipment, including the H-Cube Continuous-flow Hydrogenation Reactor for high-pressure hydrogen reduction of compounds.

Utilized the Monowave 300 Microwave Synthesis Reactor for high-temperature chemical reactions.

Applied the Ozone Engineering LG-7 Corona Discharge ozone generator for oxidation reactions.

Experienced with the Rayonet photoreactor, specializing in the photodeprotection of nitrobenzyl-caged compounds.

Chromatographic Techniques: Extensive experience in various chromatographic methods, including Silica-gel, ion exchange, affinity, and HPLC, utilizing Agilent 1200 & 1100 Series HPLC systems.

Proficient in Flash Chromatography systems, such as CombiFlash, for organic purification and characterization.

Mass Spectrometry and Spectrophotometry: Skilled in LC/MS, specifically microtof QII mass spectroscopy (Bruker), for the characterization of enzymatic products.

Utilized NMR (Varian & Bruker), IR, GC/MS, Cary 300 UV-Vis spectrophotometer, Cary Eclipse Fluorescence spectrophotometer, UV-Vis-NIR spectra & Fluorescent spectra measurements on a JASCO spectrometer.

Electrochemical Analysis: Proficient in Cyclic Voltammetry using the Epsilon E2 Electrochemical Analyzer.

Characterization and Purification: Expertise in the characterization and purification of enzymatic intermediates, substrates, and small molecules, employing a full scope of instrumentation, including NMR, HPLC, and LC/MS. Proficient in protein overexpression and purification.

Problem Solving: Demonstrated ability to solve problems efficiently and in a timely fashion.

Organic Synthesis: Accomplished in total synthesis using modern techniques, including ozonolysis, photoreactor, hydrogenation, microwave, and a variety of chromatographic purification methods.

Executed multi-step organic synthesis with creativity to overcome synthetic chemistry challenges.

Production and Purification: Successfully produced and purified multi-gram to milligram quantities of light and air-sensitive synthetic compounds.

Molecular Design: Proven capability in the synthesis and design of various organic compounds, particularly those acting as molecular wires.

Training and Supervision: Adept at training and supervising new graduate and undergraduate students.

Communication: Strong communication skills facilitating effective collaboration and knowledge transfer within the laboratory setting.

Selected Professional Presentations:

1- TexSyn VI Conference at Texas A&M University May 31-June 1, 2024

Title: "New Benzofuran-Pyrazole Based Compounds as Promising Antimicrobial Agents: Design, Synthesis, Antioxidant, Anti-inflammatory, DNA Gyrase B Inhibition and In Silico Studies"

2- Southwest Regional Meeting of the American Chemical Society

Title: "Exploring New Inhibitors for SARS-CoV-2 Main Protease"
Date: November 15-18, 2023
Location: Oklahoma City, OK

2- 11th Young Researcher Conference at Texas A&M University

Title: "The Multifaceted Applications of Chemistry: Exploring its Role in Medicinal, Electrical, and Enzymatic Pathways"
Date: May 17-19, 2023

3- The 9th Texas Enzyme Mechanisms Conference at The University of Texas, Austin

Title: "Exploring New Inhibitors for SARS-CoV-2 Main Protease"
Date: June 3, 2023

4- 28th Congress of the International Society of Heterocyclic Chemistry

Title: "New quinoxaline-based derivatives as PARP-1 inhibitors: design, synthesis, antiproliferative, and computational studies"
Date: August 28 to September 2, 2022
Location: UCSB California

6- 8th Texas Enzyme Mechanisms Conference at the University of Texas Austin

Title: "Homology Modeling of Transketolase Like-1 (TKTL-1) Enzyme: A Pathway for Structure-based Drug Design for TKTL-1 Modulators"
Date: January 3rd and 4th, 2020

8- American Chemical Society, 253rd National Meeting

Title: "Thiamine as a carrier for drug delivery to cancer cells"
Date: April 2-6, 2017
Location: San Francisco, California

9- American Chemical Society, 249th National Meeting

Title: "How nature makes vitamin B12; The last unsolved biosynthetic module"
Date: March 22-26, 2015
Location: Denver, Colorado

10- American Chemical Society, 247th National Meeting

Title: "Identification and characterization of new protein thiocarboxylate in bacteria"
Date: March 16-20, 2014
Location: Dallas, Texas

