Requirements specification

Requirements specification for the invitation by the Danish Emergency Management Agency (DEMA) to submit tenders for a contract concerning the purchase of a mass spectrometer system

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Content

1 Requirements specification for instrument A or A1 and B

This chapter contains a description of the technical, software and service specifications.

Tenderers are - with regards to both minimum requirements (MR), scored requirements (SR) and wishes (W) - required to:

a) Give reference to the relevant part of tender with regards to a detailed description of the fulfilment/non-fulfilment of the MR, SR or W.

b) Give a full description of how the offered equipment fulfils the requirement or why the offered equipment does not fulfil the requirement.

The descriptions in the tender are used for evaluation purposes. Therefore, tenderers are encouraged to be as specific as possible with regards to all descriptions (simple yes/and no answers could result in lower scores).

Please note that a minimum requirement (MR) is a demand that must be fulfilled by the Tenderer in order for the offer to be taken into account (need to have), while it is not necessary to fulfil a wish (W) in order for the offer to be taken into account. The scored requirements (SR) are used for evaluation of the tenders. The wishes (W) show options that do not influence on the evaluation, but prices for the options are wanted and the options can be chosen to compliment the tenders.

All scored requirement will be graded on the following general scale:

Grade 5: State of the art quality with great added value to DEMA.

Grade 4: Good quality with added value to DEMA .

Grade 3: Quality as expected from DEMA.

Grade 2: Quality not quite up to DEMA’s expectation.

Grade 1: Minimal accepted quality.

Weight			
Low	Means that this requirement has a Low weight. Grade x 1.		
Medium	Means that this requirement has a Medium weight. Grade x 3.		
High	Means that this requirement has a High weight. Grade x 5.		
Very High	Means that this requirement has a Very High weight. Grade x 10.		

Technical specifications

Title	ID	Description If not a specific instrument is noted, the requirement applies to both instruments (A or A1 and B)	Type of requirement	Points and weights
Scope of delivery	1.1	For this purchase there is a need for: A system consisting of two individual instruments A and B. Both instruments should be flexible and highly sensitive Gas Chromatograph – Mass Spectrometers (GC-MS). Instrument A and instrument B should be delivered at Danish Emergency Management Agency, Chemical Division in Copenhagen. The gas chromatographs should use a capillary column with a temperature programmable oven. The basic call is for two single quadrupole GC-MS instruments A and B. The instruments require different configuration for autosampler, inlets and extra detectors. DEMA will strongly encourage the suppliers to give one or more additional offers for an alternative Gas Chromatograph - Mass Spectrometer for instrument A, here after called instrument A1. Instrument A1 is defined as an instrument capable of doing GC-high resolution MS (High resolution definied as better than 13,000 FWHM) with ppm mass accuracy at m/z = 200. DEMA will prioritize as first choice a combination of instrument A1 and B as long as it is within our economical frame. If such a combination is not within our economical frame a combination of instrument A and B will be chosen.	**MR**	

		The price for each GC-MS system must be specified, but it is only the total price that is used for the evaluation of the tender.		
General	2.1	Full on-site installation and verification. Delivery and installation must be included in the tender. Acceptance test must be specified and included in the tender.	**MR**	
	2.2	We want instruments from the same provider to facilitate the ease of use of the system. The instruments do not need to be identical, but the user interface, software for instrument control and data handling must be identical.	**MR**	
	2.3	The tenderer must specify the installation requirements in the tender, including the dimensional need for delivery on 7th floor (elevator) for instruments A or A1 and B.	**MR**	
	2.4	Removal of the two present GC-MS instruments from DEMA at 7th floor must be included in the tender. The two present GC-MS systems are a Waters GCT instrument and a Thermo DSQ-II instrument.	**MR**	
	2.5	Describe acceptance tests. They must include:	**MR**	

		• Sensitivity test for electron ionization (EI) and chemical ionization (CI). • Isotope ratio test for electron ionization (EI) and chemical ionization (CI).		
	2.6	The tender must include technical manuals and detailed descriptions of the equipment.	**MR**	
	2.7	The tender must include dimensions and weight of the equipment.	**MR**	
	2.8	Instruments must be able to work under normal laboratory conditions with a temperature span up to 5°C per 24 hr. Instruments must use air cooled turbo-pumps and not water cooled.	**MR**	
	2.9	Specify noise levels.	**MR**	
	2.10	Describe how noise reduction of pumps and fans are done.	**MR**	
	2.11	Instruments must be supplied with oil free fore pumps (Dry scroll pumps).	**MR**	
	2.12	Option for delivery of noise reduction boxes with the instruments	**W**	

