

LIMITED SOURCES JUSTIFICATION

ORDER >\$3,000

FAR PART 8.405-6(g)

2237 Transaction # or Vista Equipment Transaction #: 541-13-2-250-0020

This acquisition is conducted under the authority of the Multiple Award Schedule Program. The material or service listed in par. 3 below is sole source, therefore, consideration of the number of contractors required by FAR Subpart 8.4 – Federal Supply Schedules, is precluded for the reasons indicated below.

Restricted to the following source: Provide original manufacturer's name for material or contractor's name for service. (If a sole source manufacturer distributes via dealers, ALSO provide dealer information.)

Manufacturer/Contractor: Waters Associates

Manufacturer/Contractor POC & phone number: 800-252-4752

Mfgr/Contractor Address: 34 Maple Street, Milford, MA 01757

Dealer/Rep address/phone number: N/A

☒ The requested material or service represents the minimum requirements of the Government.

(1) AGENCY AND CONTRACTING ACTIVITY:

Department of Veterans Affairs

Network Contracting Office (NCO) 10

6150 Oak Tree Blvd. Suite 300

Independence, Ohio 44131-2569

VISN:

10

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(2) NATURE AND/OR DESCRIPTION OF ACTION BEING APPROVED:

The Department of Veteran Affairs (VA), Cleveland Veterans Affairs Medical Center (VAMC), has a requirement for a firm fixed price contract for mass spectrometers.

(3) (a) A DESCRIPTION OF THE SUPPLIES OR SERVICES REQUIRED TO MEET THE AGENCY'S NEED:

A mass spectrometer is used to determine the mass of any molecule by ionizing the sample to create charged fragments that are read by a mass analyzer and detector. Mass spectrometry can be used for anything from identifying the molecular mass of a known protein to determining the composition of an unknown sample. Mass spectrometry in the agency's hands will be used to: 1. Verify the molecular weights of purified proteins, which is required prior to further *in vitro* studies of that protein. 2. Identify any post-translation modifications to purified proteins. 3. Determine interactions between proteins and drugs, including but not limited to identifying chemical rearrangements in drug compounds as well as understanding mechanisms of protein-drug interactions. 4. Identify unknown proteins. 5. Identify which specific amino acid or region of a protein that a drug has bound to or has been post-translationally modified. For protein mass spectrometry, the agency requires an electrospray ionization (ESI) quadrupole time-of-flight (Q-TOF) instrument. Additionally, the

instrument must be capable of tandem mass spectrometry (MS/MS) technology. The Q-TOF instrument must possess the following set of critical specifications: 1. MS mass resolution is the ability of a mass spectrometer to differentiate between ions very close in m/z ratio and is measured in full width at half maximum values (FWHM). FWHM must be an average $\geq 35,000$ m/z. 2. Internal mass accuracy must be <1 ppm. 3. Linear dynamic range must be ≥ 4 orders of magnitude.

An ultra performance or high performance high pressure liquid chromatography system (HPLC) that allows for >96 samples to be desalted and injected onto the mass spectrometer in an automated cooled process with a heater to maintain the column temperature is required.

A superior approach to mass accuracy is required. Signal and sensitivity are critical when working with proteins and drugs that are limiting in concentration. An internal reference of known mass (calibrant) is used during the ionization process to correct for changes in environment or experimental conditions over the course of the analysis. The choice of calibrant compounds is made based on several criteria including: sufficient number of peaks in the mass range of interest, ease of ionization and detection with the instrument, and compatibility with the analyte of interest. The major advantage of a system that has two independent sprayers, one for the calibrant and the other for the sample (analyte) is that it separates the analyte from the calibrant, thus relaxing the selection rules described above. The calibrant can be in an entirely different solvent and it can have peaks that overlap with the analyte which greatly simplifies internal calibration for ESI. A system that has two independent sprayers is a required feature to meet the agency's needs.

A method is required to prevent unionized and unvaporized (harmful) components in the sample from reaching the lenses that focus the ion beam or the detector.

The capability of ion mobility, analogous to electrophoresis, but in the gas phase is absolutely required. This feature would be a fundamental enhancement to the agency's work examining drug binding sites on a protein and/or if the protein is post-translationally modified as well as looking at mutant proteins.