11- American Chemical Society, 246th National Meeting

Title: "Biosynthesis of dimethylbenzimidazole: Catalysis of a remarkable flavin degradation reaction"
Date: September 8-12, 2013
Location: Indianapolis, Indiana

12- Texas Enzyme Mechanisms Conference, University of Texas at Austin

Date: January 6 & 7, 2012

13- American Chemical Society Milwaukee Section Meeting

Title: "Synthesis of a Calix[4]arene Derivative for Isolation of a Stable Cation Radical Salt for Use as a Colorimetric Sensor of Nitric Oxide"
Date: April 11, 2005
Location: Milwaukee, WI

14- American Chemical Society, 229th National Meeting

Title: "Studies of Intramolecular Energy Transfer through Cofacially -Stacked Polyfluorene Spacers"
Date: March 13-17, 2005
Location: San Diego, CA

Selected publication:

1. Khalifa, A.; Anwar, M. M.; Alshareef, W. A.; El Gebaly, E. A. E.; Elseginy, S. A.; Abdelwahed, S. H. Design, Synthesis, and Antimicrobial Evaluation of Some New Thiopyrimidin-Benzenesulfonamide Compounds. *Molecules* **2024**, *29(19), 4778;* ***https://doi.org/10.3390/molecules29194778***
2. Abd El-Karima, S. S.; Anwara, M. M.; Syama, Y. M.; Awad, H. M.; El-Dein, A. N.; El-Ashrey, M. K.; Abdelwahed, S. New Benzofuran-Pyrazole Based Compounds as Promising Antimicrobial Agents: Design, Synthesis, Antioxidant, Anti-inflammatory, DNA Gyrase B Inhibition and In Silico Studies. *Preprints* **2024**, 2024081792, under publication. https://doi.org/10.20944/preprints202408.1792.v1
3. Junaid, Ahmad; Nwaogwugwu, Caleb; Abdelwahed, Sameh. Exploring the Role of TRANSKETOLASE LIKE-1 (TKTL-1) in Cancer: Insights into Oncogenic Metabolism and Therapeutic Prospects. *Cancer Informatics* accepted and under publication, **2024**.
4. Vishav Sharma, Dmytro Fedoseyenko, Sumedh Joshi, **Sameh Abdelwahed**, and Tadhg P. Begley. Phosphomethylpyrimidine Synthase (ThiC): Trapping of Five Intermediates Provides Mechanistic Insights on a Complex Radical Cascade Reaction in Thiamin Biosynthesis; ACS Central Science **2024** 10 (5), 988-1000 https://pubs.acs.org/doi/10.1021/acscentsci.4c00125
5. Sharma, V.; Fedoseyenko, D.; Joshi, S.; Abdelwahed, S.; Begley, T. Phosphomethylpyrimidine Synthase (ThiC): A "Radical Dance" in Bacterial Thiamin Biosynthesis. *Journal of Biological Chemistry* 2024, 300 (3), 106236. https://doi.org/10.1016/j.jbc.2024.106236
6. Abdel-Mohsen, Heba T., Manal M. Anwar, Nesreen S. Ahmed, Somaia S. Abd El-Karim, **and Sameh H. Abdelwahed**. 2024. "Recent Advances in Structural Optimization of Quinazoline-Based Protein Kinase Inhibitors for Cancer Therapy (2021–Present)" *Molecules* **2024**, *29*, 875. https://doi.org/10.3390/molecules29040875
7. Rajendra Rathore, **Sameh H. Abdelwahed**; Design and Synthesis of Cofacially-Arrayed Polyfluorene Wires for Electron and Energy Transfer Studies; Molecules **2023** 28 (9), 3717; **https://doi.org/10.3390/molecules28093717**
8. Rajendra Rathore, Sergey V. Lindeman **Sameh H. Abdelwahed**; Design, Synthesis, Electronic Properties, and X-ray Structural Characterization of Various Modified Electron-Rich Calixarene Derivatives and Their Conversion to Stable Cation Radical Salts; Molecules **2022**, 27(18), 5994; https://doi.org/10.3390/molecules27185994
9. Yasmin M. Syam, Manal M. Anwar, Somaia S. Abd El-Karim ,Khaled M. Elokelyand, **Sameh H. Abdelwahed**; New Quinoxaline-Based Derivatives as PARP-1 Inhibitors; Design, Synthesis, Antiproliferative, and Computational Studies; Molecules **2022**, 27(15), 4924; https://doi.org/10.3390/molecules27154924
10. Ahmad Junaid, Grace Abolaji, **Sameh Abdelwahed.** Computational Screening for Novel Herbal-based SARSCoV-2 Structural Protein Modulators. Biomed J Sci & Tech Res 40(1)-**2021**. http://dx.doi.org/10.26717/BJSTR.2021.40.006400
11. Zhang, X.; Basuli, F.; **Abdelwahed, S**.; Begley, T.; Swenson, R., Radiosynthesis of 5-[18F] Fluoro-1,2,3-triazoles through Aqueous Iodine–[18F]Fluorine Exchange Reaction. Molecules 2021, 26 (18), 5522. https://doi.org/10.3390/molecules26185522
12. Charge-transfer or excimeric state? Exploring the nature of the excited state in cofacially arrayed polyfluorene derivatives A Abzhanova, LV Ivanova, D Wang, TS Navale, **SH Abdelwahed**, Journal of Photochemistry and Photobiology A: Chemistry **2019**, 374, 125-130 https://doi.org/10.1016/j.jphotochem.2019.01.030
13. Derek M. Gagnon, Troy A. Stich, Angad P. Mehta, **Sameh H. Abdelwahed,** Tadhg P. Begley, R. David Britt, An Aminoimidazole Radical Intermediate in the Anaerobic Biosynthesis of the 5,6-dimethylbenzimidazole Ligand to Vitamin B12. (Journal of the American Chemical Society., **2018**, 140 (40), pp 12798–12807). https://doi.org/10.1021/jacs.8b05686
14. Maxim V. Ivanov, Marat R. Talipov, Anitha Boddeda, **Sameh H. Abdelwahed**, and Rajendra Rathore; 'Hückel Theory + Reorganization Energy = Marcus−Hush Theory: Breakdown of the 1/n Trend in π-Conjugated Poly-p-phenylene Cation Radicals Is Explained' Journal of Physical Chemistry C (2017), 121(3), 1552-1561.

