

# THE SEARCH FOR CHEMICAL COMPLEXITY IN PROTOPLANETARY DISKS



## ALMA Wideband Preview of HL Tauri

**Master's Thesis Project by:**

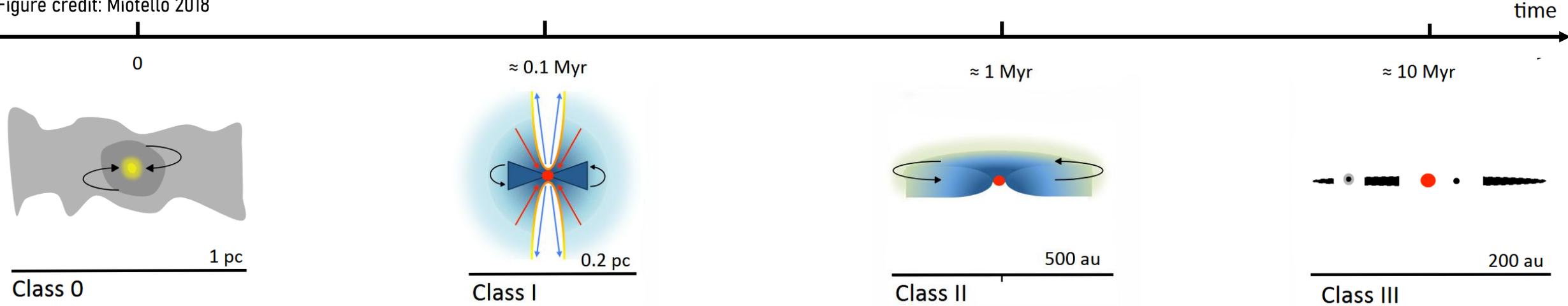
| Davide Napolitano

**Supervisors & Supporting Team:**

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## 1.1 Astrochemistry in YSOs

Figure credit: Miotello 2018

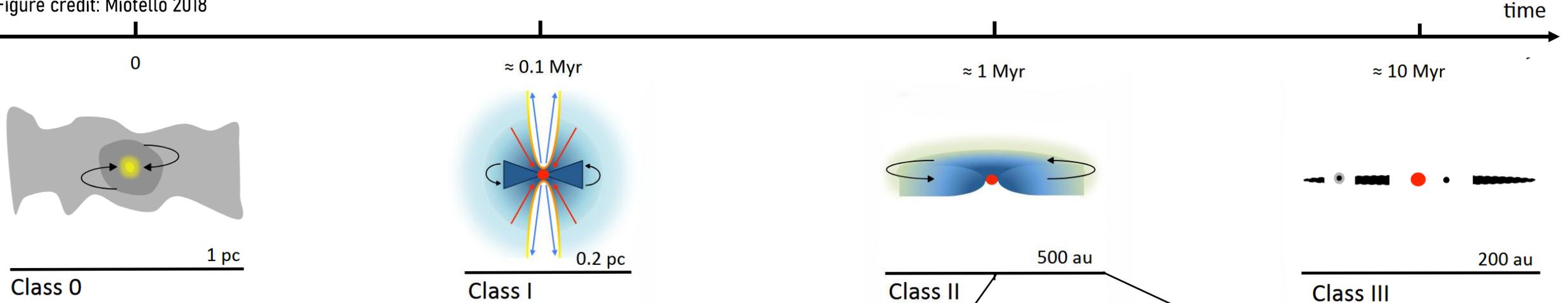


Understanding the evolution of chemical complexity from star formation to planets

- Combination of **in situ** processes and **inheritance**
- Chemistry governed by **temperature** and exposure to ionizing **radiation**
- Species of pre-biotic interest (**COMs**) widely detected in Class 0-I YSOs (Frediani 2023, de Simone 2022)

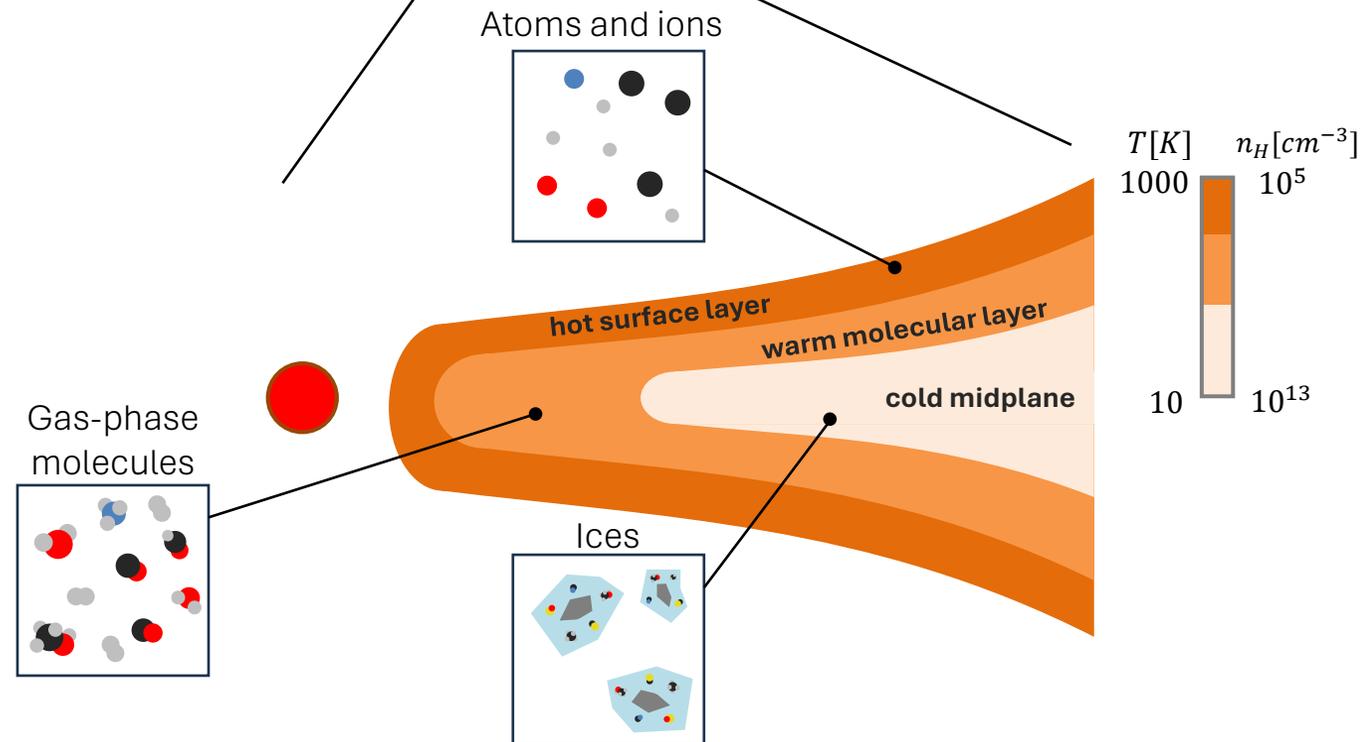
## 1.1 Astrochemistry in YSOs

Figure credit: Miotello 2018



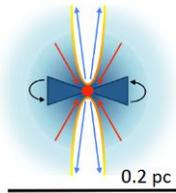
### Astrochemistry in protoplanetary disks

- Difficulty in detecting COMs (**colder systems**)
- Weak lines that require **large SNR**
- **Dust continuum opacity** contributes to hide faint molecular emission
- ➔ **COM budget in disks is still uncertain**

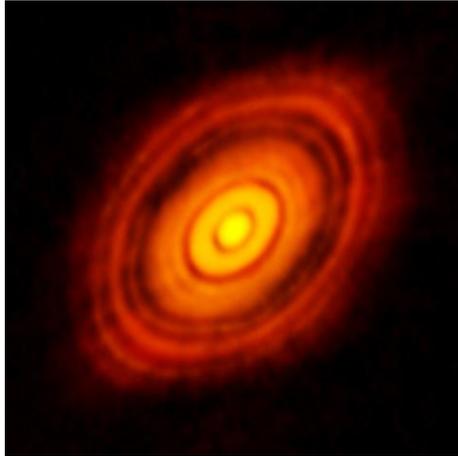


## 1.2 HL Tau and its protoplanetary disk

≈ 0.1 Myr



Class I

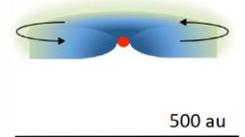


ALMA partnership 2015

HL Tau - Intermediate Class I/II

- Very **young**, partially embedded disk
- Substructures (ALMA partnership 2015). Active **planet formation?**
- Interactions with envelope in the form of **accretion streamers** (Yen et al. 2019)

