

# Quadrupole Ion Trap Mass Spectrometer (QITMS) for the Supercritical CO<sub>2</sub> and Subcritical H<sub>2</sub>O Analysis instrument (SCHAN)

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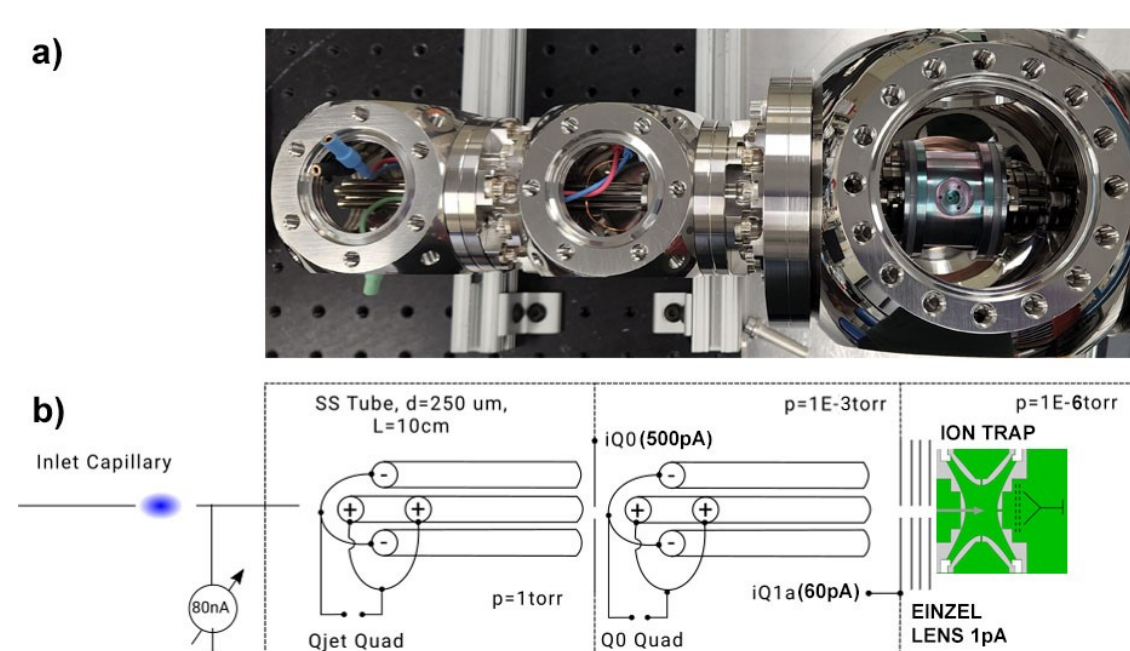
Program: FY22 R&TD Strategic Initiative

Strategic Focus Area: In-Situ Extant Life Detection Technology - Strategic Initiative Leader: Victor S. Abrahamsson