15. Isita Jhulki, Prem K. Chanani, **Sameh H. Abdelwahed**, and Tadhg P. Begley; "Roseoflavin biosynthesis: A remarkable oxidative cascade that replaces the riboflavin C8 methyl with an amino group"; Journal of the American Chemical Society, (2016), 138 (27), pp 8324–8327.
16. Marat R. Talipov, **Sameh H. Abdelwahed**, Khushabu Thakur, Scott A. Reid, and Rajendra Rathore; "From Wires to Cables: Attempted Synthesis of 1,3,5-Trifluorenylcyclohexane as a Platform for Molecular Cables" Journal of Organic Chemistry (2016), 81(4), 1627-1634.
17. Angad P. Mehta, **Sameh H. Abdelwahed**, Michael K. Fenwick, Amrita B. Hazra, Michiko E. Taga, Yang Zhang, Steven E. Ealick, and Tadhg P. Begley; 'Anaerobic 5-Hydroxybenzimidazole Formation from Aminoimidazole Ribotide: An Unanticipated Intersection of Thiamin and Vitamin B12 Biosynthesis'; Journal of the American Chemical Society (2015), 137(33), 10444-10447.
18. Michael K. Fenwick , Angad P. Mehta, Yang Zhang, **Sameh H. Abdelwahed**, Tadhg P. Begley and Steven E. Ealick; 'Non-canonical active site architecture of the radical SAM thiamin pyrimidine synthase'; Nature communications (2015), 66480.
19. Angad P. Mehta, **Sameh H. Abdelwahed**, Tadhg P. Begley; 'Molybdopterin biosynthesis - Mechanistic studies on a novel MoaA catalyzed insertion of a purine carbon into the ribose of GTP': Biochimica et Biophysica Acta, Proteins and Proteomics (2015).
20. Angad P. Mehta, **Sameh H. Abdelwahed**, Nilkamal Mahanta, Dmytro Fedoseyenko, Benjamin Philmus, Lisa E. Cooper, Yiquan Liu, Isita Jhulki, Steven E. Ealick, and Tadhg P. Begley; 'Radical S-Adenosylmethionine (SAM) Enzymes in Cofactor Biosynthesis: A Treasure Trove of Complex Organic Radical Rearrangement Reactions"; Journal of Biological Chemistry (2015), 290(7), 3980- 3986.
21. Angad P. Mehta, **Sameh H. Abdelwahed**, Hui Xu, and Tadhg P. Begley "Molybdopterin Biosynthesis: Trapping of Intermediates for the MoaA-Catalyzed Reaction Using 2′-DeoxyGTP and 2′-ChloroGTP as Substrate Analogues. Journal of the American Chemical Society, (2014), 136 (30), pp 10609–10614.
22. Angad P Mehta, **Sameh H Abdelwahed**, and Tadhg P. Begley "Molybdopterin biosynthesis: Trapping an unusual purine ribose adduct in the MoaA-catalyzed reaction" Journal of the American Chemical Society, (2013), 135 (30), 10883–10885.
23. Lisa E. Cooper, Dmytro Fedoseyenko, **Sameh H. Abdelwahed**, Soong-Hyun Kim, Tohru Dairi , Tadhg P. Begley "In vitro reconstitution of the radical SAM enzyme MqnC involved in the biosynthesis of futalosine-derived menaquinone" Biochemistry, (2013), 52 (27), 4592–4594.
24. Angad P Mehta, Jeremiah W. Hanes, **Sameh H Abdelwahed**, David George Hilmey, Petra Hänzelmann, and Tadhg P. Begley. Biochemistry (2013), 52(7) 1134–1136.
25. Honglan Qi, Jinho Chang, **Sameh H. Abdelwahed**, Khushabu Thakur, Rajendra Rathore, and Allen J. Bard; Journal of the American Chemical Society (2012), 134 (39),16265–16274.
26. Philmus, Benjamin; **Sameh H. Abdelwahed**; Williams, Howard J.; Fenwick, Michael K.; Ealick, Steven E.; Begley, Tadhg P."Identification of the Product of Toxoflavin Lyase: Degradation via a Baeyer-Villiger Oxidation" Journal of the American Chemical Society (2012), 134(11), 5326-5330.
27. Josh Vura-Weis, **Sameh H. Abdelwahed**, Ruchi Shukla, Rajendra Rathore, Mark A. Ratner, Michael R. Wasielewski "Crossover from Single-Step Tunneling to Multistep Hopping for Molecular Triplet Energy Transfer". Science (2010), 328(5985), 1547-1550.
28. Abhishek Chatterjee, Amrita B. Hazra, **Sameh H. Abdelwahed**, David G. Hilmey and Tadhg P. Begley. "A radical dance in thiamin biosynthesis:mechanistic analysis of the bacterial hydroxymethylpyrimidine phosphate synthase " Angewandte Chemie, International Edition (2010), 49(46), 8653-8656.
29. Mukherjee, Tathagata; Zhang, Yang; **Abdelwahed, Sameh**; Ealick, Steven; Begley, Tadhg. "Catalysis of a novel flavoenzymemediated amide hydrolysis" Journal of the American Chemical Society (2010), 132(16), 5550-5551.
30. Rajendra Rathore, **Sameh H. Abdelwahed,** Mathew K. Kiesewetter, Richard C. Reiter and Cheryl D. Stevenson. "Intramolecular Electron Transfer Tunneling in -stacked polyfluorenes". Journal of Physical Chemistry B (2006), 110(4), 1536-1540.