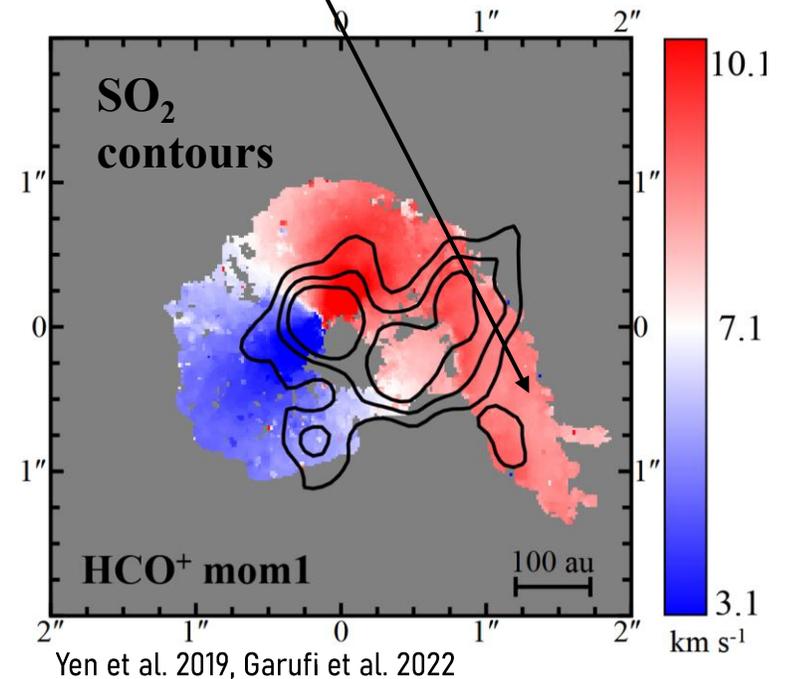
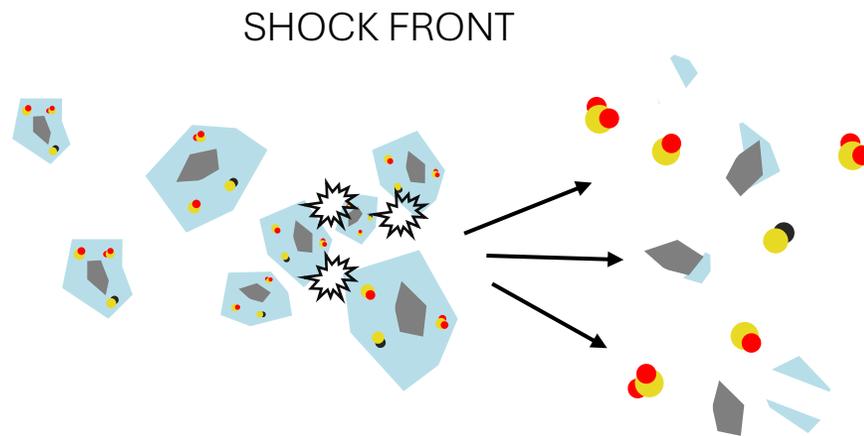
≈ 1 Myr



Class II

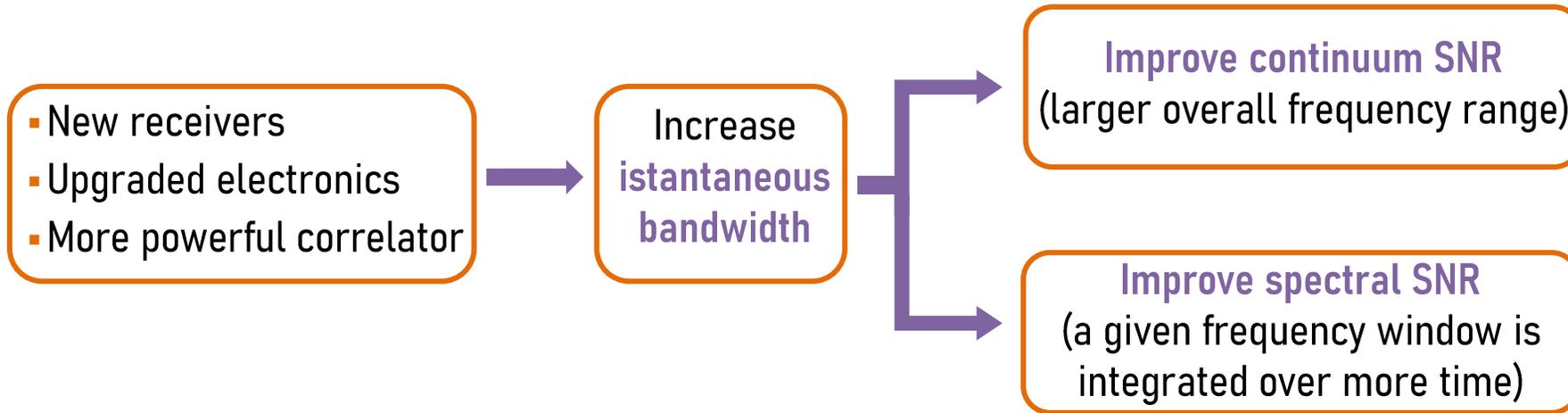
Late accretion events (Garufi et al. 2022)

- Detection of **S-bearing molecules** at the impact location between disk and accretion streamer
- Not compatible with thermal desorption → **mechanical desorption** (sputtering of icy matles) as a result of slow shocks



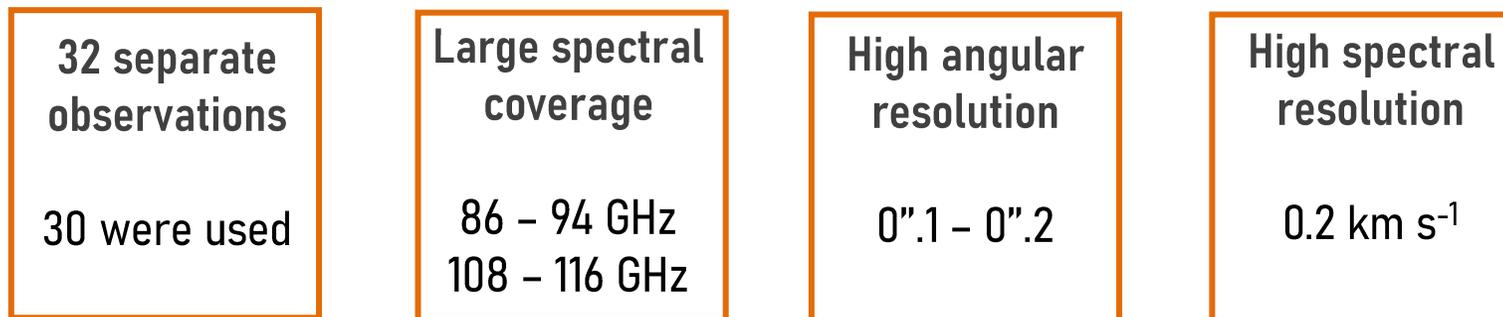
### 2.1 ALMA and the WSU

#### The Wideband Sensitivity Upgrade



#### The Dataset

Demonstration dataset in preparation for the WSU (PI: R. Loomis). Science target: **HL Tau**



Largest dataset **ever made for any protoplanetary disk** → Standard size post-WSU!

