UNIVERSITY of SOUTH FLORIDA

SINGLE SOURCE CERTIFICATION

Authority is requested to make the following purchase under the provision of USF System Regulation USF4.02010(IV)(A)(2)(b) as a non-competitive purchase available from only one source. By submitting this form, department acknowledges that existing exemptions will not apply to this purchase. Single source requests exceeding $75,000 must be signed by a Procurement Director and posted publicly for (3) business days.

DATE: 01/13/2023

ITEM(S): SPINSOLVE 60 Multi-X PLUS

PRICE: $ 76,900 **FUND #:** TPA 10000 121300 000000 (

SUPPLIER ID: _____ **REQUISITION#:** _____

SUPPLIER NAME: Magritek

FEDERAL GRANT: ○ Y ◉ N

In your words, describe the equipment, commodity, or contractual service. Explain how these specifications are essential to the accomplishment of your work:

This NMR is going to be used for inorganic undergraduate classroom. It will serve as a teaching tool for future professionals. This is the leading hardware and software on the field and its manufactured by Magritek.This instrument would be used for the undergraduate Inorganic, Analytical, and Methods labs for specific experiments, especially on experiments of some paramagnetic metal complexes and interactions of metal with various molecules. Dr. Ming verified the feasibility of this particular instrument for such experiments. The built-in four-channel system in the Magritek NMR allows the desired experiments of paramagnetic metal complexes to be conducted in the Inorganic labs smoothly.

In your own words, describe the reason(s) the item is not subject to competition from other sources and how the stated specification(s) restrict the requisition to only one supplier. Description may include unique features/compatibility/specifications/availability/delivery time frame etc. (Note: Price is not a valid reason).

The Magritek is the manufacturer of the Spinsolve 60 Multi X NMR spectrometer. This is highly specialized piece of equipment.

In your own words, describe the due diligence conducted to validate this supplier as Single Source. Description SHOULD list all other suppliers with item(s)/service(s) with similar functions, your efforts to identify other suppliers, and why these suppliers would not qualify to submit a competitive quote.

Alternatives by Dr. Ming and Dr. Figueroa were searched however the Spinsolve Multi X NMR Spectrometer is a Magritek product.

Michael A. Hernandez Digitally signed by Michael A. Hernandez Date: 2023.02.09 08:32:20 -05'00'

Approved By (Procurement) **DATE**

START 2/8/23 END 2/13/23_

PUBLIC POSTING DATES

Authority: USF4.02010(IV)(A)(2)(b)

Last Modified: 05/10/2021

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Basic NMR Specification	Value	Explanation
NMR Resonance Frequency	minimum 60 MHz	Proton NMR Frequency of the NMR Spectrometer
Detectable Nuclei	**^{1}H, ^{19}F, ^{13}C,^{31}P**	4 nuclei on one single system switched in a fully automati simply selecting the nuclei in the software (no manual matching required / no user intervention needed).
Queued Experiments	**All Protocols available without intervention**	User should be able to queue any number of experiments av the instrument without having to tune or match manually intervention should be required.
Resolution / Linewidth Line width at 50% Peak height (Standard sample: 20% chloroform dissolved in deuterated acetone)	**< 0.35 Hz**	Reached without sample spinning and determined mathematical post-processing – Magritek realized th manufacturers apply so-called Reference Deconvolution - a algorithm that improves the resolution by a mathematical m This specification shall display the resolution without appl mathematical procedures.
Resolution / Linewidth Line width at 0.55 % Peak height (Standard sample: 20% chloroform dissolved in deuterated acetone)	**< 10 Hz**	Reached without sample spinning and determined mathematical post-processing – Magritek realized th manufacturers apply so-called Reference Deconvolution - a algorithm that improves the resolution by a mathematical m This specification shall display the resolution without appl mathematical procedures.
^{1}H Sensitivity (Standard sample 1% Ethyl Benzene in deuterated Chloroform)	**> 130:1**	Magritek calculates SNR according to ASTM method E386–9 Determination of the Sensitivity of NMR Instruments. For spectrum of a 1% Ethyl benzene sample in deuterated chlo recorded with a single scan. For S/N calculation the amplitu highest peak of the methylene quartet is divided by the deviation of the noise. For noise calculation an area of so between the methylene and the aromatic signals is chosen amplitude of the noise band is determined. The reciprocal n amplitude is multiplied with the signal amplitude of the hig of the methylene quartet and the calculated value is then inc S/N (SNR) or sensitivity.
NMR Magnet, Shim and Lock …	**Value**	**Explanation**
Magnet Geometry	Halbach	Any Spinsolve NMR System possesses patented Halbach magnet technology. The following Patents apply: US201000 US8148988, EP2144076A1, EP2144076B1. Halbach mag compact and have a low weight as compared to other magn
Magnet Shielding	Multi-layer mu-metal cylinder	Magnet sits into a multi-layer mu-metal cylinder that sh magnet from outside magnetic field changes / disturbance required to assure a stable NMR system performance.
Magnet Stray Field	< 2 Gauss	The stray field of the Magnet is completely inside the hou Gauss). Given such a low stray field, credit cards will not be d in the vicinity of the apparatus. Also operators with implantations are not in danger when working with the NI the Earth magnetic field is approximately about 0.5 G (de location – typical value in Germany).
Magnet Temperature Control	< 1 mK	The Spinsolve magnet sits inside the mu-metal cylinder hou within this housing the temperature is controlled to better t Important for instrument stability.