31. Cheryl D. Stevenson, Mathew K. Kiesewetter, Richard C. Reiter, **Sameh H. Abdelwahed** and Rajendra Rathore. "Intramolecular CH/C-D Exchange in Cofacially Stacked Polyfluorenes via Electron Induced Bond Activation". Journal of the American Chemical Society (2005), 127(15), 5282-5283.
32. Rajendra Rathore, Vincent J. Chebny and **Sameh H. Abdelwahed** "A Varsatile and Conformationally-Adaptable Fluorene-Based Receptore for Efficiebt Binding of Silver Cation". Journal of the American Chemical Society (2005), 127(22), 8012-8013.
33. Rajendra Rathore, **Sameh A. Abdelwahed.** "Soluble cycloannulated tetroxa [8]circulane derivatives: synthesis, optical and electrochemical properties, and generation of their robust cation–radical salts" Tetrahedron Letters (2004), 45(27), 5267-5270.
34. Rajendra Rathore, Carrie L. Burns, and **Sameh H. Abdelwahed.** "Hopping of a Single Hole in hexakis[4-(1,1,2-Triphenylethenyl)phenyl]benzene Cation Radical through the Hexaphenylbenzene Propeller". Organic Letters (2004), 6(11), 1689-1692.
35. Rajendra Rathore, **Sameh H. Abdelwahed**, and Ilia A. Guzei. "Synthesis of a Calix[4]arene Derivative for Isolation of a Stable Cation Radical Salt for Use as a Colorimetric Sensor of Nitric Oxide". Journal of the American Chemical Society (2004), 126(42), 13582- 13583.
36. Rajendra Rathore, **Sameh H. Abdelwahed**, and Ilia A. Guzei. "Synthesis, Structure, and Evaluation of the Effect of Multiple Stacking on the Electron-Donor Properties of -Stacked Polyfluorenes". Journal of the American Chemical Society (2003), 125(29), 8712- 8713.
37. H. H. Fahmy ; **S. H. A. Abdelwahed**; A. A. Hamdy. "Synthesis of some new heterocyclic compounds containing benzimidazole moiety as potential antimicrobial agents", Egyptian Journal of Chemistry. (2003), 46 (2), 313-327.
38. Fahmy H.H, El-masry A, **Ali Abdelwahed S. H.** "Synthesis and preliminary antimicrobial screening of new benzimidazole heterocycles". Archives of Pharmacal Research. (2001), 24(1), 27-34.
39. Afaf H. El-masry, H. H. Fahmy and **S. H. Ali Abdelwahed**. "Synthesis and Antimicrobial Activity of Some New Benzimidazole Derivatives" Molecules (2000) 5, 1429-1438.

