Minutes of Technical Sub Committee meeting

Tender reference: IICB/PUR/24-25/599/574/T&PC/28

The pre-bid meeting for the procurement for "NMR (600 MHz) Spectrometer" was held on 22.08.2024. Representatives from two firms, namely Bruker and Jeol, participated in the meeting. They have raised certain requests, which they have submitted through email subsequently. The Technical Sub Committee (TSC) met on 27.08.2024 to discuss the requests from them and to finalize the technical specifications. The response from Bruker and Jeol are present in the below Table 1 and Table 2, respectively. The response from the TSC is also present in the tables. The updated technical specification is attached with the document.

Table 1. Request from Bruker

	Tender Specifications	Request / Recommendation from Bruker	**Response from TSC**
1	Magnet :- Specs mentioned as Liquid Helium hold time of at least 250 days or more.	Liquid Helium Hold Time of 365 days or more, due to global scarcity of Liquid Helium, it is always recommended to opt for a higher hold time magnet.	The committee examined the specifications of both Bruker and Jeol. The committee expects both vendors quote latest model with and best available technical features from their end. The committee notes that Bruker magnet has "Maximum liquid helium refill volume/total volume of 114/129 liter" and "Minimum helium hold time of 365 days". In comparison, as per the documents available, the magnet from Jeol from has a hold time of 200 days with refill volume of 85 L for liquid helium. The committee **does not agree** with the request. The updated specification (1.iii) reads: "Liquid Helium hold time of 200 days or more"
2	Multi Receiver Technology for sequential as well as parallel acquisition of nuclei at a time. This technology	Without this technology it is very difficult to distinguish between new generation NMR spectrometer with old generation spectrometers. This is highly recommended by our Application Team and	The committee is fully aware of that NOAH (Nuclear magnetic resonance by Ordered Acquisition using 1H detection) experimental scheme for acquiring certain multiple experiments in a single combined pulse sequence with a single relaxation delay is possible by the latest

	enhance the technical benefit of the spectrometer and subsequently reduces time for the experiment. Please treat this as a recommendation to include in your specs.	our factory and both the bidders can provide this.	available instruments from both Bruker and Jeol. Accordingly, the committee **does not agree** with the request, and the decision is not restrictive.
3	Software Controlled Power up and power down of the entire spectrometer. Please treat this as a recommendation to include in your specs.	This point is recommended for safety reasons.	The committee **does not agree** with this request as well. The committee is fully aware of the safety standards of the instruments from both Bruker and Jeol, and the decision is not restrictive.

Table 2. Request from Jeol

	Tender specifications	Request from Jeol	**Response from TSC**
1	1. Magnet System (standard bore) iii. Liquid Helium hold time of at least 250 days or more.	We are requesting you to kindly amend the specification as follows: A Liquid Helium hold time of at least 200 days or more. Our 600 MHz NMR system features a magnet with a hold time of 200 days or more (No other options are available with us). Additionally, we've developed this magnet system with low cryogen consumption in mind.	As stated in the Response to the entry 1 in the Table 1, the committee examined the liquid helium capacity and hold time from the latest available magnets from both Bruker and Jeol. Accordingly, the committee **accepts** the request. The updated specification (1.iii) reads ". Liquid Helium hold time of 200 days or more"

		New magnet specification is Liquid Helium capacity 85L/200 days and a Liquid Nitrogen capacity 82L/18 day. Hence requesting you to kindly amend the specification with 200Days hold time.	
2	Spectrometer console: High-power linear amplifier broadband amplifier 100 W or better for 1H channel; 500 W or better, for X channels to provide the shortest possible pulse-widths. Please specify all relevant parameters including power (wattage), frequency range, duty cycle, maximum pulse duration, etc.	We request you to kindly amend the spec as below: High-power linear amplifier broadband amplifier 100 W or better for 1H channel; 300 W or better, for X channels to provide the shortest possible pulse-widths. Please specify all relevant parameters including power (wattage), frequency range, duty cycle, maximum pulse duration, etc. Explanation: The LF(/X) channel with a 300W amplifier is good for both solution and solid-state NMR applications at 600MHz. Although solid-state NMR requires high-power pulses for low gamma nuclei, such as 15N, even in these cases, 250W is typically more than enough. Since the IICB Tender specifies solution NMR applications, a 300W amplifier for the LF(/X) channel will easily meet these requirements. Therefore, we request that the specification for the X channel power amplifier be changed to 300W. This adjustment will not affect the performance or quality of NMR data.	The committee considers the requirement of 500 W amplifier for the detection of X nuclei (13C, 19F, 11B, 31P, and all other magnetically active nuclei) is essential. Based on the experience with the existing instrument, the committee **does not agree** with the request, and the decision is not restrictive.
3	Spectrometer console:	We request you to kindly amend the spec as below:	The committee considers the requirement of 50G/cm, or higher, from