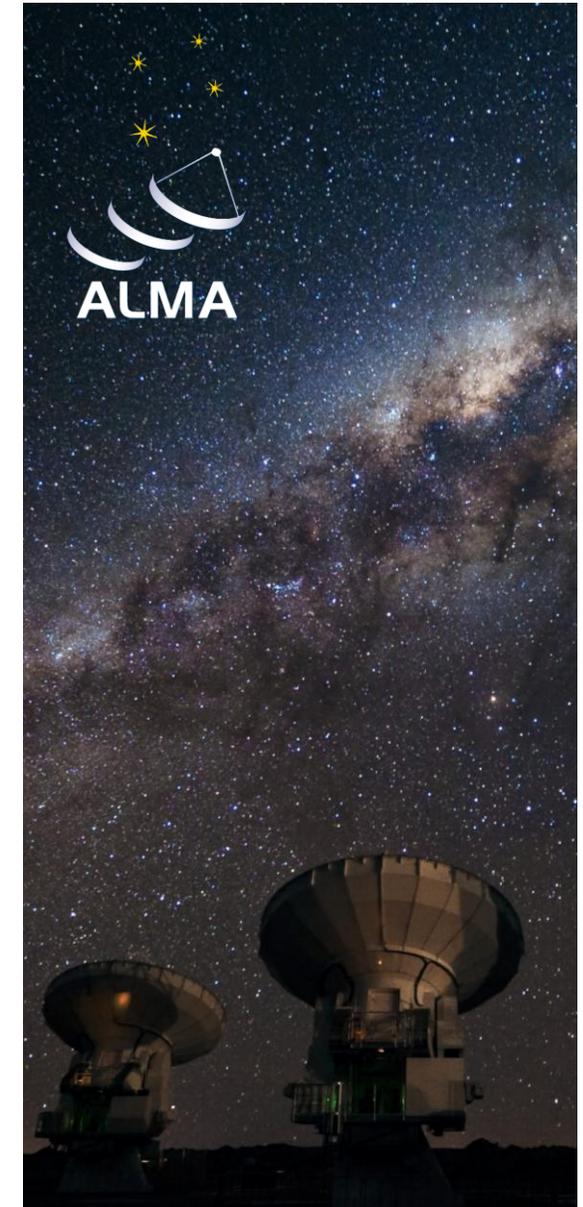
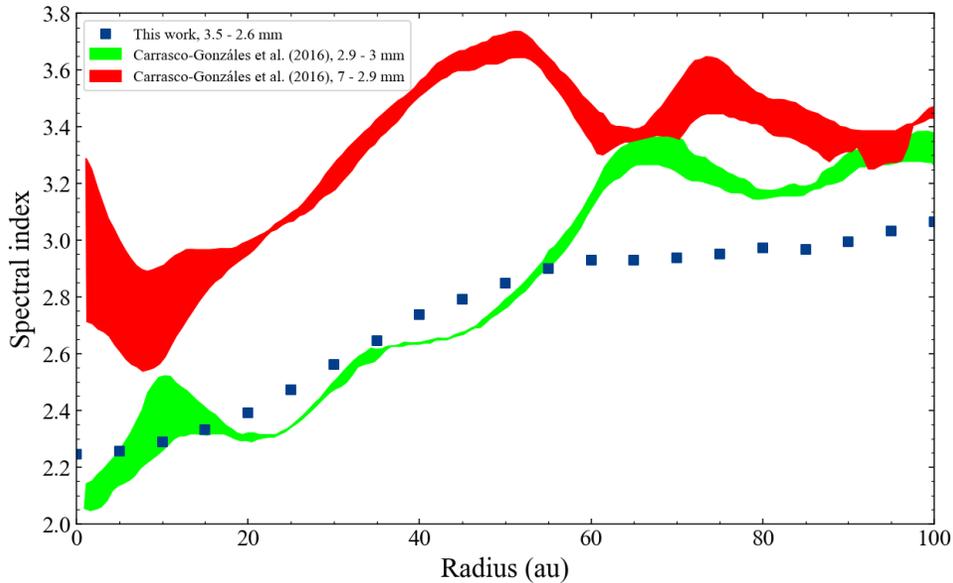
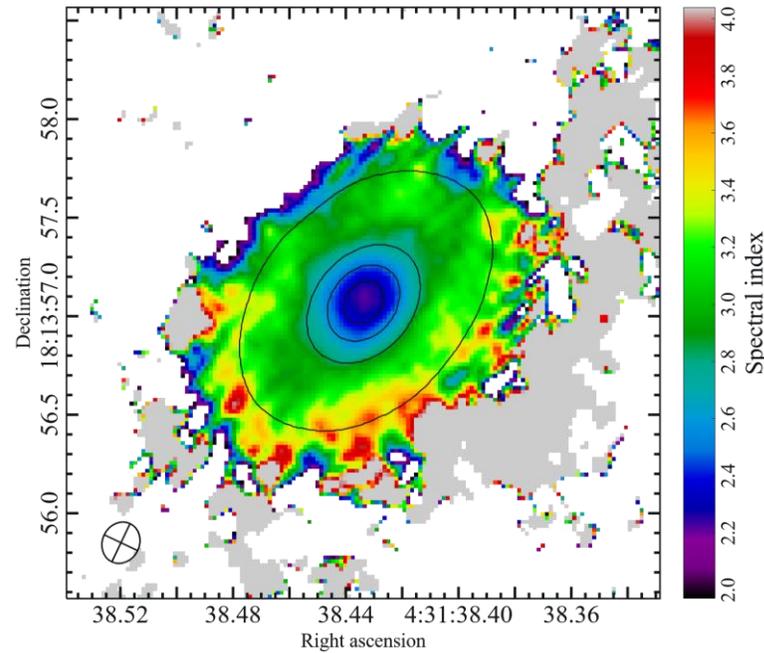
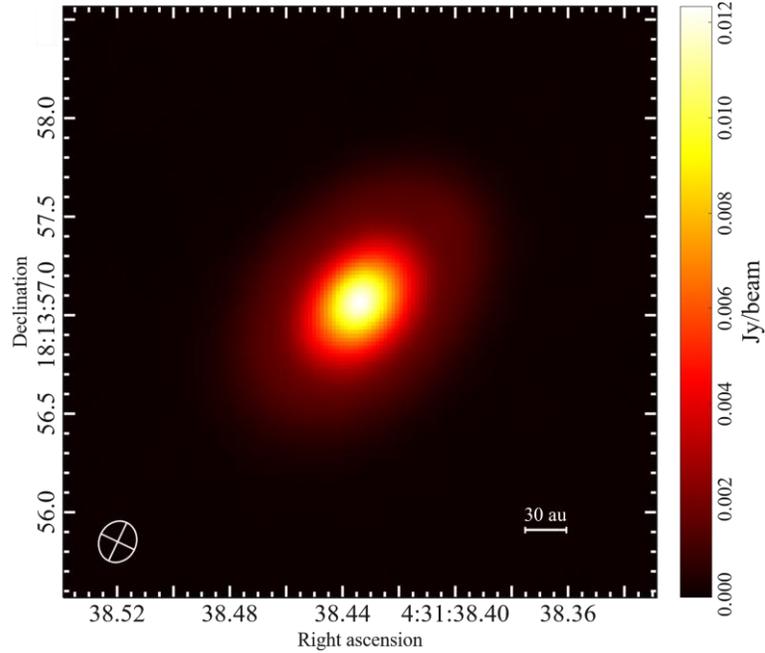


Figure credit: ESO

## 3.1 Continuum imaging & spectral index



Rayleigh-Jeans approximation

$$F_\nu \sim F_0 (\nu/\nu_0)^\alpha$$

$$2 \leq \alpha \leq 2 + \beta$$

Optically thick

Optically thin, with  $\beta$  depending on dust size (and ignoring scattering)

Channel and time average of the calibrated datacubes



Wideband imaging with tclean and MT-MFS



Single combined image at the central frequency + Spectral index map

## 3.2 Molecular lines in HL Tau

Time average of the calibrated continuum-subtracted datacubes



Cleaning with CASA's tclean and automasking



Searching for lines with the help of GoFish (Teague 2019)

### Emission lines

6 emission lines from 6 molecules:



Four CO isotopologues



HCO<sup>+</sup>



SO

Emitting mostly from the rotating disk

→ Signal boosting using keplerian model (GoFish)

Localized near the streamer

### Absorption lines

10 absorption lines from 3 molecules:



CN



HCN



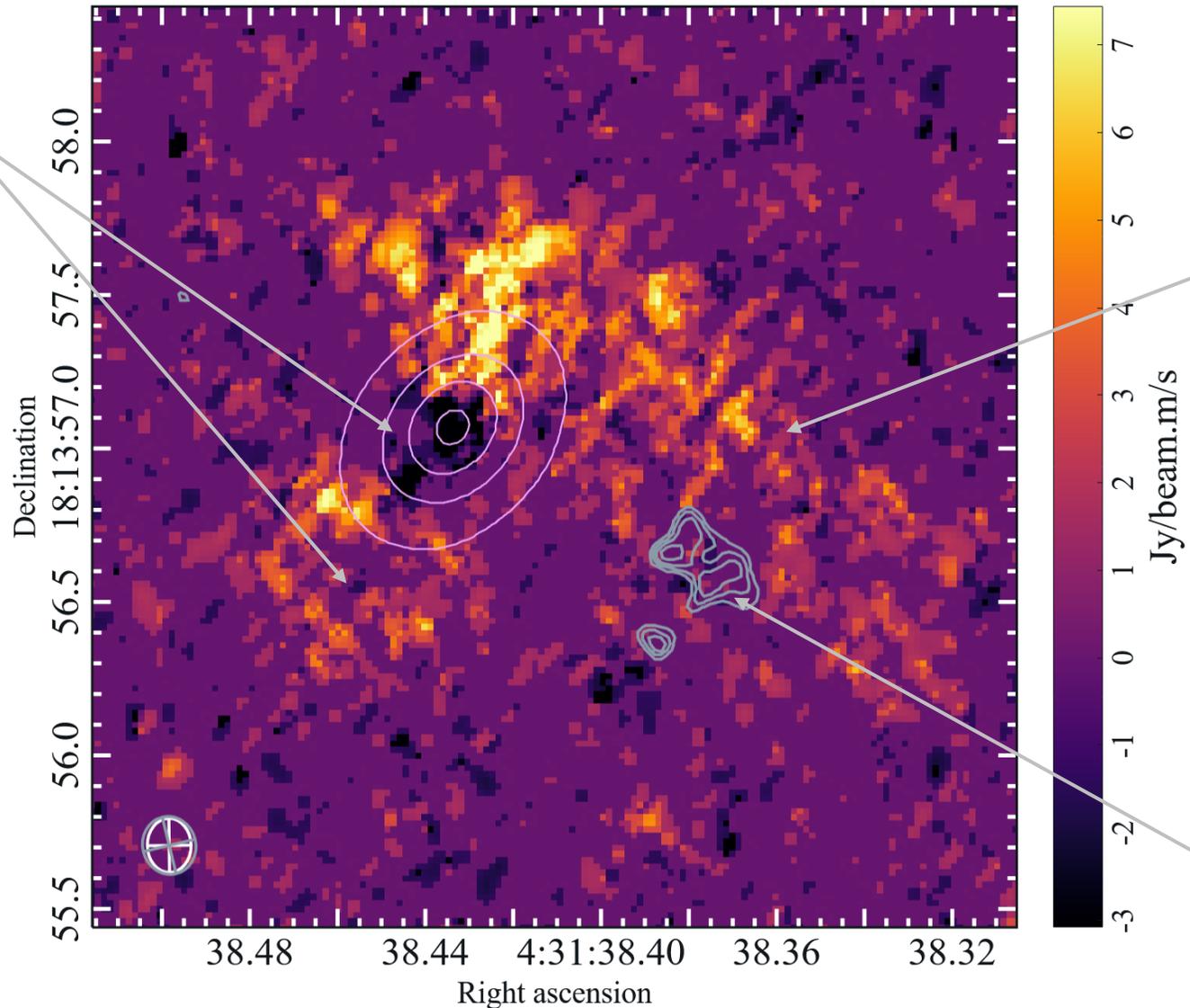
HNC

Absorbing from the envelope

| Molecule                        | Transition    | $\nu_{rest}$ (GHz) |
|---------------------------------|---------------|--------------------|
| Emission                        |               |                    |
| <sup>12</sup> C <sup>16</sup> O | 1 – 0         | 115.27120          |
| <sup>13</sup> C <sup>16</sup> O | 1 – 0         | 110.20135          |
| <sup>12</sup> C <sup>18</sup> O | 1 – 0         | 109.78217          |
| <sup>12</sup> C <sup>17</sup> O | 1 – 0         | 112.35928          |
| HCO <sup>+</sup>                | 1 – 0         | 89.18852           |
| SO                              | 3 2 – 2 1     | 109.25222          |
| Absorption                      |               |                    |
| CN                              | 1 1 1 – 0 1 2 | 113.14416          |
| CN                              | 1 1 2 – 0 1 1 | 113.17049          |
| CN                              | 1 1 2 – 0 1 2 | 113.19128          |
| CN                              | 1 2 2 – 0 1 1 | 113.48812          |
| CN                              | 1 2 3 – 0 1 2 | 113.49097          |
| CN                              | 1 2 2 – 0 1 2 | 113.50890          |
| HCN                             | 1 1 – 0 1     | 88.63042           |
| HCN                             | 1 2 – 0 1     | 88.63185           |
| HCN                             | 1 0 – 0 1     | 88.63394           |
| HNC                             | 1 – 0         | 90.66357           |