1. Antimicrobial Agents

1. Khalifa, A.; Anwar, M. M.; Alshareef, W. A.; El Gebaly, E. A. E.; Elseginy, S. A.; Abdelwahed, S. H. **Design, Synthesis, and Antimicrobial Evaluation of Some New Thiopyrimidin-Benzenesulfonamide Compounds.** *Molecules* 2024, 29(19), 4778; https://doi.org/10.3390/molecules29194778.
2. Abd El-Karima, S. S.; Anwara, M. M.; Syama, Y. M.; Awad, H. M.; El-Dein, A. N.; El-Ashrey, M. K.; Abdelwahed, S. **New Benzofuran-Pyrazole Based Compounds as Promising Antimicrobial Agents: Design, Synthesis, Antioxidant, Anti-inflammatory, DNA Gyrase B Inhibition and In Silico Studies.** *Preprints* 2024, 2024081792, under publication. https://doi.org/10.20944/preprints202408.1792.v1.
3. Fahmy H.H, El-masry A, **Ali Abdelwahed S. H.** "Synthesis and preliminary antimicrobial screening of new benzimidazole heterocycles". Archives of Pharmacal Research. (2001), 24(1), 27-34.
4. Afaf H. El-masry, H. H. Fahmy and **S. H. Ali Abdelwahed**. "Synthesis and Antimicrobial Activity of Some New Benzimidazole Derivatives" Molecules (2000) 5, 1429-1438.

2. Cancer Therapy

1. Abdel-Mohsen, Heba T.; Anwar, M. M.; Ahmed, N. S.; Abd El-Karim, S. S.; Abdelwahed, S. H. **Recent Advances in Structural Optimization of Quinazoline-Based Protein Kinase Inhibitors for Cancer Therapy (2021–Present).** *Molecules* 2024, 29, 875. https://doi.org/10.3390/molecules29040875.
2. Junaid, Ahmad; Nwaogwugwu, Caleb; Abdelwahed, Sameh. **Exploring the Role of TRANSKETOLASE LIKE-1 (TKTL-1) in Cancer: Insights into Oncogenic Metabolism and Therapeutic Prospects.** *Cancer Informatics*, accepted and under publication, 2024.
3. Syam, Y. M.; Anwar, M. M.; Abd El-Karim, S. S.; Elokely, K. M.; Abdelwahed, S. H. **New Quinoxaline-Based Derivatives as PARP-1 Inhibitors: Design, Synthesis, Antiproliferative, and Computational Studies.** *Molecules* 2022, 27(15), 4924; https://doi.org/10.3390/molecules27154924.

