Dr. Gennadii Grabovyi, PhD CURRICULUM VITAE

Personal Information

Nationality	Ukrainian
USA Legal Status	Permanent resident
Residence	San Diego, CA
Phone	+1 (312) 589-8369
E-mail	gengrab@gmail.com

Education

08/**2013**–11/**2019** **Ph.D. in Chemistry**
University of Illinois at Chicago, Chicago, USA

05/**2010**–05/**2012** **M.S. in Chemistry**
Lomonosov Moscow State University, Moscow, Russia

08/**2007**–05/**2010** **B.S. in Chemistry**
Lomonosov Moscow State University, Moscow, Russia

Overview

14 years of experience in synthetic and analytical organic chemistry, 4 years of post-PhD experience in medicinal chemistry and drug discovery with the specialty in total synthesis of novel biologically active compounds of medicinal importance (*in silico* library screening, hit identification, hit → lead work, lead optimization, preclinical studies). Areas of expertise include small molecule drug discovery, synthetic and analytical organic chemistry, medicinal chemistry, pre-clinical pharmacology (ADME, PK, tox and efficacy studies), computational chemistry, CRO management, and talent acquisition.

Professional Research Experience

09/**2022**–present **Investigator in Drug Discovery, The Scripps Research Institute, Calibr division**
Leading the chemistry and pharmacology efforts both in the house and with CRO for the drug discovery in the following disease areas:
- Cancer, neurodegenerative, cardiovascular diseases (development of novel NRF2/KEAP1 activators)
- Diabetes and obesity (development of a novel peptide agonist of GLP-1R, GIPR, and GCGR)
- 2019 Novel Coronavirus (SARS-CoV-2; COVID-19) (targeting PL^{pro} and CL^{pro} of the virus)
- Niemann-Pick disease (*in silico* → *in vitro* studies to restore the function of NPC1 protein)
- Chagas disease.

05/**2020**–09/**2022** **Postdoctoral Researcher in Drug Discovery, The Scripps Research Institute, Calibr division**
(Research advisor Dr. Arnab K. Chatterjee)
- Early → late-stage drug discovery for treatment of 2019 Novel Coronavirus (SARS-CoV-2; COVID-19) targeting CL^{pro} and RdRp of the virus. Proposed and synthesized ~ 300 novel CL^{pro} inhibitors guided by computational and experimental SAR data. Optimized targets for *in vitro* potency (calu-3, hela), efficacy (ADME on various animal cell lines), and *in vivo* pharmacokinetic properties (PK in mouse, hamster, rat, dog, monkey). All synthesized compounds were patented (3 patents)
- Proposed and synthesized a COVID-19 drug-candidate CMX990 that went into Phase 1 clinical trials in a partnership with AbbVie
- Early-stage drug discovery and synthesis of drug-candidates in a field of proteolysis targeting chimeras (PROTAC)
- Late-stage drug optimizations using Hippo-YAP signaling pathway.

02/**2019**–05/**2019** **Visiting Doctoral Researcher in Organic Chemistry, California Institute of Technology**
(Research advisor Prof. B. M. Stoltz)
- Copper-catalyzed enantioselective alkylation of dienol silyl ethers
- Nickel-catalyzed enantioselective alkylation and arylation of dienol silyl ethers.

02/**2014**–05/**2020** **Doctoral Researcher in Organic Chemistry, University of Illinois at Chicago**
(Research advisor Prof. J. T. Mohr)
- Total synthesis of biologically active natural products using α,γ-functionalization of cyclic vinylogous esters (including total synthesis of grifolin, grifolic acid, ilicicollinic acid A, LL-Z1272α, LL-Z1272β, colletochlorins A–G, colletorin A–C, cylindrocarpol, chlorocylindrocarpol, aspergillusenes B, aeroplysinin-1, and amorfrutin A)
- Development of novel nickel-catalyzed transformations on electronically rich aryl chlorides to access bioactive natural alkaloids
- Enantioselective formal synthesis of (–)-platencin (collaboration with Prof. B. M. Stoltz).