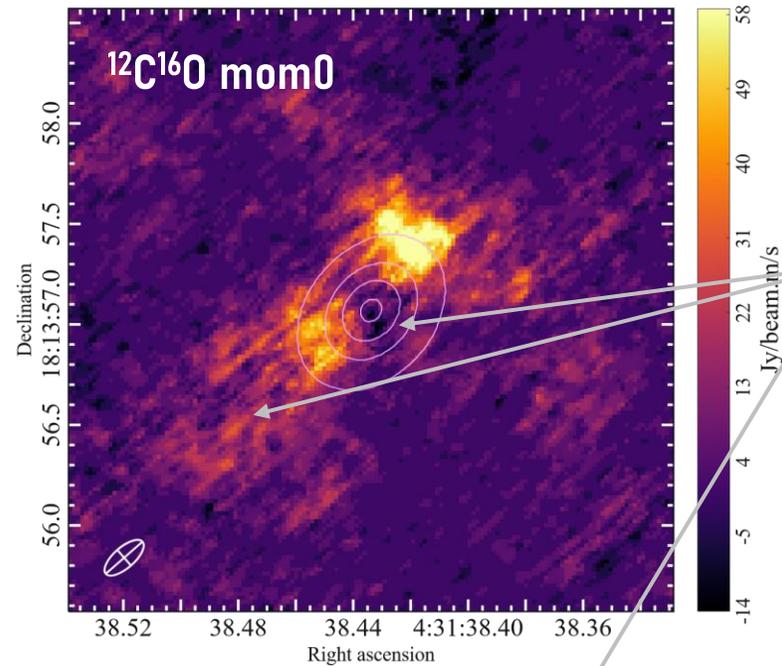
# HCO<sup>+</sup> mom0, with SO contours and continuum contours

Absorption and fainter emission



Accretion streamer

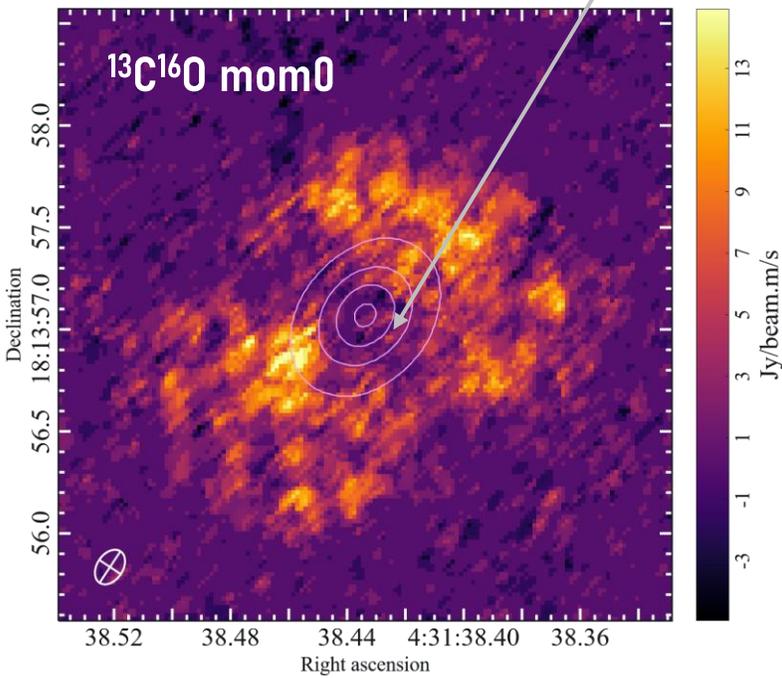
Localized SO emission  
↓  
Likely not thermally desorbed