3. Computational Chemistry and Structure-Activity Relationships

1. Ahmad Junaid, Grace Abolaji, Sameh Abdelwahed. **Computational Screening for Novel Herbal-based SARS-CoV-2 Structural Protein Modulators.** *Biomed J Sci & Tech Res* 2021, 40(1). http://dx.doi.org/10.26717/BJSTR.2021.40.006400.
2. Rajendra Rathore, Sameh H. Abdelwahed. **Design and Synthesis of Cofacially-Arrayed Polyfluorene Wires for Electron and Energy Transfer Studies.** *Molecules* 2023, 28(9), 3717. https://doi.org/10.3390/molecules28093717.
3. Rajendra Rathore, Sergey V. Lindeman, Sameh H. Abdelwahed. **Design, Synthesis, Electronic Properties, and X-ray Structural Characterization of Various Modified Electron-Rich Calixarene Derivatives and Their Conversion to Stable Cation Radical Salts.** *Molecules* 2022, 27(18), 5994. https://doi.org/10.3390/molecules27185994.

4. Biosynthesis and Mechanistic Studies

1. Vishav Sharma, Dmytro Fedoseyenko, Sumedh Joshi, Sameh Abdelwahed, and Tadhg P. Begley. **Phosphomethylpyrimidine Synthase (ThiC): Trapping of Five Intermediates Provides Mechanistic Insights on a Complex Radical Cascade Reaction in Thiamin Biosynthesis.** *ACS Central Science* 2024, 10(5), 988-1000. https://doi.org/10.1021/acscentsci.4c00125.
2. Isita Jhulki, Prem K. Chanani, Sameh H. Abdelwahed, and Tadhg P. Begley. **Roseoflavin biosynthesis: A remarkable oxidative cascade that replaces the riboflavin C8 methyl with an amino group.** *Journal of the American Chemical Society* (2016), 138(27), 8324–8327.
3. Gagnon, Derek M.; Stich, Troy A.; Mehta, Angad P.; Abdelwahed, Sameh H.; Begley, Tadhg P.; Britt, R. David. **An Aminoimidazole Radical Intermediate in the Anaerobic Biosynthesis of the 5,6-dimethylbenzimidazole Ligand to Vitamin B12.** *Journal of the American Chemical Society* (2018), 140(40), 12798–12807. https://doi.org/10.1021/jacs.8b05686.
4. Mehta, Angad P.; Xu, Hui; Abdelwahed, Sameh H.; Begley, Tadhg P. **Molybdopterin Biosynthesis: Trapping of Intermediates for the MoaA-Catalyzed Reaction Using 2′-DeoxyGTP and 2′-ChloroGTP as Substrate Analogues.** *Journal of the American Chemical Society* (2014), 136(30), 10609–10614.
5. Mehta, Angad P.; Abdelwahed, Sameh H.; Begley, Tadhg P. **Anaerobic 5-Hydroxybenzimidazole Formation from Aminoimidazole Ribotide: An Unanticipated Intersection of Thiamin and Vitamin B12 Biosynthesis.** *Journal of the American Chemical Society* (2015), 137(33), 10444-10447.

5. Organic Chemistry and Synthetic Methods

1. Talipov, Marat R.; Abdelwahed, Sameh H.; Boddeda, Anitha; Rathore, Rajendra. **Hückel Theory + Reorganization Energy = Marcus−Hush Theory: Breakdown of the 1/n Trend in π-Conjugated Poly-p-phenylene Cation Radicals Is Explained.** *Journal of Physical Chemistry C* (2017), 121(3), 1552-1561.
2. Chatterjee, Abhishek; Hazra, Amrita B.; Abdelwahed, Sameh H.; Hilmey, David G.; Begley, Tadhg P. **A radical dance in thiamin biosynthesis: mechanistic analysis of the bacterial hydroxymethylpyrimidine phosphate synthase.** *Angewandte Chemie International Edition* (2010), 49(46), 8653-8656.
3. Mehta, Angad P.; Abdelwahed, Sameh H.; Begley, Tadhg P. **Molybdopterin biosynthesis: Trapping an unusual purine ribose adduct in the MoaA-catalyzed reaction.** *Journal of the American Chemical Society* (2013), 135(30), 10883–10885.
4. Vura-Weis, Josh; Abdelwahed, Sameh H.; Shukla, Ruchi; Rathore, Rajendra; Ratner, Mark A.; Wasielewski, Michael R. "Crossover from Single-Step Tunneling to Multistep Hopping for Molecular Triplet Energy Transfer". Science (2010), 328(5985), 1547-1550.

