



Application Note: In-situ NMR Illuminator for Precision Photochemistry in Fixed-Field NMR

Introduction

The **In-situ NMR Illuminator**, manufactured by **Field Cycling Technology Ltd.**, is a compact and high-efficiency solution designed for photochemical experiments within fixed-field Nuclear Magnetic Resonance (NMR) spectrometers. Unlike traditional laser-based setups that often involve complex optical paths or place the light source outside the critical detection volume, this system is engineered to provide superior illumination efficiency and uniformity directly inside the sample.

Key Features and Advantages

The system overcomes several limitations inherent in "home-built" laser/fiber optic setups:

- **Homogeneous Irradiation:** Utilizing non-coherent LED sources, the system delivers radially uniform irradiance, eliminating interference patterns and uneven illumination common with coherent laser light.
- **Minimized Power Loss:** High-power LEDs are positioned proximally to the sample, circumventing the significant power losses associated with long optical fiber transmissions.
- **Seamless Integration:** The device is designed for effortless installation onto commercially available standard 5 mm liquid-state NMR tubes **without requiring any modifications to the magnet hardware.**
- **Industrial-Grade Stability:** The system provides stable power control and a standardized 4 mm light guide that minimizes reflection variability and angular misalignment inside the tube.

Primary Applications

The In-situ NMR Illuminator is optimized for a wide range of light-driven NMR investigations, including:

- **Photo-CIDNP** (Chemically Induced Dynamic Nuclear Polarization) for drastic signal enhancement.
- **In-situ Photoreactions:** Monitoring reaction kinetics and mechanisms in real-time.
- **Biomolecular Research:** Metabolic pathway illumination, radical-pair photochemistry, and **in-cell NMR** photo-activation.
- **Optogenetics:** Studying molecular behavior and signaling pathways under controlled light influence.

Technical Specifications



- **Light Source:** High-power LEDs with adjustable power levels (200 levels via software).
- **Available Wavelengths:** Royal Blue (450nm, max. 2000mW), Blue (475nm, max. 1500mW), Green (530nm, max. 750mW), and Red (625nm, max. 800mW), Closed UV (410nm, max. 500mW); custom wavelengths available upon request.
- **Power Delivery:** Up to 2000±200 mW delivered through a 4 mm diameter high-efficiency light guide.
- **Synchronization:** Integrated TTL trigger interface for precise coordination with NMR pulse programs.

Installation and Operation

To ensure high-quality, reproducible data, the system follows a standardized workflow:

1. **Assembly:** The light guide is secured to the tube holder with silicon O-rings. It is recommended to clean the exposed part of the guide before installing the NMR tube to prevent contamination.
2. **Precision Centering:** Users must use the spectrometer provided **sample gauge** to ensure the sample is precisely positioned at the center of the RF coil before insertion into the magnet.
3. **Synchronization:** The timing of illumination program is controlled via the FCNMR GUI, allowing for automated triggering via the NMR console.
4. **Irradiation Durations:** Adhere to suggested safety limits for continuous irradiation (power adjusted within 200 levels via software):
 - **Low Power (Levels 1–3):** Up to 30 s.
 - **Intermediate (Levels 4–12):** 2 s to 10 s.
 - **High Power (Levels >25):** Maximum **200 ms** per cycle.
5. **Calibration:** A dedicated **optical power meter** is included to calibrate the light source monthly, ensuring "Total Power in Sample" readouts remain accurate over time.

Conclusion

The FCNMR In-situ NMR Illuminator unlocks new experimental dimensions for existing high-field and bench-top NMR spectrometers, enabling photo-CIDNP signal enhancement, real-time photoreaction monitoring, and light-driven biomolecular studies that were previously inaccessible without complex custom setups. With standardized hardware, software-controlled illumination, and seamless integration into existing probe configurations, researchers can expand into new experimental directions immediately, without rebuilding their infrastructure.

Contact Information:

For technical consultations or quotes, please contact shuttle@fcnmr.com or visit www.fcnmr.com