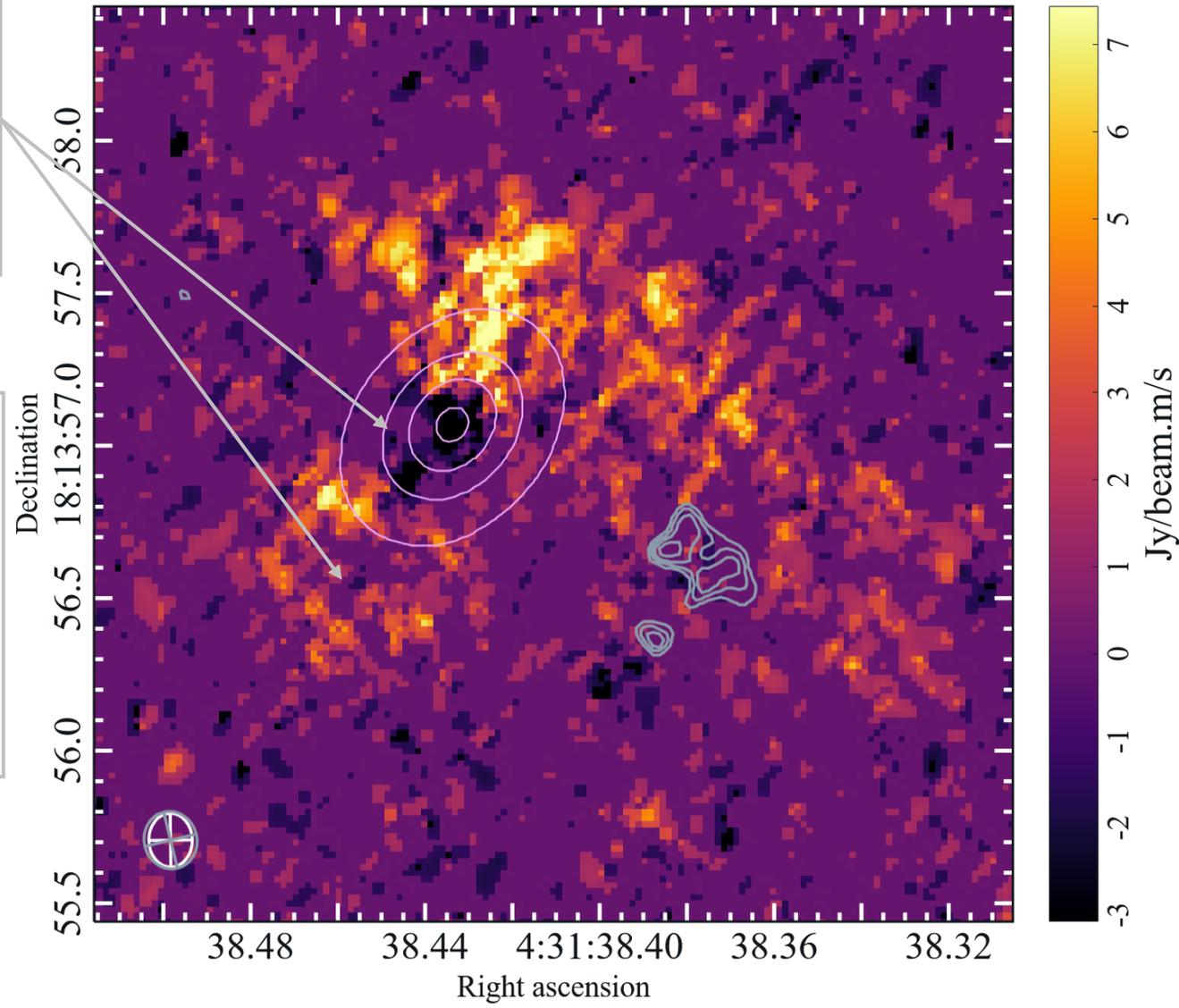
Absorption and fainter emission



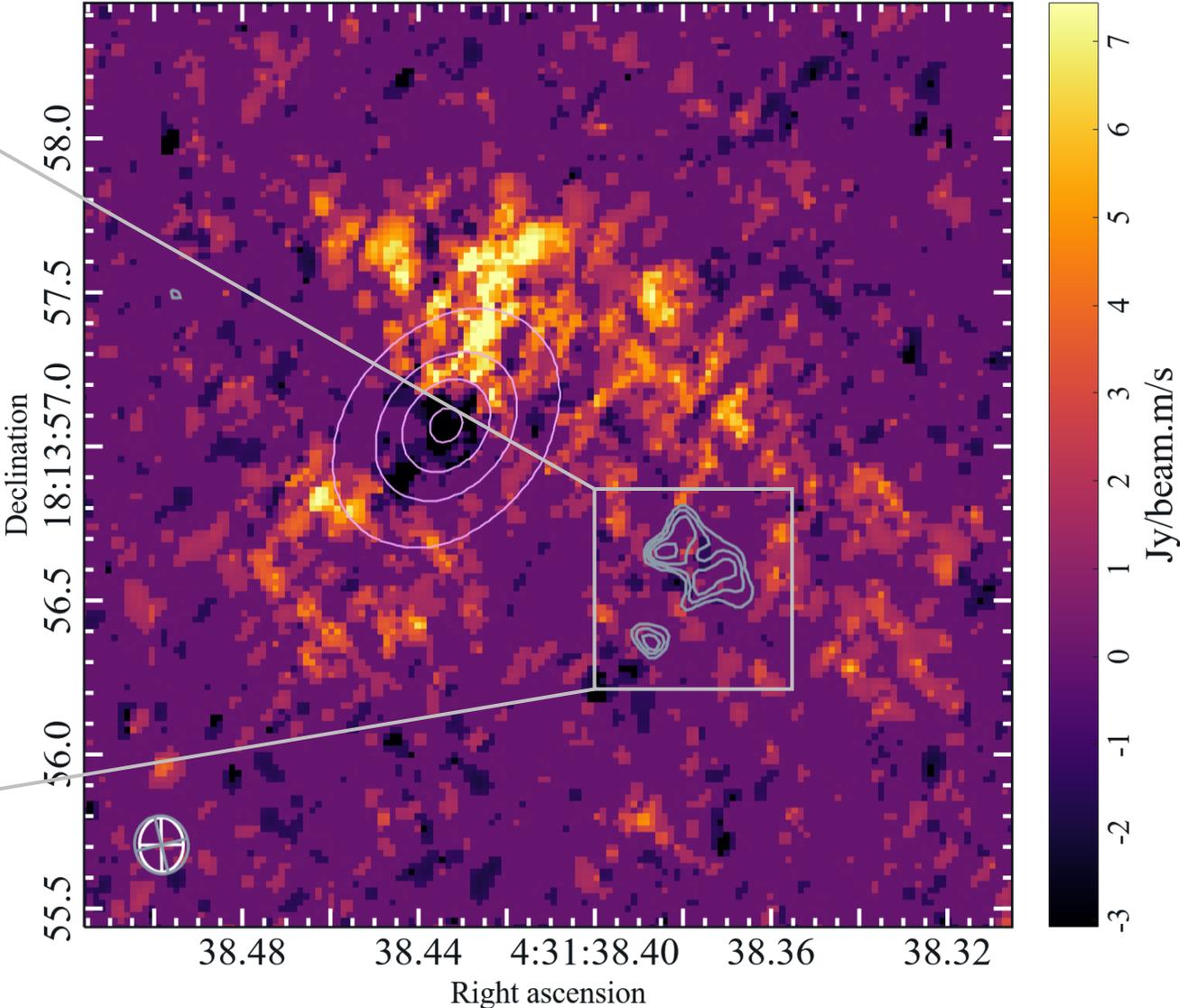
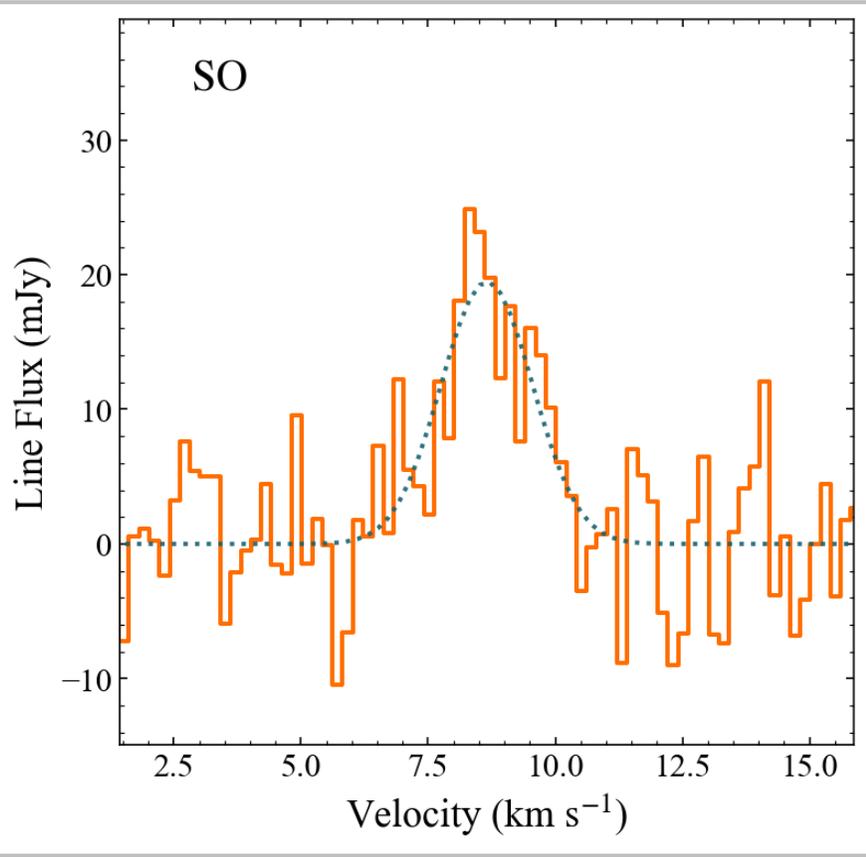
Absorption from  
**dust**  
+  
Molecules in the  
surrounding  
**envelope**



**$\text{HCO}^+$  mom0, with SO contours and continuum contours**



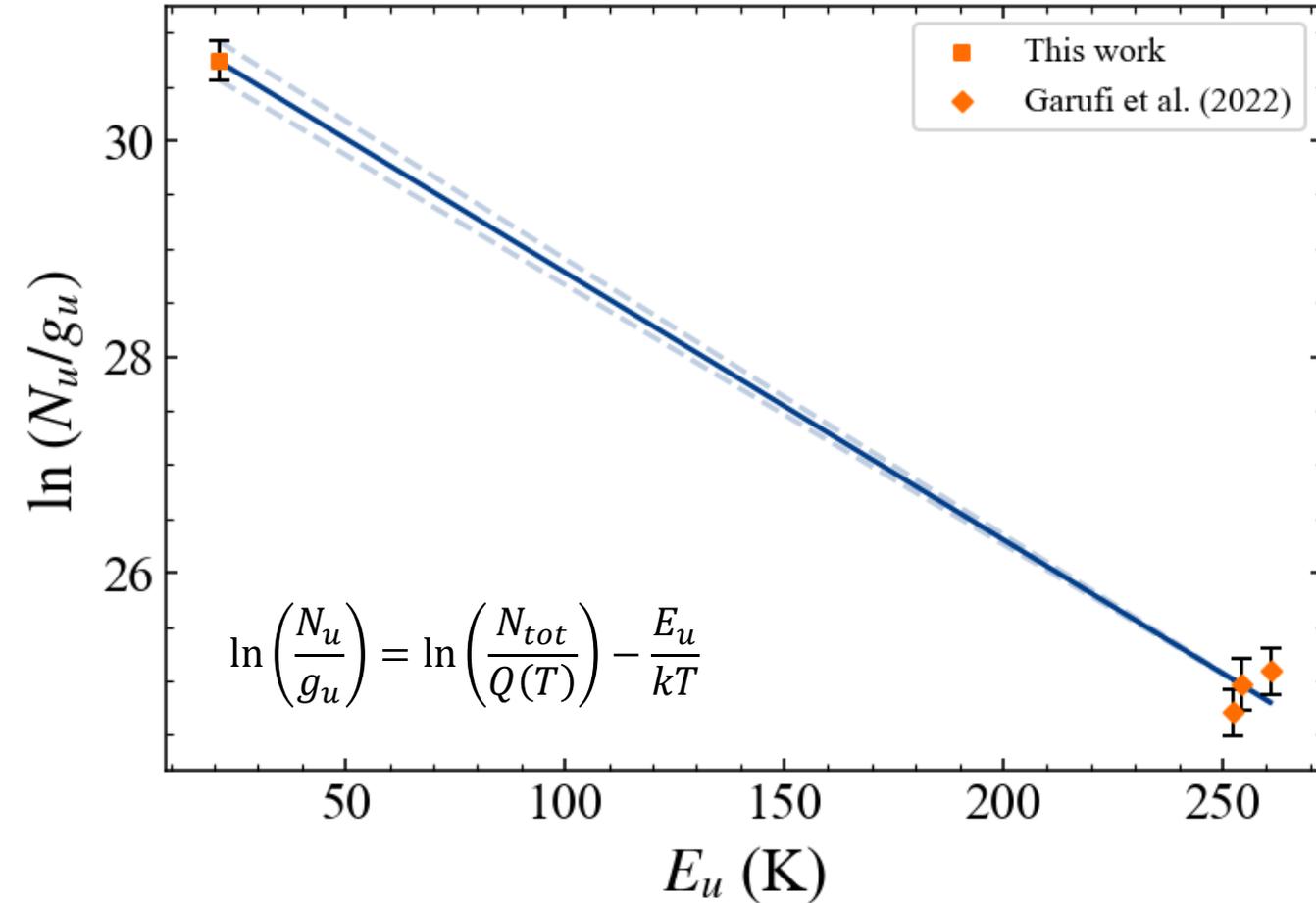
HCO<sup>+</sup> mom0, with SO contours and continuum contours



| Molecule | Transition | $\sigma_{rms}$<br>(mJy) | Line peak<br>( $\sigma_{rms}$ ) | $V_{sys}$<br>( $\text{km s}^{-1}$ ) | $\Delta V$<br>( $\text{km s}^{-1}$ ) | Line Flux<br>( $\text{mJy km s}^{-1}$ ) |
|----------|------------|-------------------------|---------------------------------|-------------------------------------|--------------------------------------|---|
| SO       | 32 - 21    | 4.8                     | 5.2                             | 8.65 (0.11)                         | 5.4                                  | 44.5 (6.6)                              |

