

Jackson State University
Notice of Proposed Sole Source Purchase 26-03
Small Molecule Drug Discovery Suite Software
RFX 3150007041

Jackson State University anticipates purchasing the item listed below as a sole source purchase. Anyone objecting to this purchase shall follow the procedures outlined below.

Product Overview:

The Schrödinger Small Molecule Drug Discovery Suite is a comprehensive software suite designed for the investigation of chemical systems. It includes tools for target preparation, ligand preparation, workflow automation, and virtual modeling. The suite will be available for use by faculty, staff, and students at Jackson State University.

Explanation of need to be fulfilled by this item, how it is unique from all other options, and why it is the only one that can meet the specific needs of the department:

The Agency conducted a market review of available platforms for small molecule drug discovery and advanced molecular modeling and found that Schrödinger is the only provider offering a fully integrated suite — combining quantum chemistry, molecular dynamics, machine learning, and biologics modeling through proprietary modules such as Glide, DeepAutoQSAR, and LigPrep — within a single, validated, and seamlessly compatible workflow that no other vendor can replicate with equivalent depth or performance. This exclusivity was confirmed directly by Schrödinger in a sole source letter.

Name of company selling the item and why that source is the only possible source that can provide:

The name of the company is Schrödinger, LLC 101 SW Main Street, Suite 1300 Portland, OR 97204. Schrödinger is the sole manufacturer of the molecular modeling software. No other vendor provides this breadth of functionality within a unified, validated framework.

Estimated cost of item and explanation of why the amount to be expended is considered reasonable:

The estimated total cost of \$65,318.25 reflects a fair and strategic investment given the scope of included tools and the long-term value they provide. To ensure the best possible price, the department negotiated directly with Schrödinger and

secured academic and volume-based discounts, including a significant reduction tied to a five-year license term. This long-term commitment, combined with a floating license model and bundled access, provides favorable pricing, cost predictability, and efficient shared use across the research programs. Given the breadth of proprietary, integrated capability covered under this single procurement and the reduced infrastructure and per-seat costs made possible by the hosted, shared license model — with first-year server hosting included at no additional charge — the Agency has determined the negotiated price to be fair and reasonable.

Explanation of the efforts taken by the department to determine that this is the only source and efforts used to obtain the best possible price:

1. With departmental need at front of mind, the department researched the marketplace and found that this item is the only one that will adequately meet the needs for research and curriculum purposes and determined that Schrödinger, LLC is the only manufacturer of this product.
2. Office of Purchasing and Travel searched DFA for item and vendor to no avail. Also, the web was searched for alternate vendors to no avail as all listings of the product linked to Schrödinger, LLC as the sole purveyor of the item.

Any person or entity that objects and proposes that the commodity listed is not sole source and can be provided by another person or entity shall submit a written notice to:

Kimberly R. Harris, CMPA, MHSA Director
of Procurement Services
kimberly.r.harris@jsums.edu
Subject Line must read "Sole Source Objection"

The notice shall contain a detailed explanation of why the commodity is not a sole source procurement. Appropriate documentation shall also be submitted if applicable.

If after a review of the submitted notice and documents, JSU determines that the commodity in the proposed sole source request can be provided by another person or entity, then JSU will withdraw the sole source request publication from the procurement portal website and submit the procurement of the commodity to an advertised competitive bid or selection process.