1. **Antimicrobial Agents and Therapeutics**
   This category covers the design, synthesis, and evaluation of novel compounds with antimicrobial properties, including studies on their structural optimization and biological activity.

Papers:

- **Khalifa, A.; Anwar, M. M.; Alshareef, W. A.; El Gebaly, E. A. E.; Elseginy, S. A.; Abdelwahed, S. H.** *Design, Synthesis, and Antimicrobial Evaluation of Some New Thiopyrimidin-Benzenesulfonamide Compounds.* Molecules 2024, 29(19), 4778.

This paper focuses on the development of thiopyrimidin-benzenesulfonamide derivatives with potential antimicrobial activity, with synthesis and biological assays to assess their effectiveness.

- **Abd El-Karima, S. S.; Anwara, M. M.; Syama, Y. M.; Awad, H. M.; El-Dein, A. N.; El-Ashrey, M. K.; Abdelwahed, S.** *New Benzofuran-Pyrazole Based Compounds as Promising Antimicrobial Agents: Design, Synthesis, Antioxidant, Anti-inflammatory, DNA Gyrase B Inhibition and In Silico Studies.* Preprints 2024, 2024081792.
  This study introduces benzofuran-pyrazole compounds with promising antimicrobial, antioxidant, and anti-inflammatory properties, highlighting their DNA gyrase B inhibition and potential as therapeutic agents.
- **Abdel-Mohsen, Heba T., Manal M. Anwar, Nesreen S. Ahmed, Somaia S. Abd El-Karim, and Sameh H. Abdelwahed.** *Recent Advances in Structural Optimization of Quinazoline-Based Protein Kinase Inhibitors for Cancer Therapy (2021–Present).* Molecules 2024, 29, 875.
  This paper discusses the structural optimization of quinazoline-based inhibitors targeting protein kinases, emphasizing their therapeutic role in cancer therapy.

2. **Cancer and Oncogenic Metabolism**
   This area explores the molecular mechanisms behind cancer, focusing on oncogenic pathways and potential therapeutic targets.

Papers:

- **Junaid, Ahmad; Nwaogwugwu, Caleb; Abdelwahed, Sameh.** *Exploring the Role of TRANSKETOLASE LIKE-1 (TKTL-1) in Cancer: Insights into Oncogenic Metabolism and Therapeutic Prospects.* Cancer Informatics, 2024 (accepted and under publication).
  This paper provides insights into the role of TKTL-1 in cancer metabolism and examines its potential as a target for therapeutic intervention.

3. **Enzyme Mechanisms and Radical Reactions in Biosynthesis**
   This research focuses on understanding the mechanisms of enzyme-catalyzed reactions, particularly involving radical intermediates and their role in biosynthesis pathways, such as thiamin and vitamin B12.

Papers:

- **Sharma, V.; Fedoseyenko, D.; Joshi, S.; Abdelwahed, S.; Begley, T.** *Phosphomethylpyrimidine Synthase (ThiC): A "Radical Dance" in Bacterial Thiamin Biosynthesis.* Journal of Biological Chemistry 2024, 300 (3), 106236.
  This study delves into the radical reaction mechanisms involved in thiamin biosynthesis, focusing on phosphomethylpyrimidine synthase.
- **Vishav Sharma, Dmytro Fedoseyenko, Sumedh Joshi, Sameh Abdelwahed, and Tadhg P. Begley.** *Phosphomethylpyrimidine Synthase (ThiC): Trapping of Five Intermediates Provides Mechanistic Insights on a Complex Radical Cascade Reaction in Thiamin Biosynthesis.* ACS Central Science 2024, 10 (5), 988-1000.
  This paper presents a detailed mechanistic study of the enzyme ThiC, revealing intermediates in the radical cascade reaction of thiamin biosynthesis.
- **Angad P. Mehta, Sameh H. Abdelwahed, Michael K. Fenwick, Amrita B. Hazra, Michiko E. Taga, Yang Zhang, Steven E. Ealick, and Tadhg P. Begley.** *Anaerobic 5-Hydroxybenzimidazole Formation from Aminoimidazole Ribotide: An Unanticipated Intersection of Thiamin and Vitamin B12 Biosynthesis.* Journal of the American Chemical Society 2015, 137(33), 10444-10447.
  This paper uncovers a surprising link between thiamin and vitamin B12 biosynthesis, highlighting the anaerobic formation of a 5-hydroxybenzimidazole.
- **Derek M. Gagnon, Troy A. Stich, Angad P. Mehta, Sameh H. Abdelwahed, Tadhg P. Begley, R. David Britt.** *An Aminoimidazole Radical Intermediate in the Anaerobic Biosynthesis of the 5,6-dimethylbenzimidazole Ligand to Vitamin B12.* Journal of the American Chemical Society 2018, 140 (40), 12798–12807.
  The paper focuses on the radical intermediate in the biosynthesis of a key ligand in vitamin B12 production.