### 3.3 Constraining the physical conditions of SO

SO rotational diagram



Only works assuming **optically thin lines** and **LTE!**

- Using this work's SO line and the three higher-energy detections from Garufi et al. 2022

**This work**

$$T_{SO} = (40.4 \pm 1.2) K \quad N_{tot,SO} = 3.6_{-0.7}^{+0.9} \times 10^{15} \text{ cm}^{-2}$$

**Garufi et al. (assuming  $T_{SO} = T_{SO_2}$ )**

$$T_{SO} = (58 \pm 19) K \quad N_{tot,SO} = (0.2 - 2) \times 10^{16} \text{ cm}^{-2}$$

- The detections of Garufi et al. lie in an energy range too narrow for a rotational diagram
- ➔ They assumed an SO temperature equal to that of  $\text{SO}_2$

This result confirms their assumption and **agrees with a non-thermal origin of the SO gas**

### SOME PROMISING RESULTS ...

- Derived the intra-band **spectral index of HL Tau within the full Band 3** using a WSU-like dataset
- Confirmed the assumptions of Garufi et al. regarding the **co-spatial nature** of SO and SO<sub>2</sub> and their origin as **mechanically desorbed** species
- Highlighted the **importance of late accretion events and slow shocks** in the enrichment of the gas phase with otherwise frozen-out molecules

### ... DESPITE LARGE LIMITATIONS

- Demonstration dataset – not meant for science!
  - Very **low SNR**
  - Lack of short baselines and **loss of extended emission**
- COMs remain undetected in HL Tau
- Will the SNR improvements of Band 2 finally reveal the elusive complexity in HL Tau? Maybe, but **compromises on the angular resolution** might still be required

**Thank you**



## A.1 The rotational diagram

Assuming  
LTE

$$N_{tot} = \frac{e^{E_u/k_B T}}{g_u} N_u Q(T)$$



$$\ln\left(\frac{N_u}{g_u}\right) = \ln\left(\frac{N_{tot}}{Q(T)}\right) - \frac{E_u}{kT}$$

Slope  $m$

Intercept  $q$

$$N_{tot} = e^q Q(T)$$

$$T = -1/m$$

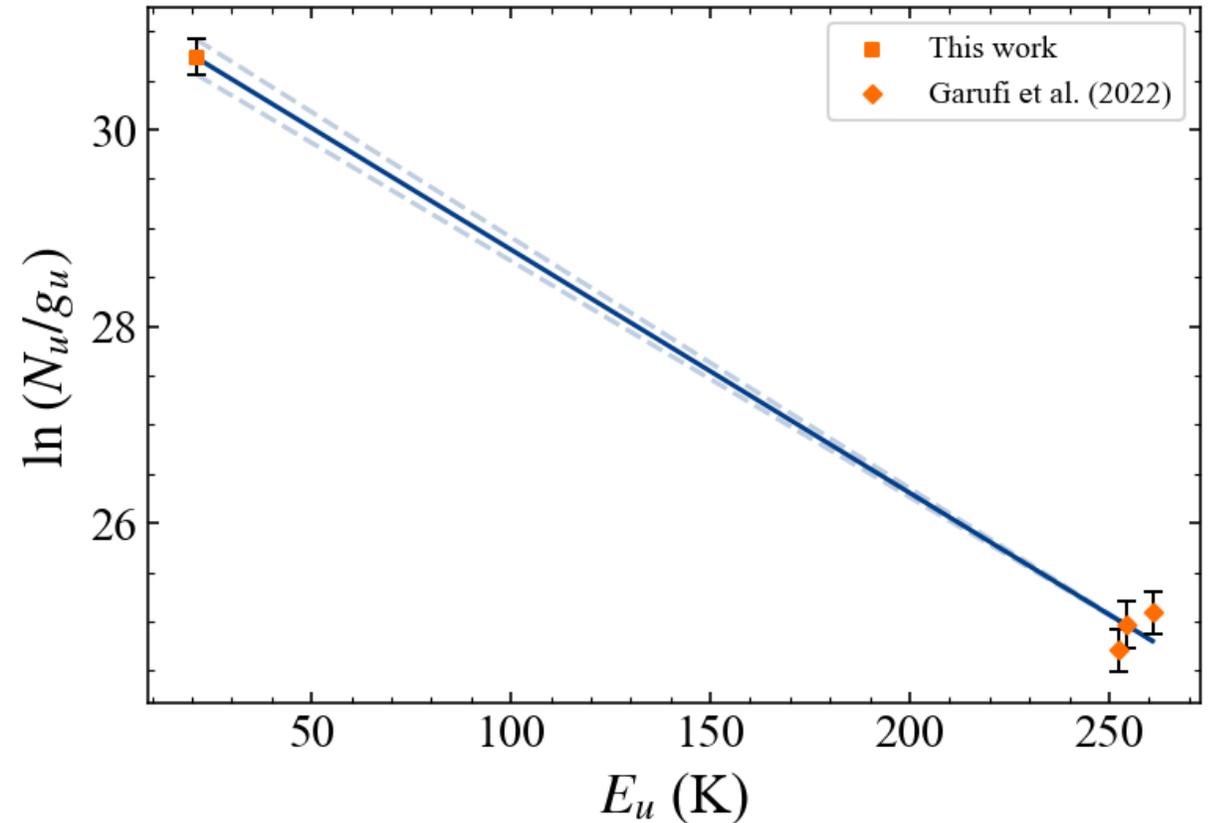
$$Q(T) = \sum_i g_i e^{-E_i/k_B T}$$

Partition function

$$N_u = \frac{8\pi k_B \nu^2}{hc^3 A_{ul}} \int T_b d\nu$$

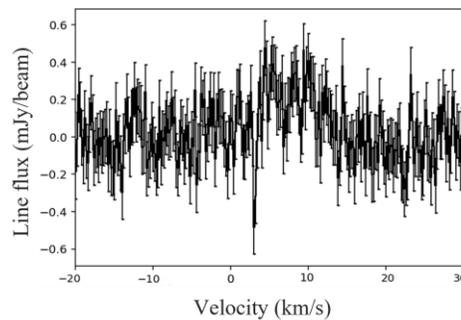
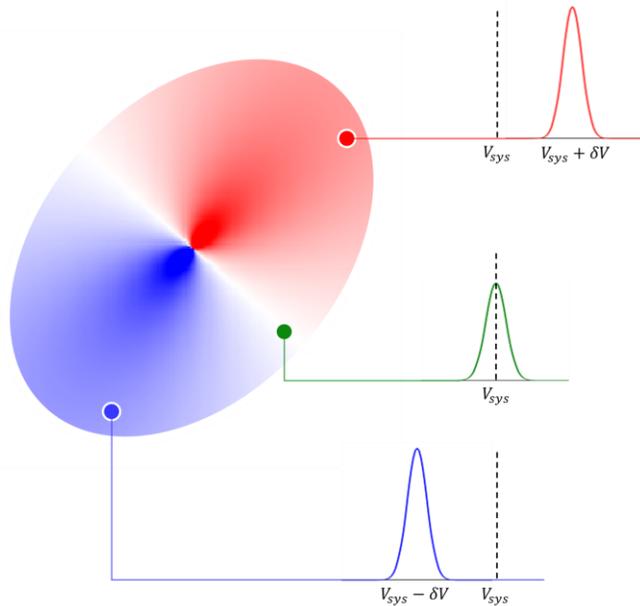
Upper-level column density

Assuming optically thin lines

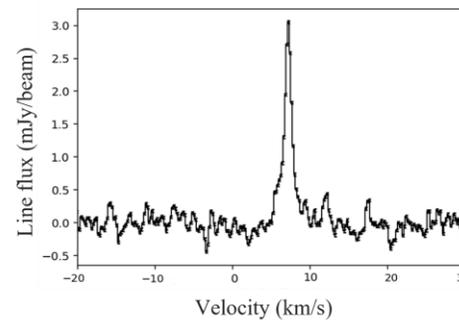
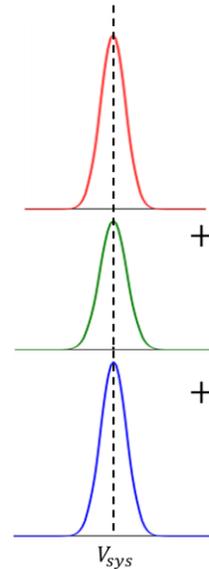


## A.2 SNR boosting with GoFish

### WITHOUT ALIGNMENT



### WITH ALIGNMENT AND STACK



Spectrum of  $C^{18}O$  in HL Tau before and after shift-and-stack (this work)

### Requires:

- Stellar mass
- Disk inclination angle
- Disk Position Angle
- Distance from the observer