## Objectives:

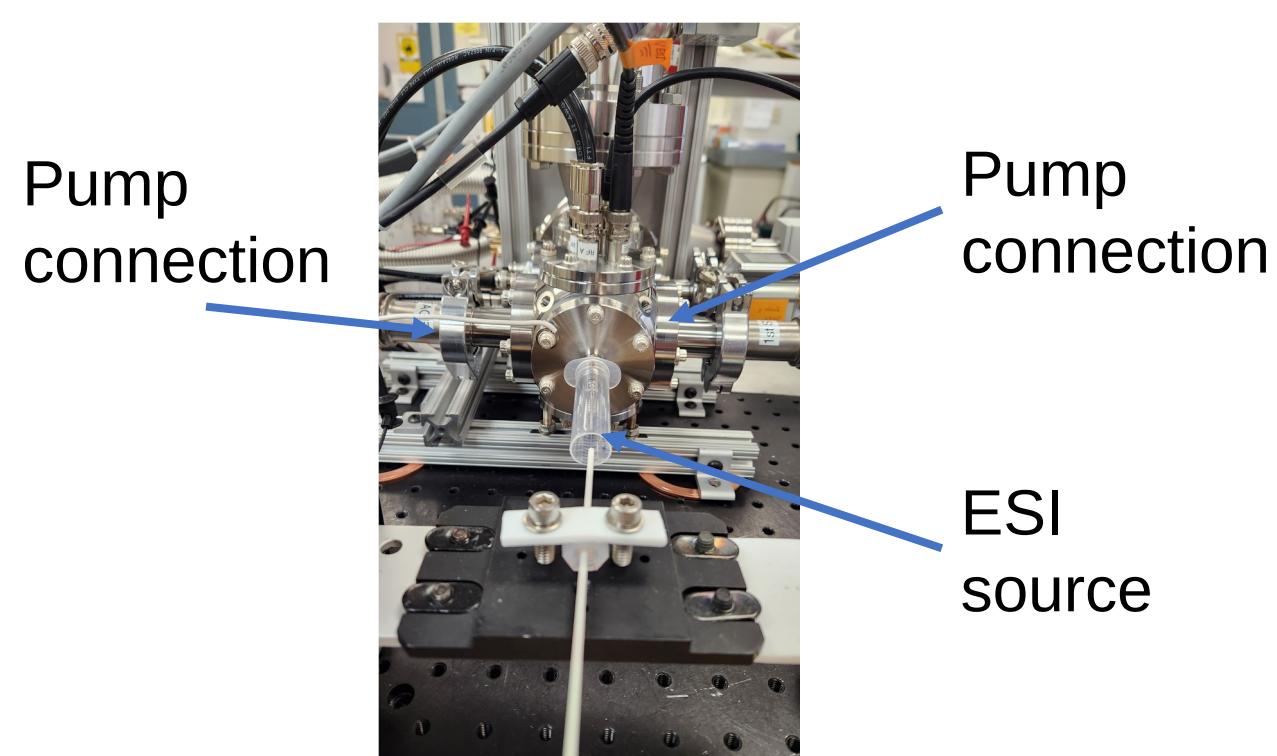
- 1) Develop an interface between the Quadrupole Ion Trap Mass Spectrometer (QITMS) and the Supercritical CO<sub>2</sub> and Subcritical H<sub>2</sub>O Analysis (SCHAN) instrument;
- 2) Extend the mass/charge ( $m/z$ ) range of the QITMS up to  $m/z$  600, to be able to detect key organic biosignatures in the context of future Discovery, New Frontiers, or flagship missions exploring Enceladus or Mars.