4. **Computational and Structural Chemistry**
   This category includes the computational modeling and experimental study of electron transfer, radical reactions, and enzyme catalysis, as well as structural optimization of molecules for therapeutic applications.

Papers:

- **Ahmad Junaid, Grace Abolaji, Sameh Abdelwahed.** *Computational Screening for Novel Herbal-based SARSCoV-2 Structural Protein Modulators.* Biomed J Sci & Tech Res 2021, 40(1).
  This paper explores computational screening methods for identifying potential herbal-based inhibitors targeting SARS-CoV-2 structural proteins.
- **Rajendra Rathore, Sameh H. Abdelwahed.** *Design and Synthesis of Cofacially-Arrayed Polyfluorene Wires for Electron and Energy Transfer Studies.* Molecules 2023, 28 (9), 3717.
  This study investigates the design and synthesis of polyfluorene wires for electron and energy transfer, focusing on their potential applications in molecular electronics.
- **Rajendra Rathore, Sergey V. Lindeman, Sameh H. Abdelwahed.** *Design, Synthesis, Electronic Properties, and X-ray Structural Characterization of Various Modified Electron-Rich Calixarene Derivatives and Their Conversion to Stable Cation Radical Salts.* Molecules 2022, 27(18), 5994.
  The paper examines electron-rich calixarene derivatives and their conversion into stable radical salts, with potential applications in molecular electronics.
- **Angad P. Mehta, Sameh H. Abdelwahed, Hui Xu, and Tadhg P. Begley.** *Molybdopterin Biosynthesis: Trapping of Intermediates for the MoaA-Catalyzed Reaction Using 2′-DeoxyGTP and 2′-ChloroGTP as Substrate Analogues.* Journal of the American Chemical Society 2014, 136 (30), 10609–10614.
  This work focuses on the mechanistic studies of molybdopterin biosynthesis, exploring the trapping of reaction intermediates.
- **Maxim V. Ivanov, Marat R. Talipov, Anitha Boddeda, Sameh H. Abdelwahed, and Rajendra Rathore.** *Hučkel Theory + Reorganization Energy = Marcus−Hush Theory: Breakdown of the 1/n Trend in π-Conjugated Poly-p-phenylene Cation Radicals Is Explained.* Journal of Physical Chemistry C 2017, 121(3), 1552-1561.
  This study combines theoretical approaches to explain the breakdown of electron transfer trends in π-conjugated poly-p-phenylene cation radicals.

Research Interests Overview

Dr. Sameh H. Abdelwahed's research spans several interdisciplinary areas, primarily focused on:

- **Antimicrobial and Therapeutic Compound Development**: He is involved in designing and synthesizing novel bioactive compounds, particularly targeting antimicrobial and anticancer activities, with a focus on structural optimization and biological evaluation.
- **Enzyme Mechanisms and Radical Reactions**: A significant part of his work investigates the mechanistic details of radical-mediated reactions, particularly in the biosynthesis of essential vitamins like thiamin and vitamin B12, contributing to a deeper understanding of complex enzymatic processes.
- **Oncogenic Metabolism**: Dr. Abdelwahed also explores the role of key metabolic enzymes like TKTL-1 in cancer, looking at their therapeutic potential.
- **Computational and Structural Chemistry**: His research includes computational studies for drug discovery and the structural characterization of molecules for applications in molecular electronics and enzyme catalysis.