

Unlocking New Insights Into Targeting LRRK2 For Parkinson's Disease: Advancing Drug Discovery With The CAS BioFinder Discovery Platform™

E. Detta,^a J. Raymond,^a J. Al-Saleem,^a

CAS 2540 Olentangy River Road Columbus, Ohio 43202 U.S.A

edetta@acs-i.org

Effective drug discovery for any medical condition requires informed decision-making based on comprehensive, structured, and harmonized data. We herein showcase how the CAS BioFinder Discovery Platform™--a solution designed to streamline the overall drug design, discovery, and development process by integrating key resources in one platform—can enable the efficient exploration of leucine-rich repeat serine/threonine-protein kinase 2 (LRRK2) as a therapeutic target for the treatment of Parkinson's disease. To be specific, we demonstrate that CAS BioFinder™ facilitates:

- Access to all published activity data for ligands targeting specific proteins and diseases, such as LRRK2 and Parkinson's disease
- Identification of molecular scaffolds from the most potent ligands against a target, such as LRRK2
- Analysis of local structure-activity relationships (SAR) to investigate how well-defined structural modifications influence compound properties
- Prioritization of known and novel compounds based on predictive molecular characteristics and off-target activity assessments
- Visualization of protein crystal structures to analyze binding pockets and guide rational drug design
- Exploration of disease modulation strategies through access to relevant biomarkers

By consolidating these critical research components, our approach could enhance the efficiency of target evaluation and accelerate the development of novel therapeutics for Parkinson's disease.