Ionization	3.1	The following ionization modes must be possible with the delivered ion source(s). **EI** (electron ionization) **CI** (+/-) (chemical ionization positive and negative modes, with methane, isobutane and ammonia).	**MR**	
	3.2	Option for alternative ionisation such as Low Energy EI.	**W**	
	3.3	Describe the exchanging between EI and CI mode and how fast it can be done.	**SR**	High 0 – 30 min = 5 30 – 60 min = 4 60 – 90 min = 3 90 – 120 min = 2 > 120 min = 1
Mass spectrometer	4.1	The detector dynamic range must be specified.	**SR**	Medium 10x6 or greater = 5 10x5 = 4 10x4 = 3

				10x3 = 2 < 10x3 = 1
	4.2	Mass range 20 – 1000 dalton. Specify possible scan ranges.	**MR**	
	4.3	EI-spectra should be of high quality, non skewed and library searchable for a known mixture as defined below.	**MR**	
	4.4	The resolution should be specified both at 50% and 10% valley	**MR**	
	4.5	Performance and sensitivity for EI and CI must be tested on full GC-MS system with split/splitless injection on standard column (5%-phenyl-methylpolysiloxane).	**MR**	

	4.6	Performance EI Full Scan (m/z <= 40 - >= 600): QC test sample of own choice with at least 10 organic compounds injected with 1- 10 ng on the instrument. There must be at least 1 compound with 1 chlorine atom, and at least 1 compound with 1 sulfur atom. The test must fulfil the following: 1. The signal-to-noise (S/N) ratio for each test chemical is >10:1 in the total ion chromatogram (TIC). 2. The m/z values of the major ions in EI spectra of each test chemical are correct when compared to NIST library spectra and no extra ions above 5% are present (the mass range to be printed must extend 10 m/z beyond the molecular mass, so that the whole relevant mass spectrum is registered). 3. The intensity ratios of the isotopic ions are within the following limits (the values are expressed as percentages of the less abundant isotopic ions relative to the more abundant ones ± the acceptable error limits): - (37Cl/35Cl) for chlorine containing peak in compound with 1 chlorine atom is 32.6±3.0% - (34S/32S) for sulfur containing peak in compound with 1 atom sulfur is 5.3±1.0%.	**SR**	Very High Complete fulfilment of the test criteria including all relevant chromatograms and spectra for both 1 ng and 10 ng of each compound on both instruments gives a score of 5. Complete fulfilment of the test criteria including spectra for 10 ng of each compound on both instruments gives a score of 3. Report with missing data or deviations from the fulfilment criterias gives a score of 2. No report gives a score of 1.

		Report with data for evaluation of performance should be provided with the tender.		
	4.7	Sensitivity Positive CI Full Scan (Methane as CI-gas m/z <= 60 - >= 600): QC test sample of own choice with at least 10 compounds injected with 10 ng on the instrument. There must be at least 1 compound with 1 chlorine atom and at least 1 compound with 1 sulfur atom. The test must fulfil the following: 1. The signal-to-noise (S/N) ratio for each test chemical >10:1 in the total ion chromatogram (TIC). 2. The intensity ratios of the isotopic ions are within the following limits (the values are expressed as percentages of the less abundant isotopic ions relative to the more abundant ones ± the acceptable error limits): - (37Cl/35Cl) for chlorine containing peak in compound with 1 chlorine atom is 32.6±3.0% - (34S/32S) for sulfur containing peak in compound with 1 atom sulfur is 5.3±1.0%.	**SR**	High Complete fulfilment of the test criteria including all relevant chromatograms for each compound on both instruments gives a score of 5. Report with missing data or deviations from the fulfilment criterias gives a score of 2. No report gives a score of 1.

		Report with data for evaluation of performance should be provided with the tender.		
	4.8	Sensitivity Negative CI Full Scan (Methane as CI-gas m/z <= 40 - >= 400) This test can be conducted on a column of the tenders choice: When tested on a mix containing (all chemicals can be optained from Sigma-Aldrich as certified reference solutions): Ethylene glycol dinitrate EGDN (CAS 628-96-6) 1 ng/µl Nitroglycerine NG (CAS 55-63-0) 1 ng/µl Pentaerythritol tetranitrate PETN (CAS 78-11-5) 1 ng/µl RDX (CAS 121-82-4) 1 ng/µl Trinitrotoluene TNT (CAS 118-96-7) 1 ng/µl The test must fulfil the following: 1. The signal-to-noise (S/N) ratio for each test chemical >10:1 in the relevant extracted ion chromatogram (EIC): EGDN (m/z 62; 46) NG (m/z 46; 62) PETN (m/z 101) RDX (m/z 102)	**SR**	High Complete fulfilment of the test criteria including all relevant chromatograms for each compound on both instruments gives a score of 5. Report with missing data or deviations from the fulfilment criterias gives a score of 2. No report gives a score of 1.