**Figure 1. Experimental setup**

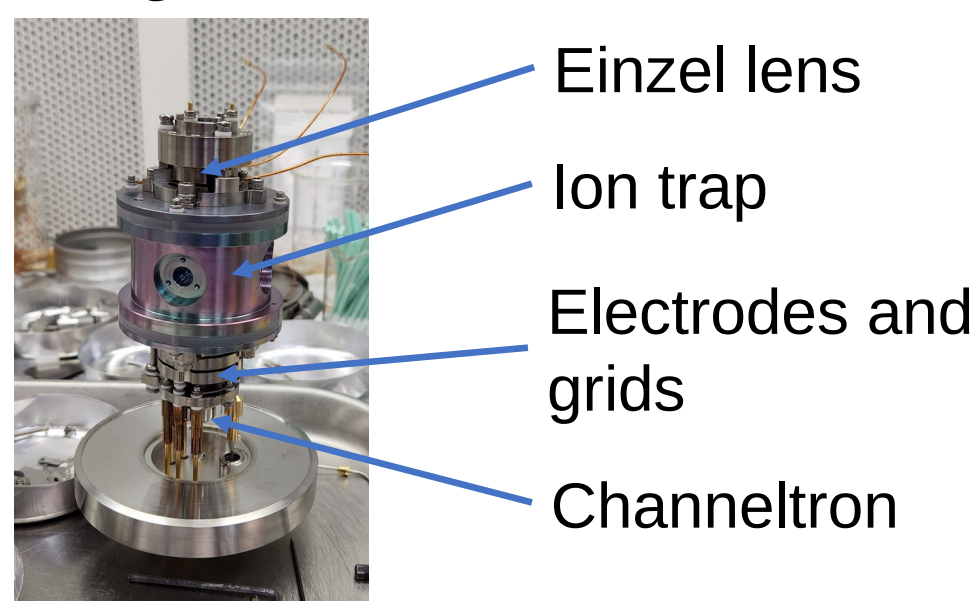


a) Photograph of the ITS and QITMS  
 b) Scheme of the experimental setup

**Figure 2. Front view of the setup**



**Figure 3. QITMS sensor**

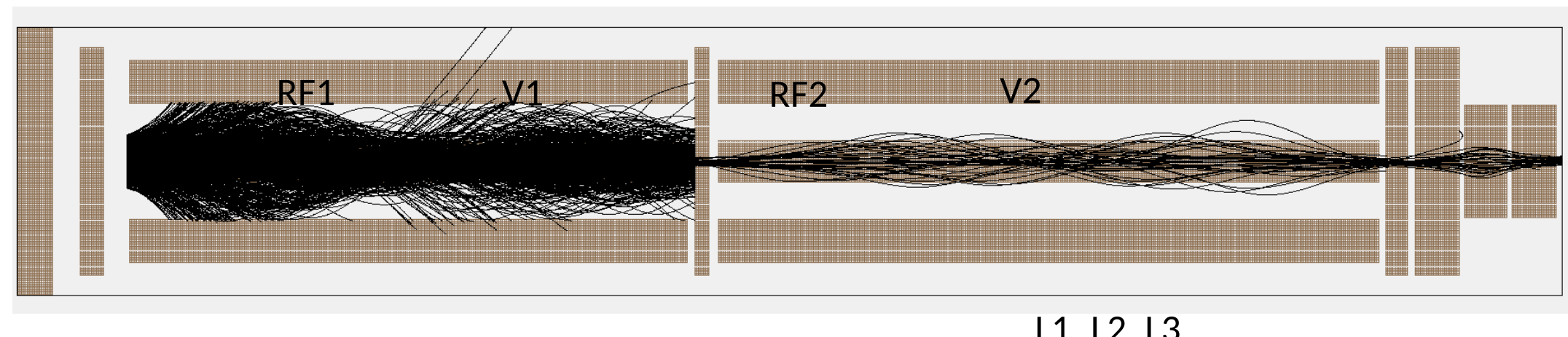


**Background:** This work is directly in line with 4x's goal to "Develop science instruments for life detection in ocean worlds.". The next-generation of life detection instruments such as SCHAN or the Ocean World Life Surveyor (OWLS) instrument require MS detection for sensitive analysis, identification of organic biosignatures, and agnostic life detection. These wet-chemistry instruments require an atmospheric-vacuum interface because ions are generated at atmospheric pressure, a capability that all wet-chemistry instruments using MS require but that does not exist for spaceflight.