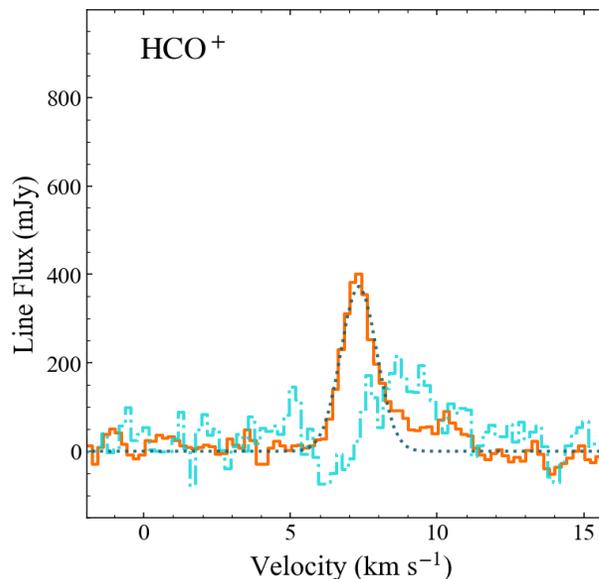
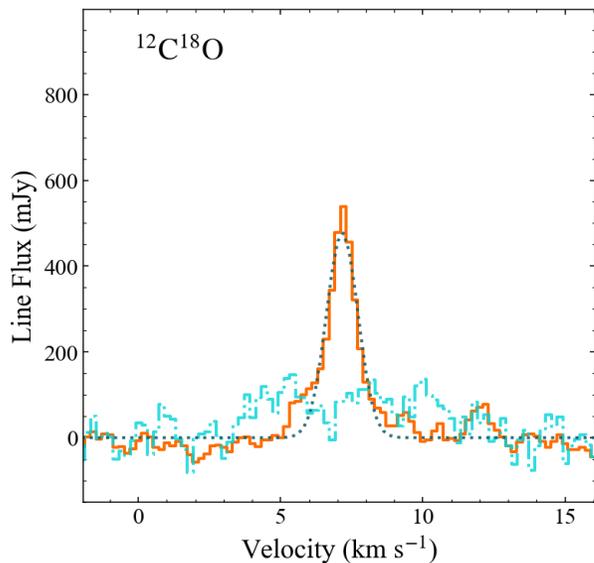
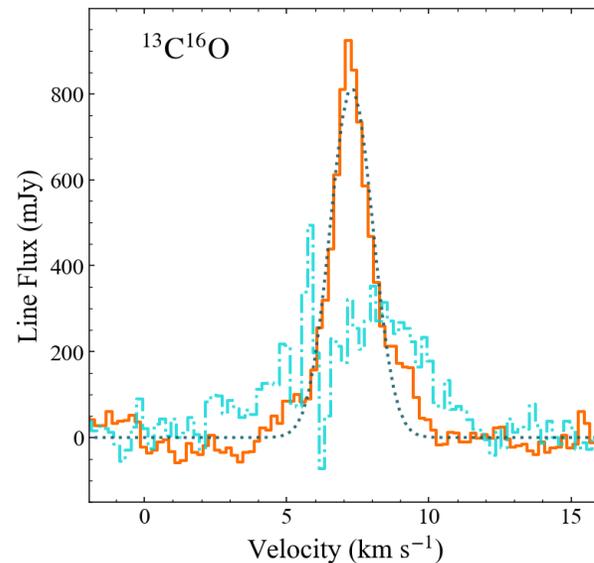
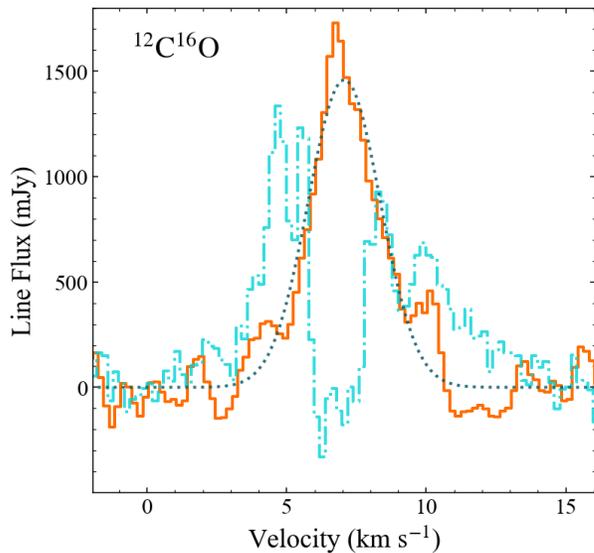
### Allows to:

- Boost the SNR of detected lines
- Detect otherwise invisible lines

Accessible through the **GoFish**  
Python module by Teague (2019)

## A.3 Spectra and fluxes

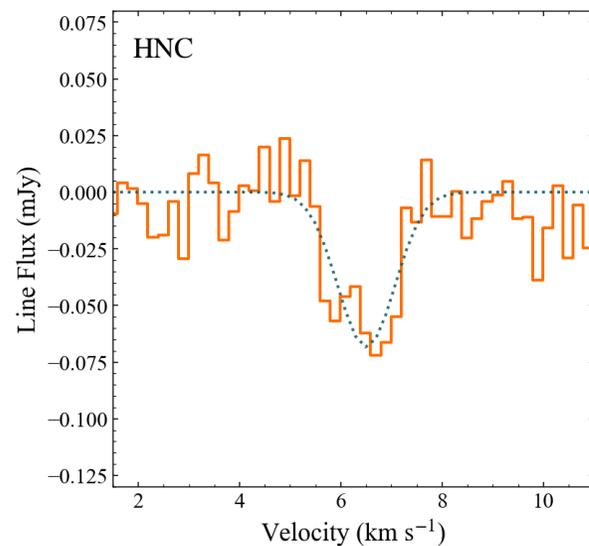
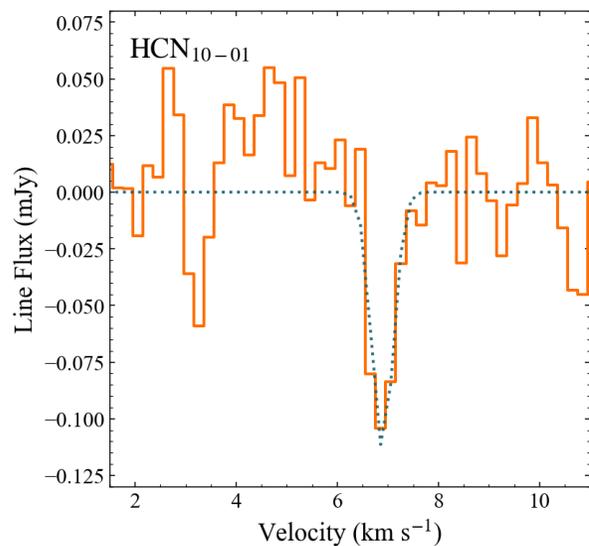
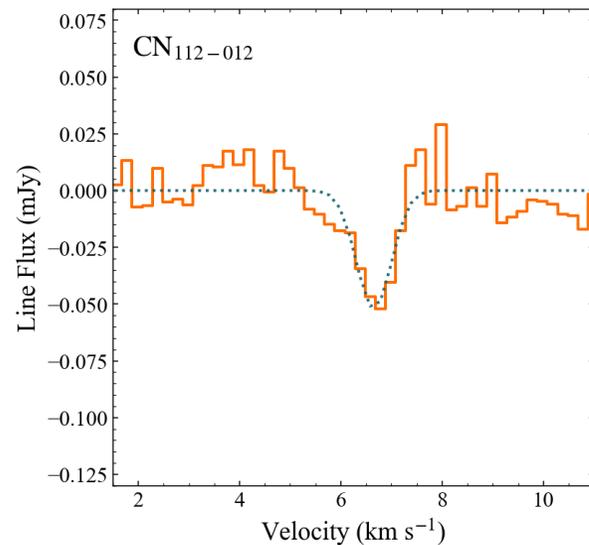
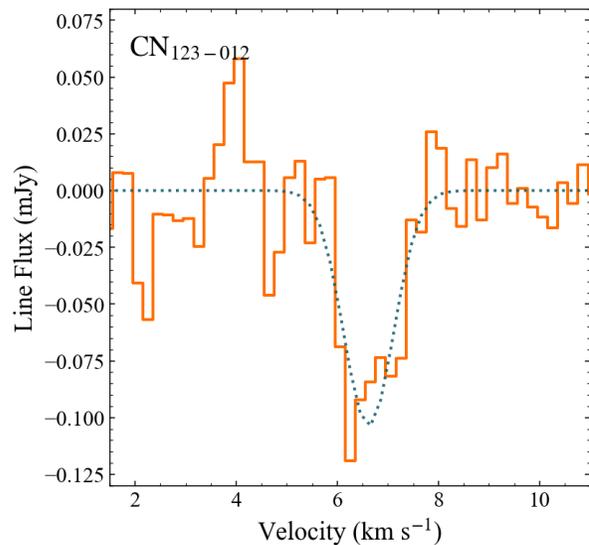
### Disk spectra with and without shift-and-stack