05/**2010**–05/**2013** **Master's Researcher in Organic Chemistry, Lomonosov Moscow State University**
(Research advisor Prof. I. P. Beletskaya)
- Synthesis of nitrogen-containing derivatives of bile acids and their application as novel amphiphilic ligands.

08/**2007**–05/**2010** **Bachelor's Researcher in General Chemistry, Lomonosov Moscow State University**
- Synthesis and property investigation of Cu-doped CdSe colloidal quantum dots (research advisor Prof. T. A. Kuznetsova)
- Developing of new spectroscopic methods of investigation of algae microorganisms (research advisor Prof. M. A. Proskurnin)
- Synthesis of 3-amino-7,12-dihydroxydeoxycholan-24-oate (research advisor Prof. N. V. Lukashev).
- The quantum-chemical calculation of thermodynamic properties of organic azides (research advisor Prof. O. V. Dorofeeva).

Patents

1. Chatterjee, A. K.; Chen, J. J.; Nakath, E.; Rahimi, A.; Gupta, A.; Grabovyi, G. A.; Wilson, K.; Ghorai, S.; Nazarian, A.; Pedroarena, J.; Mazumdar, W.; Weiss, F.; Song ,L.; Bakowski, M. A.; Riva, L.; Wolff, K.; McNamara, C. W.; Rogers, T. F. Protease Inhibitors for Treatment of Coronavirus Infections. U.S. Patent WO 2022266363, December 22, 2022.

2. Chatterjee, A. K.; Chen, J. J.; Nakath, E.; Rahimi, A.; Gupta, A.; Grabovyi, G. A.; Wilson, K.; Ghorai, S.; Nazarian, A.; Pedroarena, J.; Mazumdar, W.; Weiss, F.; Song ,L.; Bakowski, M. A.; Riva, L.; Wolff, K.; McNamara, C. W.; Rogers, T. F. Protease Inhibitors for Treatment of Coronavirus Infections. U.S. Patent WO 2022261473, December 15, 2022.

3. Chatterjee, A. K.; Petrassi, M.; Chen, J. J.; Gupta, A.; Wilson, K.; Grabovyi, G. A. U. S. Patent Application No. 63/284,952 filed December 1, 2021 "Antiviral Prodrugs and Formulations Thereof" TSRI Case 2117.0 / CIB0454P.

Publications

1. Nakath, E.; Wolff, K. C.; Riva, L.; Woods, A. K.; Grabovyi, G. A; Wilson, K.; Rahimi, A.; Pedroarena, J.; Ghorai, S.; Gupta, A. K.; Nazarian, A.; Weiss, F.; Liu, Y.; Mazumdar, W.; Song, L.; Okwor, N.; Malvin, J.; Bakowski, M. A.; Beutler, N.; Kirkpatrick, M. G.; Gebara-Lamb, A.; Huang, E.; Nguyen-Tran, V.; Chi, V.; Li, S.; Rogers, T. F.; McNamara, C. W.; Chen, J. J.; Joseph, S. B.; Schultz, P. G.; Chatterjee, A. K. 2023. Discovery of CMX990: A Potent SARS-CoV-2 3CL Protease Inhibitor Bearing a Novel Covalent Warhead. *J. Med. Chem.* **2024***, 67,* 2369−2378.