		TNT (m/z 210). Report with data for evaluation of performance should be provided with the tender.		
GC-system	5.1	Fitted with 2 temperature programmable injectors (e. g. PTV-injectors, MMI-injectors or equivalent).	**MR**	
	5.2	Describe GC temperature ramp and cooling time	**MR**	
	5.3	Possibility for analysis of sample tubes e.g. Tenax for air sampling should be presented as an option on one of the instruments.	**MR**	
	5.4	Option for analysis of air samples from canisters or tedlar-bags on one of the instruments.	**W**	
	5.5	Possibility of later change of mass analyser to different mass analyser from same or a different manufacturer.	**SR**	Low 1 – no 3 yes, MS can be upgraded . New MS can only come from same manufacturer 5 – yes, MS can be upgraded . New MS can

				come from same manufacturer or from third party manufacturer
	5.6	Possibility for dual column system with alternative detectors like FID, FPD, NPD, PFPD on one of the columns.	**MR**	
	5.7	Option for 1 FPD, dFPD or PFPF and 1 NPD with one detector mounted on each instrument.	**W**	
	5.8	Possibility for back flush of GC-columns both from mid--column or end-column. It must be possible to change between mid-column and end-column back flush.	**MR**	
	5.9	Possibility for one column with split flow to two detectors: mass analyser and alternative detector e.g. FID.	**MR**	
	5.10	Possibility for manual injection of gas samples by syringe	**MR**	
Autosampler	6.1	Autosampler can do automatic switching of syringes/tools for different analytical tasks – liquid samples, Head Space and SPME.	**MR**	
	6.2	Autosampler configured for 2 ml liquid vials and 20 ml Head Space vials.	**MR**	

	6.3	Autosampler for liquid vials must have room for at least 40 individual vials.	**MR**	
	6.4	Option for autosampler fitted with SPME fibre preconditioning station.	**W**	
	6.5	Autosampler fitted with station for heating and shaking of Head Space and SPME vials.	**MR**	
	6.6	Option for autosampler fitted with cooled vial holder as an option.	**W**	
	6.7	2 syringes/tools for liquid samples, 1 syringe/tool for Head Space and 1 syringe/tool for SPME must be included in the offer.	**MR**	
	6.8	Option for extra Head Space and SPME syringes/tools.	**W**	
Computer	7.1	The computer must be able to run under Windows 7 or later versions.	**MR**	
	7.2	The computer hardware shall have one “RJ45”-connector reserved for a local area network patch.	**MR**	
	7.3	The computer must be equipped with monitor with a size of at least 24’’.	**MR**	
Training	8.1	Specify the plan for on-site introduction training course for the full instrument and software followed by an extended training after 6-12	**SR**	High

		months after installation, for at least 9 persons. The training should be divided in a general part and a part for more advanced users for three or four persons.		Detailed description of content with possibility of customization: 5 Non-detalied description and/or fixed content: 1
	8.2	Describe the training material available, such as instructions, quick guides and video guides.	**SR**	Medium None = 1 Only printed guides = 2 Only written material = 3 Written and video material supplied by physical medium (eg. CD-ROM or similar) = 4 Written and video material supplied by physical medium (eg. CD-ROM or similar) as well as on-line (ie. World wide web) = 5.
Optional	9.1	Specify extended instrument possibilities to be included in the tender. Eg. additional equipment/spare parts, software etc.	**W**	

Software Specifications

Title	ID	Description	Type of requirement	Points and weights
	10.1	Fully integrated software for hardware control of GC, auto sampler and MS as well as data handling.	**MR**	
	10.2	Qualitative ID software package must be included, possibilities for library search. Latest version of NIST software and library must be provided.	**MR**	
	10.3	Software for automatic deconvolution combined with library search.	**MR**	
	10.4	Quantification software package must be included.	**MR**	
	10.5	Export of RAW-Data files to NetCDF and possibly other open source formats. Export of parameter files and log files in open source formats.	**MR**	