Ancillary characteristics of the instrument: The instrument must fit into a 7'X10' horizontal space with 10' of vertical space. The instrument must possess the ability to upgrade. A nitrogen generating source for the mass spectrometer must be supplied. Two computers/monitors for both data acquisition and data analyses as well as the software for the acquisition, analyses, and deconvolution must be included with the instrument systems. Three years of top tier or second highest tier of warranty including 1 performance maintenance visit per year and 10 days of training are required.

The Waters Synapt G2-S/Si instrument is the only one that currently offers ion mobility, has a superior calibration approach for mass accuracy, offers the most robust LC system, and has the potential to be upgraded as the agency's research questions evolve.

Transaction 541-13-2-250-0085 Equipment:

1 SYNAPT G2-S SYSTEM With the following configuration: 1 EA

SYNAPT G2-Si MS 8K
Synapt G2-S US Mains cable kit
SYNAPT G2-S roughing pump option
LockSpray source with ESI probe
MassLynx Performance Workstation
MONITOR, Lenovo Thinkvision Flat Panel
MS Ref Stds: TOF G2-S MS Install

Mass Lynx Software Options

Transform v4.1
MaxEnt 1 v4.1
MaxEnt 3 v4.1
BioLynx v4.1
MassLynx Process-Only PC
Monitor, Lenovo ThinkVision Flat Panel

ACQUITY UPLC H-Class Systems

ACQUITY UPLC H-Class Core System

Analytical Column Options

ACQUITY UPLC BEH C18 1.7 um 2.1 X 100mm col

Installation, Training and Plans

Synapt HDMS Installation Certificate

2 Lic.,MassLynx Supl. V4.1 User	1 EA
3 Synapt G2-S MS – HDMS upgrade	1 EA
4 NA-On-Site Field Apps Ed Cert (5 days)	2 EA
5 Nitrogen Generator NM32LA 230v	1 EA
6 TAW Synapt G2-S/Si (1PM)	1 EA
7 MassLynx Software 2 year plan	1 EA
8 TAW ACQUITY H-Class QSM (1PM)	1 EA
9 TAW ACQUITY H-Class SM-FTN (1PM)	1 EA
10 TAP Synapt G2S-Si (1PM)	1 EA
11 MassLynx Software 1 year plan	1 EA

12 TAP ACQUITY H-Class QSM (1PM)	1 EA
13 TAP ACQUITY H-Class SM-FTN (1PM)	1 EA
14 Installation Excellence kit	1 EA

(b) ESTIMATED DOLLAR VALUE: \$499,900.00

(c) REQUIRED DELIVERY DATE: August 15, 2013

(4) IDENTIFICATION OF THE JUSTIFICATION RATIONALE (SEE FAR 8.405-6), AND IF APPLICABLE, A DEMONSTRATION OF THE PROPOSED CONTRACTOR'S UNIQUE QUALIFICATIONS TO PROVIDE THE REQUIRED SUPPLY OR SERVICE.

☒ Specific characteristics of the material or service that limit the availability to a sole source (unique features, function of the item, etc.). Describe in detail why only this suggested source can furnish the requirements to the exclusion of other sources.

The Synapt G2-S/Si mass spectrometer items are made and distributed only by the Waters Corporation. The Synapt G2-S/Si from Waters combines the Stepwave ion optics and Quantitative ToF (QuanTof) technologies to provide the highest levels of sensitivity, selectivity, and speed on the market and was chosen based on the following patented instrument specifications:

1. The patented Z-spray technology allows the ion source to be of a dual orthogonal design. The nebulized sprayer is positioned orthogonally to the sampling orifice and be positioned off-axis for maximum source longevity and analyzer protection against "dirty" samples.
2. Hi-sensitivity ion optics (StepWave patent): The T-Wave based ion optics maximize sensitivity while maintaining system robustness. Neutral molecules and gas load are actively exhausted while the ion beam is actively extracted into a parallel off axis T-Wave device for enhanced transmission and to enable focusing into the analyzer.
3. The instrument has the option of an 8kDa quadrupole with the range of 20 to 8000 m/z in resolving mode and 20 to 30,000 m/z in non-resolving mode.
4. Ion arrival times are recorded using an analogue-to-digital converter (ADC) with an acquisition rate of 3G Samples/sec to provide excellent peak definition and mass accuracy. This is achieved by the ToF data acquisition system and covered under the QuanTof patent.
5. It is easy to select single or double pass geometries via the data system to provide spectral resolution >10,000 FWHM (full width half maximum) or >20,000 FWHM in single pass mode (Sensitivity and Resolution modes). This ability is covered under the QuanTof patent.
6. The mass range of the analyzer must be up to 100,000 m/z in single pass mode and 32,000 m/z in dual pass mode.
7. The TOF can acquire full spectral data at rates up to 30 spectra/sec.
8. The software offers data directed analysis (DDA) i.e., acquisitions whereby the instrument automatically switches into MS/MS mode during an acquisition based upon data acquired in the MS mode in the previous scan. The software selects up to 30 precursors for MS/MS from a Survey scan, with a maximum spectral acquisition rate of 30 MS/MS /sec. If any ion is found above a user-defined threshold in an MS survey scan, the instrument switches to acquire a product ion spectrum for that ion. Specific target masses, mass ranges and charge states may be selected for switching, or unwanted masses may be excluded. The duration of MS/MS

acquisition may be determined by either the signal intensity or by a user-defined switching time. This function allows product ion data to be acquired without prior knowledge of the sample composition or constituent retention times.

9. The software is capable of MS^E data acquisitions whereby high and low collision energy data is acquired simultaneously to provide fragmentation data for all detectable molecular ions. The instrument alternates between low and high-energy in the collision cell at user-defined intervals. In the low-energy acquisition it records the mass spectrum exhibiting mainly precursor ions, and in the high-energy acquisition their respective fragment ions. This capability is covered in Water's PID/MS^E patent.
10. The software offers exact parent ion discovery and exact neutral loss: It should describe acquisitions where, at user-defined intervals, the instrument alternates between low and high-energy conditions. In the low-energy acquisition it records the mass spectrum exhibiting mainly precursor ions, and in the high-energy acquisition their respective fragment ions. In the exact parent ion discovery mode the acquisition system monitors the high-energy data for a specific, diagnostic product ion. Upon detection of the specified product ion the instrument will switch into MS/MS mode and cycle through all possible precursors, present in the low-energy data, to reveal the true precursor. In the exact neutral loss experiment the acquisition system will calculate the masses of all potential precursors in the low-energy data, before interrogating the high-energy data for neutral losses of a specified m/z difference from those calculated masses. Upon detection of the neutral loss the instrument will switch into the MS/MS mode on the suspected precursor ion to confirm its status. This technology is covered under the PID/MS^E patent.
11. Using proprietary algorithms, the software is capable of searching for metabolites of a specific compound. The search is limited with specialized functions that account for all of the de-alkylation events that potentially give rise to metabolites and subsequently the range of the exact mass differences between the starting material and those possible metabolites. This dramatically reduces the number of false positive hits.
12. The software permits navigation through a mobility data file displaying information associated with retention time, mass, intensity and drift time.
13. The software provides the ability to perform peak detection for 3D (m/z, intensity and drift time) or 4D (m/z, intensity, drift time and retention time) datasets.
14. The software provides the ability to selectively detect peaks, to export detected components as a peak list or provide the ability to directly launch elemental composition determination software and structural determination (Mass fragment) software for subsequent spectral interpretation.
15. The software provides the ability to generate an ion mobility calibration profile for a range of components of known collision cross-section which will subsequently enable the facile generation of collision cross section values for analytes under identical experimental (ion mobility separation) conditions.
16. The software enables the generation of theoretical collision cross section values from one or more pdb (protein databank) files containing the three-dimensional structure coordinates for a sample(s) of interest to facilitate comparison with T-wave derived collision cross section values.

☒ A patent, copyright or proprietary data limits competition. The proprietary data is:

CONJOINED PARALLEL RF ION GUIDES
Z-Spray Ion Source
'Z' SPRAY

GB 2455171

US 5,756,994 GB2308227

LockSpray and NanoLockSpray Sources		
MUX/LOCKSPRAY	US 6,410,915	EP0966022
T-Wave Collision Cell		
RAMPING COLLISION ENERGY	US 7,622,711	GB2421839
DRE and pDRE		
'Z' LENS ATTENUATING A CONTINUOUS BEAM	US 7,683,314	GB2413006
HDMS capability and Triwave (specific to the HDMS upgrade capability on SYNAPT MS systems)		
INTERFACING IMS WITH TOF	US 6,992,283	GB2409764
ION TUNNEL AS AN ION TRAP	US 6,903,331	GB2381948
HELIUM GATE	US 8,076,636	GB2440618
Quantitative Tof (QuanTof) analyzer		
'W' OPTICS	US 6,570,152	GB2361580
TOF DATA ACQUISITION SYSTEM	US 8,063,358	GB2429110
Accurate Mass Measurement		
ACCURATE MASS MEASUREMENT	US 7,202,473	GB2401721
'Data Independent' MS ^E and Precursor Ion Discovery Modes		
ALTERNATING HIGH AND LOW ENERGY ACQUISITIONS	US 6717130	

- ☐ These are "direct replacements" parts/components for existing equipment.
- ☐ The material/service must be compatible in all aspects (form, fit and function) with existing systems presently installed/performing. Describe the equipment/function you have now and how the new item/service must coordinate, connect, or interface with the existing system.
- ☐ The new work is a logical follow-on to an original Federal Supply Schedule order provided that the original order was placed in accordance with the applicable Federal Supply Schedule ordering procedures. The original order must not have been previously issued under sole source or limited source procedures.
- ☐ An urgent and compelling need exists, and following the ordering procedures would result in unacceptable delays.

(5) DESCRIBE WHY YOU BELIEVE THE ORDER REPRESENTS THE BEST VALUE CONSISTENT WITH FAR 8.4 TO AID THE CONTRACTING OFFICER IN MAKING THIS BEST VALUE DETERMINATION:

Per FAR 8.404(d), GSA has already determined prices of supplies and fixed-price service to be fair and reasonable.

(6) DESCRIBE THE MARKET RESEARCH CONDUCTED AMONG SCHEDULE HOLDERS AND THE RESULTS OR A STATEMENT OF THE REASON MARKET RESEARCH WAS NOT CONDUCTED:

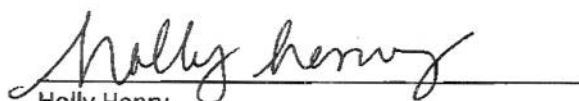
A search was conducted on NAC/GSA, no other vendor was found that could deliver the equipment needed.

(7) ANY OTHER FACTS SUPPORTING THE JUSTIFICATION: The equipment is available from a mandatory source.

(8) A STATEMENT OF THE ACTIONS, IF ANY, THE AGENCY MAY TAKE TO REMOVE OR OVERCOME ANY BARRIERS THAT LED TO THE RESTRICTED CONSIDERATION BEFORE ANY SUBSEQUENT ACQUISITION FOR THE SUPPLIES OR SERVICES IS MADE:

Eventually other vendors/manufacturers will bring comparable products to market.

(9) REQUIREMENTS CERTIFICATION: I certify that the requirement outlined in this justification is a Bona Fide Need of the Department of Veterans Affairs and that the supporting data under my cognizance, which are included in the justification, are accurate and complete to the best of my knowledge. I understand that processing of this limited sources justification restricts consideration of Federal Supply Schedule contractors to fewer than the number required by FAR Subpart 8.4. *(This signature is the requestor's supervisor, fund control point official, chief of service or someone with responsibility and accountability.)*

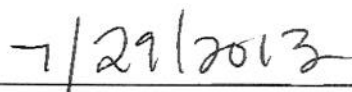


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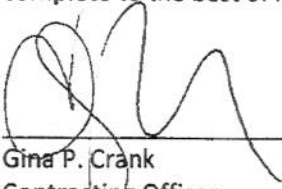
VISN 10/VHA VAMC Cleveland

DATE

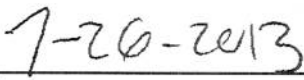


(10) APPROVALS IN ACCORDANCE WITH FAR 8.405-6(h):

a. CONTRACTING OFFICER'S CERTIFICATION (required): I certify that the foregoing justification is accurate and complete to the best of my knowledge and belief.



Gina P. Crank
Contracting Officer
NCO 10



DATE

HIGHER LEVEL APPROVAL: (REQUIRED \$3K and above)

b. NCM/PCM/DESIGNEE: I certify that the foregoing justification is accurate and complete to the best of my knowledge and belief.

Terry Spitzmiller
NCM
NCO 10

DATE