2. Nakath, E.; Wolff, K. C.; Riva, L.; Woods, A. K.; Grabovyi, G. A; Wilson, K.; Rahimi, A.; Pedroarena, J.; Ghorai, S.; Gupta, A. K.; Nazarian, A.; Weiss, F.; Liu, Y.; Mazumdar, W.; Song, L.; Okwor, N.; Malvin, J.; Bakowski, M. A.; Beutler, N.; Kirkpatrick, M. G.; Gebara-Lamb, A.; Huang, E.; Nguyen-Tran, V.; Chi, V.; Li, S.; Rogers, T. F.; McNamara, C. W.; Chen, J. J.; Joseph, S. B.; Schultz, P. G.; Chatterjee, A. K. 2023. Discovery of CMX990: A Potent SARS-CoV-2 3CL Protease Inhibitor Bearing a Novel Covalent Warhead. bioRxiv doi: 10.1101/2023.10.24.563688

3. Grabovyi, G. A.; Bhatti, A.; and Mohr, J. T. Total Synthesis of Benzofuran-Based Aspergillusene B via Halogenative Aromatization of Enones. *Org. Lett.* **2020**, *22*, 4196–4200.

4. Defieber, C.; Mohr, J. T.; Grabovyi, G. A.; Stoltz, B. M. Short Enantioselective Formal Synthesis of (–)-Platencin. *Synthesis* **2018**, *50*, 4359–4368. Dedicated to Prof. Dr. Scott E. Denmark on the occasion of his 65th birthday.

5. Grabovyi, G. A.; Mohr, J. T. Synthetic Studies Toward the Total Synthesis of Aeroplysinin. *ARKIVOC* **2018**, *part iv*, 215–230. Special Issue in honor of Prof. Gordon Gribble's retirement.

6. Lukashev, N. V.; Grabovyi, G. A.; Erzunov, D. A.; Kazantsev, A. V.; Latyshev, G. V.; Averin, A. D.; Beletskaya, I. P. Pd- and Cu-Catalyzed Approaches in the Syntheses of New Cholane Aminoanthraquinone Pincer-like Ligands. *Beilstein J. Org. Chem.* **2017**, *13*, 564–570.

7. Grabovyi, G. A.; Mohr, J. T. Total Synthesis of Grifolin, Grifolic Acid, LL-Z1272α, LL-Z1272β, and Ilicicolinic Acid A. *Org. Lett.* **2016**, *18*, 5010–5013. Highlighted by Prof. Douglass F. Taber at organic-chemistry.org, June 19, 2017.

Professional Research Skills

Management and Laboratory Operations

- on-site hiring, training, and management of junior synthetic chemists (BSc, MSc, PhD levels)
- off-site management of CRO teams of synthetic chemists (Aragen Life Sciences Ltd., Symbol Ltd., LAXAI Life Sciences)
- maintenance of laboratory equipment (rotovaps, hot plates, pumps, UPLCs, etc.)
- supervision and organization of chemical inventory.

Synthetic Organic Chemistry

- small molecule organic compounds synthesis in both air- and inert atmosphere in temperature ranges –78 to 189 °C (bench-top and glovebox)
- micro- (<1 mg) and macro-scale (>100 g) multi-step organic synthesis including batch processes (>100 reactions at a time)
- areas of synthetic expertise are total organic synthesis, reaction optimization, peptide synthesis, metal catalysis, enantioselective chemistry.

Analytical Organic Chemistry

- purification of small molecule organic compounds via normal and a reverse phase manual and automated flash-column chromatography (BioTage, Teledyle), prep-HPLC (Waters), prep-TLC, recrystallization, distillation, sublimation
- data analysis via (U)HPLC-MS (Agilent, Waters), NMR (Bruker), PLM (Nikon), Particle Size Analyzer (Malvern), TLC, GC-MS (Agilent), SFC-MS (Agilent), IR (Nicolet), XRD, UV, melting and boiling points
- data analysis software: ChemDraw, MNova, Prizm Graph Pad, MS Office Suite, Schrodinger's Maestro, and ACAS Suite.

Medicinal Chemistry and Drug Discovery

- computational methods of drug discovery via shape and structure-based molecular docking in Schrödinger (Maestro, LiveDesign)
- early-stage library design and data analysis via SAR, including potency and ADME optimization
- late-stage optimization of drug's pharmacokinetic properties (PK data analysis)
- data management via LiveDesign (Schrödinger) and ACAS (Assay Capture and Analysis System).