	Gradient unit for Auto shimming (1H/2H) to achieve good line shape of sample and to perform all-new gradient pulse program-based experiment with the capability to run DOSY and other gradient experiments having capacity of 50 G/cm, or higher.	Gradient unit for Auto shimming (1H/2H) to achieve good line shape of sample and to perform all-new gradient pulse program-based experiment with the capability to run DOSY and other gradient experiments having capacity 30 G/cm, or higher. Explanation: We would like to mention that the Gradient strength of 30 G/cm is adequate for the best gradient shimming, and high-quality water suppression. The majority of NMR pulse sequences use gradient pulses either for coherence pathway selection or rejection. For these applications in solution state uses very weak gradient strength (rarely at the max of 20G/cm) for the dephasing/rephrasing of the spin system. We believe 30G/cm is good enough to perform all the advanced higher-dimension experiments including DOSY NMR.	the gradient unit, for the challenging experiments especially DOSY among others is essential. Accordingly, the committee **does not agree** with the request, and the decision is not restrictive.
4	Probes A state-of-the-art high-sensitive 5 mm broadband probe with the ability to observe 1H, X, and 19F, with autotune and match. It should have the ability	We request IICB Technical committee that the specification include the capability to perform the 13C[1H] [19F] experiment. Fluorinated molecules are a demanding area of study, and the presence of fluorine nuclei can complicate NMR spectra and reduce sensitivity, especially for low gamma nuclei like 15N and 13C.	The committee is aware of the requirement of ability to observe 19F with 1H decoupling and to perform two-dimensional 1H/19F spectroscopy. The committee considers measuring 13C NMR with 19F coupled and 1H decoupled as advantageous on its own merit. Accordingly, the committee **does not agree** with the request.

	to observe 19F with 1H decoupling and to perform two-dimensional 1H/19F spectroscopy. It should have broadband frequency channel enabling fully automated applications on protons and the widest range of X-nuclei. The probe should allow deuterium detection experiments using short 2H 90-degree pulses, which is independent of the 2H lock channel. Operating temperature range at -100 °C to +150 °C or even improved ranges. The 1H observe sensitivity in signal to noise ratio should be 1000:1 or more and 13C sensitivity should be 340:1 or more with the standard samples. The 19F sensitivity should be 850:1 or more.	Simultaneous decoupling of 1H and 19F during 13C or 15N measurements is crucial for the complete structural elucidation of unknown molecules. A broad range of advanced 1H and 19F NMR experiments, including 1H{19F}, 19F{1H}, 13C{1H,19F}, and other unique X{1H,19F} correlation experiments, are essential for simplifying the spectral assignments of complex fluorine-containing compounds, particularly in the pharmaceutical and polymer industries. Therefore, we request technical committee that include the X[1H] [19F] experiment capability, where X represents any broadband nucleus from 31P to 15N. Please note that the nuclei in brackets indicate the decoupling or correlation nuclei.	

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5	Probe An additional high resolution 5 mm observe probe fitted with an actively shielded single axis z-gradient. The inner NMR coil is tuned to observe 13C. The outer NMR coil is tuned for 1H decoupling or observation.	Jeol request '5mm multinuclear Broad Band Direct/observe Z-gradient Probe capable of covering nuclei range 1H, 19F, 31P to 15N with computer controlled automatic tuning and matching (ATM) with S/N ratio for 1H is 480 or more, S/N ratio for 13C is 320 on standard test samples. Variable temperature ranges from –100 °C to +150 °C" Explanation: The tender requested a probe (point no. ii) which is limited to a "single vendor" and moreover this probe can only tune two nuclei (1H & 13C). Instead, we recommend you go for a broadband probe (at least 31P to 15N) routine analysis probe. This will serve as a backup probe. A probe limited to tuning just two nuclei would not be effectively utilized as a backup, especially if the main probe encounters any service issues. Hence, we request you to amend the specifications of the probe as above.	The committee considers the quoted specification is sufficiently essential, considering that this is the requirement for backup probe during any extraordinary requirement of the first probe is not functional. Otherwise, this probe is safely kept away from the instrument. The committee **does not agree** with the request. The updated the specification with the sensitivity requirement (3.ii): "The sensitivity for ^{1}H should be 400:1 or more, and ^{13}C should be 290 or more."
6	Warranty Liquid Helium supply and refilling: the vendor has to ensure that liquid helium is filled periodically	We are requesting to please consider this point as an optional item or please consider the contract of year wise liquid Helium refiling.	The committee **does not agree** with the request. The vender has to ensure that liquid helium is supplied and filled periodically during the warranty periodically, so that the instrument is fully functional without any magnet quenching.

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	during the warranty period for smooth functioning of the instrument to prevent any magnetic quenching and instrument breakdown		

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