Concept to de-couple magnet temperature from room temperature (variations)	System has 2 tempering zones whereby the magnet sits in a separate inner temperature zone which is surrounded by the 2nd zone being temperature-controlled	A constant magnet temperature is the key for a highly sta instrument. Any temperature variation will cause broader N and then causes the need for re-shimming. By de-couplin from room temperature, external locking and shielding of th very robust device results that is capable of running t demanding NMR sequences, like for instance the HSQC-I sequence.
NMR Lock system	External fast hardware lock	Deuterated solvents are not needed for system locking. The lock functions properly in any measurement situation. Other like a software lock or a Deuterium lock have severe disad While the Deuterium lock suffers from a low SNR on a Bench (and requires the use of Deuterated solvents), the software functions for measurements that have a strong NMR signal first scan) and for such NMR signals that will not shift during acquisition (like for a pH value change).
Shim Requirements	Shimming needed only once or twice a day	Due to the high stability of the Spinsolve instrument, shim system is required only once or twice a day (considerin laboratory conditions) and not whenever a sample is swapp
Sample Pre-Tempering	Not required	Samples that are being prepared in normal lab environmen need to be pre-tempered before insertion into the Spinsolve
NMR Tubes	5 mm	The instrument is designed to work with standard 5 mm NM
Infrastructural Requirements	**Value**	**Explanation**
Instrument Weight	< 60 kg	Allows easy transportation / movement of the equipmen people or lab cart
Instrument Dimensions	58 x 43 x 40 cm	Compact instrument design
No. of Instrument Compartments	1 Compartment only	PC not counted – one compartment assures a minimum o connections.
Cryogenics / Gasses	Not required	As Spinsolve works based on a permanent magnet, only ele required.
Power Requirements	100-250 V, 50/60 Hz	Spinsolve has no special power requirements.
Mobile / Flexible Use	Standard Laboratory Bench, Fume Hood or Option to place the NMR on a trolley to move it to different labs	Due to the size and the weight of the Spinsolve, the syste easily be re-positioned by 2 persons for instance to move t from the lab bench to the fume hood or vice versa. Spin systems can also be placed on a trolley to move the syst various laboratories.

Basic Specification	Value	Explanation
NMR Resonance Frequency	Minimum 60 MHz	Proton frequency of the spectrometer
Detectable Nuclei	^{1}H, ^{19}F, ^{13}C, ^{31}P	4 nuclei on one single system switched in a fully automatic way by simply selecting the nuclei in the software (no manual tuning or matching required / no user intervention needed).
Multinuclear Decoupling	$^{1}H\{^{13}C\}$, $^{1}H\{^{19}F\}$, $^{1}H\{^{31}P\}$, $^{19}F\{^{1}H\}$, $^{13}C\{^{1}H + ^{19}F\}$, $^{31}P\{^{1}H\}$	Multinuclear decoupling sequences should be able to be queued and conducted without user intervention required for tuning and matching.
Resolution / Linewidth **(Standard sample: 20% chloroform dissolved in deuterated acetone)**	Line Width at 50% of peak height = < 0.35 Hz Line Width at 0.55% of peak height = < 10 Hz	Reached without sample spinning and determined without mathematical post-processing – Magritek realized that other manufacturers apply so-called Reference Deconvolution - a software algorithm that improves the resolution by a mathematical method. This specification shall display the resolution without application of mathematical procedures.
Instrument Weight	>55 kg, 60 kg <	Total weight of the instrument should be more than 55 kg, but less than 60 kg.
Multinuclear Experiment Queue	All available 1D and 2D pulse sequences for available nuclei (^{1}H, ^{19}F, ^{13}C, ^{31}P) able to be performed without user intervention	No additional user intervention needed by the user for tuning and matching required for a queue involving up to all available nuclei. All experiments should be able to be collected through the software.