	10.6	Software updates must be included for the first two years.	**MR**	
	10.7	The tender must include license for the full qualitative and quantitative data processing software, 12 seats.	**MR**	
	10.8	The tender must include deconvolution software with possibility for target and untarget analysis, 12 seats.	**MR**	
	10.9	a. Describe if the data analysis software is capable of quantifying a number of compounds based on a single compound calibration curve. Eg. If compound 1,2,3,4 and 5 can be quantified based on standard curve made for compound A b. Additionally it is desirable if the type of quantification can be done both in MS mode as well as with other detectors such as FID. c. Additionally it is desirable if different compound calibration curves can be chosen for specific elution times, e.g. Standard A for compounds in the interval 5-10 min and standard B for compounds in the interval 10-20 min and so forth.	**SR**	Low If none = 1 If a = 3 a + b or c = 4 a +b + c = 5
	10.10	Describe if the software used for instrument control can generate a full run sequence including calibration standards, blanks and QC (quality control) samples based on a predefined template.	**SR**	Medium Not fullfilled = 1

				Fullfilled = 5
	10.11	Describe the possibilities for additional libraries to be included in the tender.	**SR**	Low 0 = 1 1 = 2 2 = 4 3+ = 5
	10.12	The software must be able to process data and quantify analytes based on a calibration curve for both the MS detector and other detectors, including FID. Describe the process. A simple process with few steps will be preferred.	**SR**	High Complex, many steps and more than one program = 1 Either complex with many steps or demand use of more than one program = 3 Simple with few steps and only one program = 5
Optional	11.1	Describe extra software packages that can be included in the tender.	**W**	

Service Specifications

Title	ID	Description	Type of requirement	Points and weights
General	12.1	The tender must include a two year full warranty and service contract including all software updates.	**MR**	
	12.2	Describe the content of the offered service contract.	**SR**	High Comprehensive and extensive plan (including annual preventive maintenance (PM); free repairs and free spare parts) = 5 Less comprehensive and extensive plan (Including annual preventive maintenance (PM) and free spare parts) = 4 Less comprehensive and extensive plan (Including annual preventive

				maintenance (PM) and free repairs) = 3 Annual preventive maintenance = 2 No detail: 1
	12.3	Specify the expected time from first contact with service organization to the time where a planned response has been agreed.	**SR**	High < 24 h = 5 24 – 48 h = 3 > 48 h = 1
	12.4	Specify the location of the nearest support office which host capable field technicians.	**MR**	
	12.5	Fast spare-part replacement. Describe the estimated delivery time for turbo pumps and detectors.	**SR**	Medium Next day = 5 Within 3 working days = 4 Within 10 working days = 3 More than 10 working days or no answer 1

Maintenance	13.1	Option for an extra 2 years full service contract (max 2 working days response time) for year 3 and 4 including spare parts, preventive maintenance, and all software updates. The option shall be valid separately for each instrument. The extension of the service contract for year 3 and 4 is entered for one year at the time if the option is accepted.	**MR**	

2 Requirements specification for the optional instrument C

This chapter contains a description of the technical, software and service specifications for the optional instrument C.

Tenderers are - with regards to both minimum requirements (MR) and wishes (W) - required to:

c) Give reference to the relevant part of tender with regards to a detailed description of the fulfilment/non-fulfilment of the MR or W.

d) Give a full description of how the offered equipment fulfils the requirement or why the offered equipment does not fulfil the requirement.

Please note that a minimum requirement (MR) is a demand that must be fulfilled by the Tenderer in order for the offer to be taken into account (need to have), while it is not necessary to fulfil a wish (W) in order for the offer to be taken into account. The wishes (W) shows options that are wanted and can be chosen to compliment the tenders.

Several of the requirements for instrument C are identical to the requirements specified for instrument A or A1 and B. It is perfectly acceptable to reuse wordings where applicable, but please note that the ID-numbering of the requirement may differ, and that all MR must be fulfilled for the tender to be conditional.

Technical specifications

Title	ID	Description	Type of requirement	Points and weights
Scope of delivery	1.1	For this purchase there is a need for: A system consisting of one flexible and highly sensitive Gas Chromatograph – Mass Spectrometer (GC-MS). The gas chromatograph should use a capillary column with a temperature programmable oven.	**MR**	
General	2.1	Full on-site installation and verification. Delivery and installation must be included in the tender. Acceptance test must be specified and included in the tender.	**MR**	
	2.2	Describe acceptance tests. They must include: • Sensitivity test for electron ionization (EI) and chemical ionization (CI). • Isotope ratio test for electron ionization (EI) and chemical ionization (CI).	**MR**	