## Significance/Benefits to JPL and NASA:

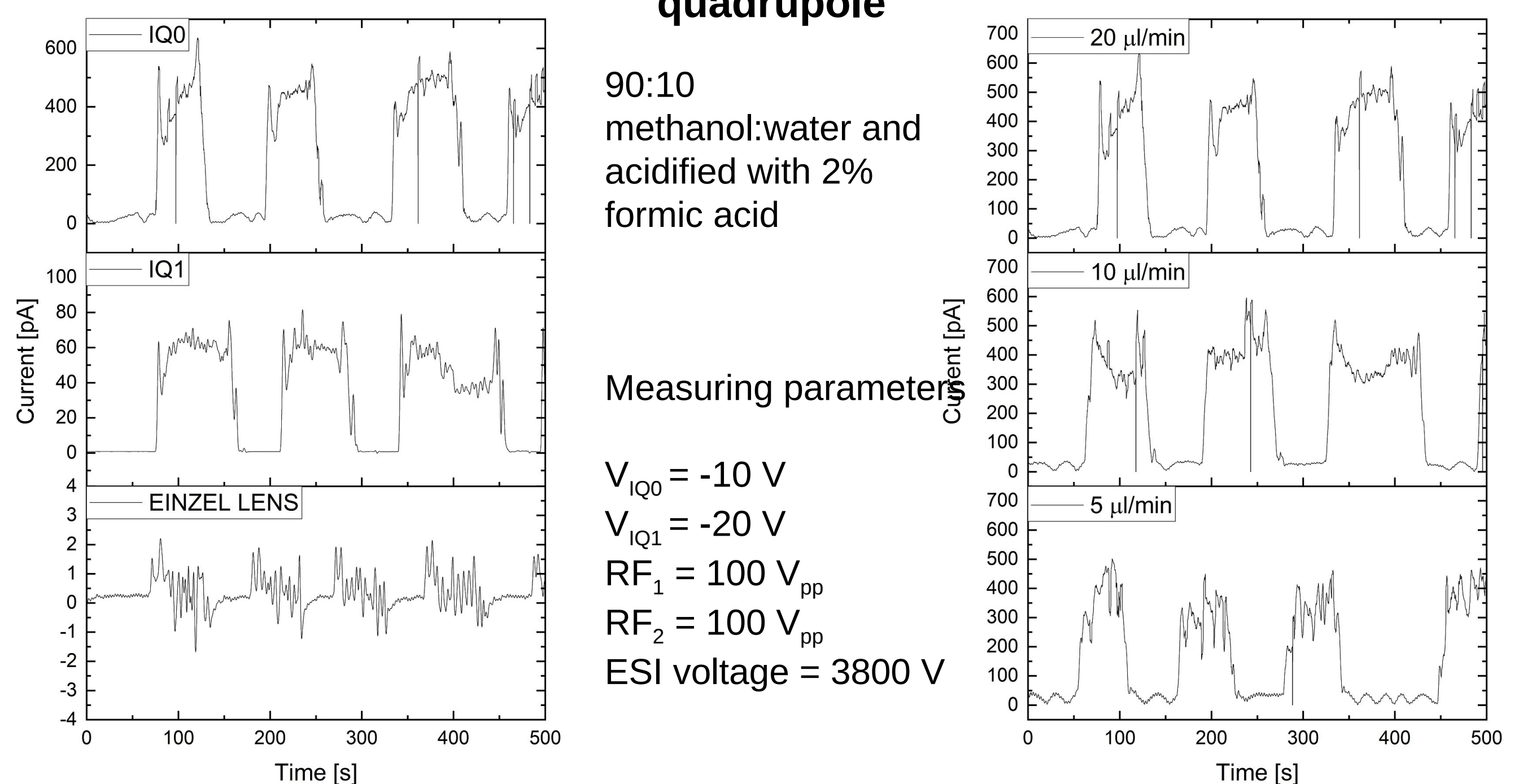
This was the first step in the development leading to the detection of the ions, generated at atmospheric pressure, in the QITMS. The next step will be the optimization of the various experimental parameters (for sensitivity) and interfacing with the SCHAN instrument. The long-term benefits for JPL will be the development of a fully integrated and compact interface and mass spectrometer for future in situ space missions dedicated to the search of organic molecules and biosignatures.

**Figure 4. SIMION Simulation of the ITS & FLS**



Parameters:  $f = 800$  kHz;  $V_{RF} = 150$  V<sub>pp</sub>;  $V_1 = -10$  V,  $V_2 = -10$  V;  $L_1 = L_3 = 0$ ;  $L_2 = +110$  V;  $m/z$  62

**Figure 5. Total ion currents measured with the capillary inside the first quadrupole**



**Approach and Results:** The experimental setup (Fig. 1) was composed of three differentially pumped vacuum chambers connected together. The ions are generated by electrospray ionization (ESI) at atmospheric pressure (Fig. 2). The ions are guided by set of electrodes through chambers, while the pressure is stepwise reduced to the third stage where the QITMS (Fig. 3) is mounted. In Fig. 4 we show one of the SIMION simulations showing the ion transfer through the system. The ions created in the ESI process are transferred by carrier gas (air in our case) through a stainless-steel capillary to the first vacuum chamber (~1 Torr). The transfer capillary is inserted into the first quadrupole. The role of this quadrupole is to transfer/guide ions through orifice between the first and the second chamber (IQ0). Then, in the second chamber (~10<sup>-3</sup> Torr), a second quadrupole is transferring the ions through a second orifice (IQ1) between the second and the third chamber. Finally, in the third and last chamber at ~10<sup>-6</sup> Torr, the ions are focused into the center of QITMS chamber through an Einzel lens. Experimental verification of ion transmission efficiencies was performed by measuring the current at the various components. The TIC measured at the two orifices IQ0, IQ1, and the Einzel lens (Fig. 5 left). The total ion current (TIC) at the orifice IQ0 at three flow rates were investigated 5, 10, and 20 μL/min (Fig. 5 right).

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