Pharmacological assessments of different fractions of Paspalidium flavidum via in vitro, in vivo, and in-silico studies

Abstract

Supercontinuum generation (SCG) is a nonlinear optical phenomenon in which intense ultrashort laser pulses propagate through nonlinear media and undergo dramatic spectral broadening, producing a continuous, ultra-wide optical spectrum. SCG has become a cornerstone technology in photonic applications including molecular spectroscopy, biomedical imaging, optical coherence tomography, and environmental sensing. The mid-infrared (MIR) spectral region is of particular importance because most chemical compounds and biomolecules exhibit strong and unique absorption fingerprints in this range, making broadband MIR sources highly valuable for sensing and diagnostics. Among nonlinear optical materials, tellurium-based chalcogenide glasses — specifically Ge-As-Se-Te and Ge-Sb-Se-Te — are promising due to their exceptionally high nonlinear refractive index, wide transparency extending beyond 20 μm, and strong optical confinement. When structured as tapered waveguides with magnesium fluoride (MgF_2) cladding, these materials allow precise dispersion engineering along the propagation direction, enabling efficient nonlinear interactions such as soliton fission, four-wave mixing, and dispersive wave generation that drive ultra-broadband spectral output. However, designing such tapered waveguides for optimal performance is a highly challenging task. The output spectrum is governed by the generalized nonlinear Schrödinger equation (GNLSE) and is acutely sensitive to the interplay of pump conditions, waveguide geometry, taper profile, and higher-order dispersion. Conventional design relies on exhaustive trial-and-error GNLSE simulations, which become computationally prohibitive when exploring the high-dimensional parameter space of a tapered structure — often requiring tens of thousands of individual simulations per optimization run. This research addresses this challenge through a two-pronged framework that combines rigorous numerical simulation with machine learning-based surrogate optimization. On the numerical side, finite element method (FEM) modeling and GNLSE simulations are used to accurately capture the full nonlinear pulse dynamics in Ge-As-Se-Te and Ge-Sb-Se-Te tapered waveguides, targeting spectral coverage from 2 μm to 20 μm with coherence and noise levels below −30 dB. On the machine learning side, a physics-guided surrogate neural network is trained on a systematically generated GNLSE dataset, enabling prediction of multiple performance outputs — bandwidth, flatness, coherence, and conversion efficiency — in milliseconds rather than seconds per evaluation. This surrogate replaces GNLSE calls during optimization, reducing computational cost by several orders of magnitude. Multi-objective optimization is then applied to the surrogate to produce a set of optimal designs that simultaneously trade off bandwidth, coherence, and propagation loss. Critically, the framework also incorporates fabrication robustness prediction, training the surrogate to estimate expected performance variance under realistic waveguide width tolerances, thereby enabling designs that are both high-performing and tolerant to fabrication imperfections. The combined numerical and ML-assisted methodology is expected to establish a systematic, efficient, and practically viable design framework for next-generation compact MIR supercontinuum sources for molecular sensing applications.