	2.3	The tender must include technical manuals and detailed descriptions of the equipment.	**MR**	
	2.4	The tender must include dimensions and weight of the equipment.	**MR**	
	2.5	The instrument must be able to work under normal laboratory conditions with a temperature span up to 5°C per 24 hr. The instrument must use air cooled turbo-pumps and not water cooled.	**MR**	
	2.6	Specify noise levels.	**MR**	
	2.7	Describe how noise reduction of pumps and fans are done.	**MR**	
	2.8	The instrument must be supplied with oil free fore pumps (Dry scroll pumps).	**MR**	
	2.9	Option for delivery of noise reduction boxes with the instrument.	**W**	
Ionization	3.1	The following ionization mode must be possible with the delivered ion source(s). **EI** (electron ionization)	**MR**	

	3.2	Option for **CI** (+/-) (chemical ionization positive and negative modes, with methane, isobutane and ammonia	**W**	
Mass spectrometer	4.1	The detector dynamic range must be specified.	**MR**	
	4.2	Mass range 20 – 1000 dalton. Specify possible scan ranges.	**MR**	
	4.3	EI-spectra should be of high quality, non-skewed and library searchable for a known mixture as defined below.	**MR**	
	4.4	The resolution should be specified both at 50% and 10% valley	**MR**	
	4.5	Performance and sensitivity for EI and CI must be tested on full GC-MS system with split/splitless injection on standard column (5%-phenyl-methylpolysiloxane).	**MR**	
GC-system	5.1	The instrument must be fitted with one split/splitless injector.	**MR**	
	5.2	Option for additional split/splitless injector.	**W**	

	5.3	Option for an additional PTV-injector.	**W**	
	5.4	Describe GC temperature ramp and cooling time	**MR**	
	5.5	Describe if it is possible to do a subsequent (post-installation) replacement of mass analyser to different mass analyser from same or a different manufacturer.	**MR**	
	5.6	Possibility for dual column system with alternative detectors like FID, FPD, NPD, PFPD on one of the columns.	**MR**	
	5.7	The instrument must be fitted with both an FID and an MS detector	**MR**	
	5.8	Possibility for back flush of GC-columns both from mid--column or end-column. It must be possible to change between mid-column and end-column back flush.	**MR**	
	5.9	Possibility for one column with split flow to two detectors: mass analyser and alternative detector e.g. FID.	**MR**	
	5.10	Possibility for manual injection of gas samples by syringe	**MR**	
Autosampler	6.1	Autosampler configured for 2 ml liquid vials	**MR**	

	6.2	Autosampler for liquid vials must have room for at least 40 individual vials.	**MR**	
Computer	7.1	The option should not include any non-specialised computer hardware, i.e. Standard cables, workstations or screens.	**MR**	
Training	8.1	Specify the plan for on-site introduction training course for the full instrument and software followed by an extended training after 6-12 months after installation, for at least 4 persons. The training should be divided in a general part and a part for more advanced users for three or four persons.	**MR**	
	8.2	Specify additional application consultancy to set up at least 2 methods using backflush.	**MR**	

Software Specifications

Title	ID	Description	Type of requirement	Points and weights
General	10.1	The software must be able to run under Windows 7 Enterprise.	**MR**	
	10.2	Fully integrated software for hardware control of GC, auto sampler and MS as well as data handling.	**MR**	
	10.3	Qualitative ID software package must be included, possibilities for library search. Latest version of NIST software and library must be provided.	**MR**	
	10.4	Software for automatic deconvolution combined with library search must be included.	**MR**	
	10.5	Quantification software package must be included.	**MR**	

	10.6	Export of RAW-Data files to NetCDF and possibly other open source formats. Export of parameter files and log files in open source formats.	**MR**	
	10.7	Software updates must be included for the first two years.	**MR**	
	10.8	The tender must include license for the full qualitative and quantitative data processing software, 4 seats.	**MR**	
	10.9	The tender must include deconvolution software with possibility for target and untarget analysis, 4 seats.	**MR**	
	10.13	The software must be able to process data and quantify analytes based on a calibration curve for both the MS detector and other detectors, including FID. Describe the process.	**MR**	

Service Specifications

Title	ID	Description	Type of requirement	Points and weights
General	12.1	The tender must include a two year full warranty and service contract including all software updates.	**MR**	
	12.2	Describe the content of the offered service contract.	**MR**	
Maintenance	13.1	Option for an extra 2 years full service contract (max 2 working days response time) for year 3 and 4 including spare parts, preventive maintenance, and all software updates. The extension of the service contract for year 3 and 4 is entered for one year at the time if the option is accepted.	**MR**	