| Molecule                     | Transition    | $\sigma_{rms}$<br>(mJy) | Line peak<br>( $\sigma_{rms}$ ) | $V_{sys}$<br>(km s <sup>-1</sup> ) | $\Delta V$<br>(km s <sup>-1</sup> ) | Line Flux<br>(mJy km s <sup>-1</sup> ) |
|------------------------------|---------------|-------------------------|---------------------------------|------------------------------------|-------------------------------------|--|
| Disk                         |               |                         |                                 |                                    |                                     |  |
| $^{12}\text{C}^{16}\text{O}$ | 1 – 0         | 69.3                    | 25.0                            | 7.06 (0.03)                        | 7.8                                 | 4999 (419)                             |
| $^{13}\text{C}^{16}\text{O}$ | 1 – 0         | 30.2                    | 30.6                            | 7.28 (0.02)                        | 4.6                                 | 1603 (42)                              |
| $^{12}\text{C}^{18}\text{O}$ | 1 – 0         | 23.7                    | 22.7                            | 7.17 (0.02)                        | 3.2                                 | 687 (35)                               |
| $^{12}\text{C}^{17}\text{O}$ | 1 – 0         | 45.9                    | 4.3                             | 7.26 (0.27)                        | 22.0                                | 1319 (132)                             |
| $\text{HCO}^+$               | 1 – 0         | 25.9                    | 15.5                            | 7.33 (0.02)                        | 3.6                                 | 578 (39)                               |
| Envelope                     |               |                         |                                 |                                    |                                     |  |
| CN                           | 1 1 1 – 0 1 2 | 0.012                   | 3.5                             | 6.85 (0.08)                        | 1.8                                 | -0.029 (0.008)                         |
| CN                           | 1 1 2 – 0 1 1 | 0.012                   | 4.0                             | 6.35 (0.12)                        | 3.2                                 | -0.040 (0.010)                         |
| CN                           | 1 1 2 – 0 1 2 | 0.012                   | 4.4                             | 6.65 (0.06)                        | 2.2                                 | -0.045 (0.008)                         |
| CN                           | 1 2 2 – 0 1 1 | 0.025                   | 3.7                             | 6.78 (0.11)                        | 2.8                                 | -0.091 (0.022)                         |
| CN                           | 1 2 3 – 0 1 2 | 0.025                   | 4.8                             | 6.62 (0.08)                        | 3.0                                 | -0.122 (0.023)                         |
| CN                           | 1 2 2 – 0 1 2 | 0.025                   | 3.9                             | 6.45 (0.13)                        | 2.6                                 | -0.064 (0.022)                         |
| HCN                          | 1 1 – 0 1     | 0.023                   | 3.9                             | 6.53 (0.18)                        | 4.0                                 | -0.080 (0.026)                         |
| HCN                          | 1 2 – 0 1     | 0.023                   | 4.0                             | 6.42 (0.11)                        | 3.6                                 | -0.120 (0.025)                         |
| HCN                          | 1 0 – 0 1     | 0.023                   | 4.4                             | 6.89 (0.03)                        | 1.2                                 | -0.054 (0.013)                         |
| HNC                          | 1 – 0         | 0.017                   | 4.2                             | 6.50 (0.09)                        | 3.4                                 | -0.090 (0.017)                         |
| Streamer                     |               |                         |                                 |                                    |                                     |  |
| SO                           | 3 2 – 2 1     | 4.8                     | 5.2                             | 8.65 (0.11)                        | 5.4                                 | 44.5 (6.6)                             |

## A.3 Spectra and fluxes

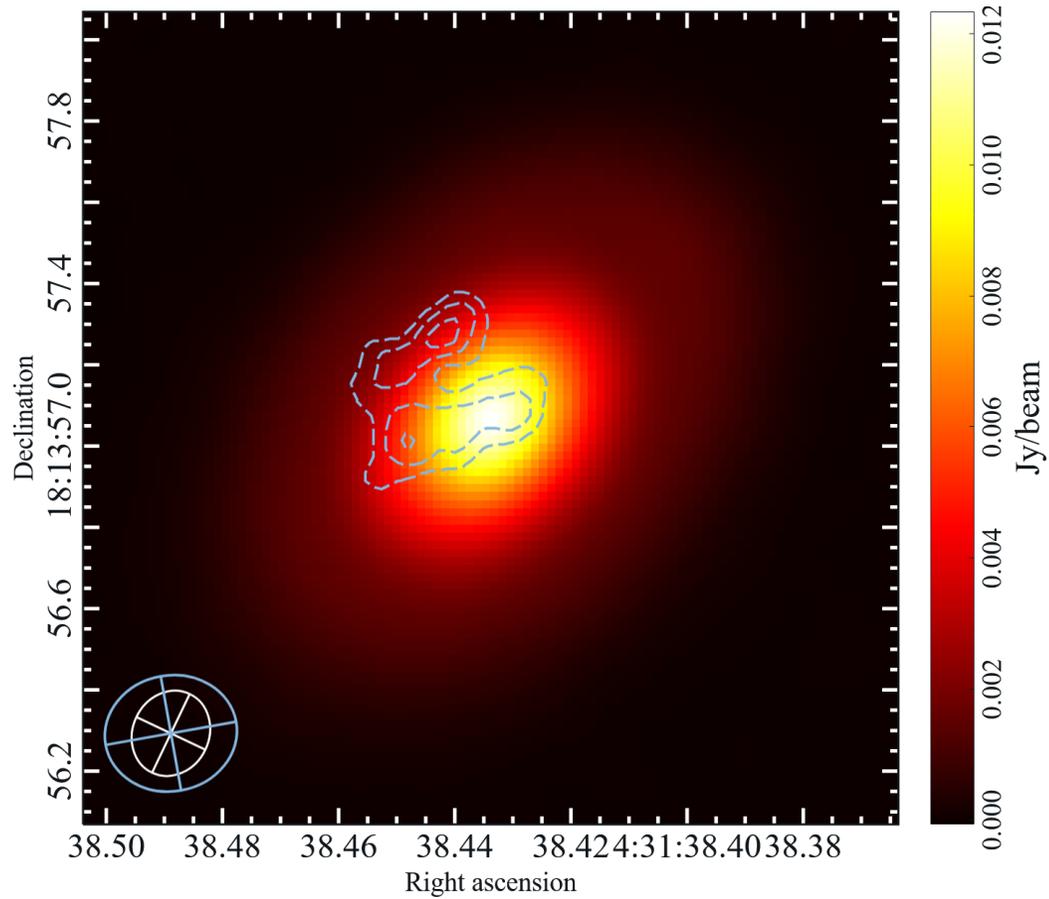
### Envelope spectra



| Molecule                        | Transition | $\sigma_{rms}$<br>(mJy) | Line peak<br>( $\sigma_{rms}$ ) | $V_{sys}$<br>(km s <sup>-1</sup> ) | $\Delta V$<br>(km s <sup>-1</sup> ) | Line Flux<br>(mJy km s <sup>-1</sup> ) |
|---------------------------------|------------|-------------------------|---------------------------------|------------------------------------|-------------------------------------|--|
| Disk                            |            |                         |                                 |                                    |                                     |  |
| <sup>12</sup> C <sup>16</sup> O | 1 - 0      | 69.3                    | 25.0                            | 7.06 (0.03)                        | 7.8                                 | 4999 (419)                             |
| <sup>13</sup> C <sup>16</sup> O | 1 - 0      | 30.2                    | 30.6                            | 7.28 (0.02)                        | 4.6                                 | 1603 (42)                              |
| <sup>12</sup> C <sup>18</sup> O | 1 - 0      | 23.7                    | 22.7                            | 7.17 (0.02)                        | 3.2                                 | 687 (35)                               |
| <sup>12</sup> C <sup>17</sup> O | 1 - 0      | 45.9                    | 4.3                             | 7.26 (0.27)                        | 22.0                                | 1319 (132)                             |
| HCO <sup>+</sup>                | 1 - 0      | 25.9                    | 15.5                            | 7.33 (0.02)                        | 3.6                                 | 578 (39)                               |
| Envelope                        |            |                         |                                 |                                    |                                     |  |
| CN                              | 111 - 012  | 0.012                   | 3.5                             | 6.85 (0.08)                        | 1.8                                 | -0.029 (0.008)                         |
| CN                              | 112 - 011  | 0.012                   | 4.0                             | 6.35 (0.12)                        | 3.2                                 | -0.040 (0.010)                         |
| CN                              | 112 - 012  | 0.012                   | 4.4                             | 6.65 (0.06)                        | 2.2                                 | -0.045 (0.008)                         |
| CN                              | 122 - 011  | 0.025                   | 3.7                             | 6.78 (0.11)                        | 2.8                                 | -0.091 (0.022)                         |
| CN                              | 123 - 012  | 0.025                   | 4.8                             | 6.62 (0.08)                        | 3.0                                 | -0.122 (0.023)                         |
| CN                              | 122 - 012  | 0.025                   | 3.9                             | 6.45 (0.13)                        | 2.6                                 | -0.064 (0.022)                         |
| HCN                             | 11 - 01    | 0.023                   | 3.9                             | 6.53 (0.18)                        | 4.0                                 | -0.080 (0.026)                         |
| HCN                             | 12 - 01    | 0.023                   | 4.0                             | 6.42 (0.11)                        | 3.6                                 | -0.120 (0.025)                         |
| HCN                             | 10 - 01    | 0.023                   | 4.4                             | 6.89 (0.03)                        | 1.2                                 | -0.054 (0.013)                         |
| HNC                             | 1 - 0      | 0.017                   | 4.2                             | 6.50 (0.09)                        | 3.4                                 | -0.090 (0.017)                         |
| Streamer                        |            |                         |                                 |                                    |                                     |  |
| SO                              | 32 - 21    | 4.8                     | 5.2                             | 8.65 (0.11)                        | 5.4                                 | 44.5 (6.6)                             |

## A.4 Absorption lines intensity maps

Continuum image with **CN contours** (three lines)



Continuum image with **HCN contours** (three lines)

