Study of cosmic-ray acceleration regions through their chemical composition

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Introduction
Cosmic-rays (CRs)

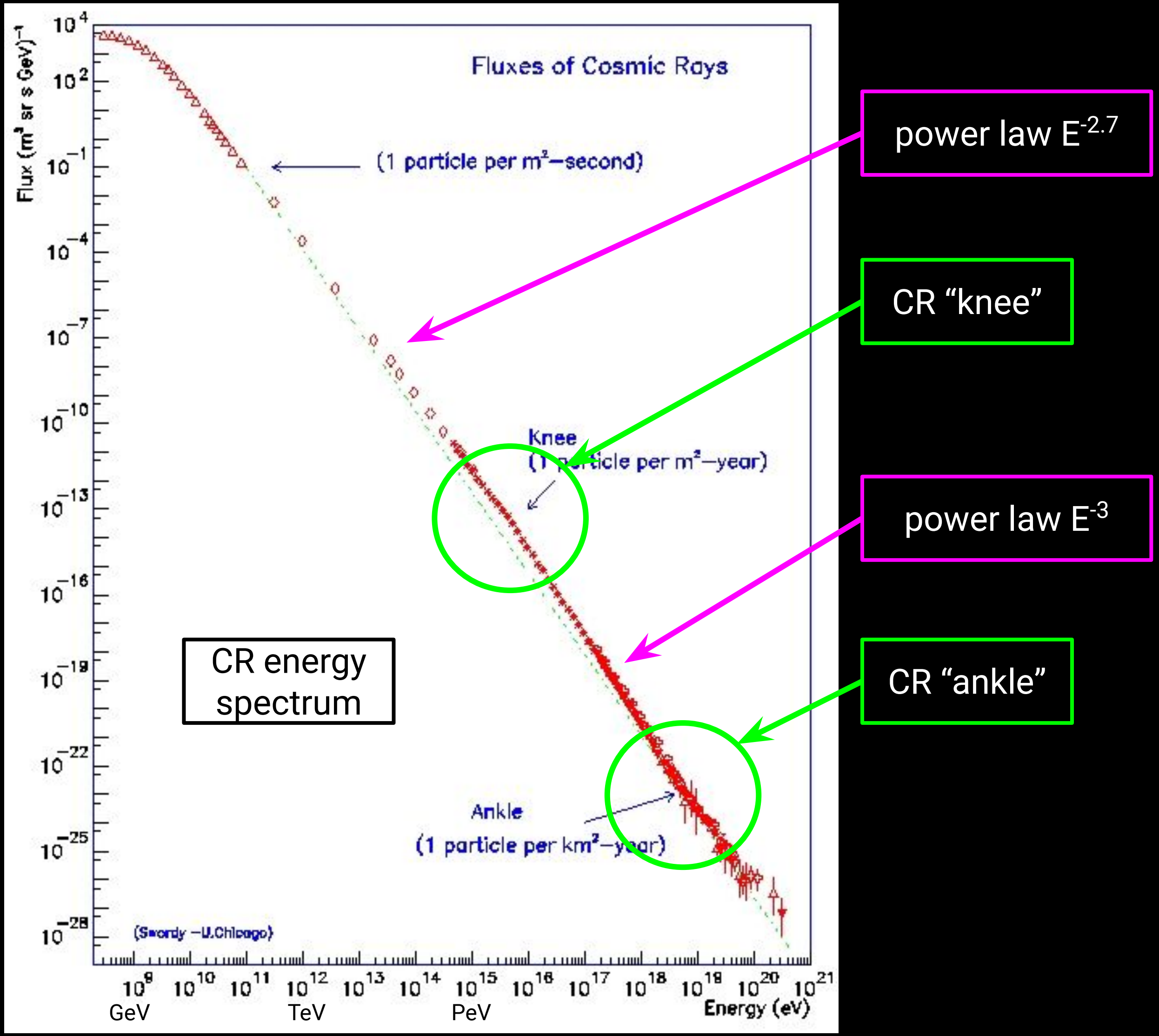
Power Law
$dN/dE \propto E^{-\gamma}$

Cosmic-ray particles:

- ✶ high-energy ionized nuclei (~90% protons + 9% alpha + heavy nuclei)
- ✶ mostly relativistic
- ✶ very few of them have ultra-relativistic energies up to 10^{20} eV

Fundamental questions of CR physics:

1) Where do they come from?
2) How are they accelerated to such high energies?
3) What is their impact on the ISM?

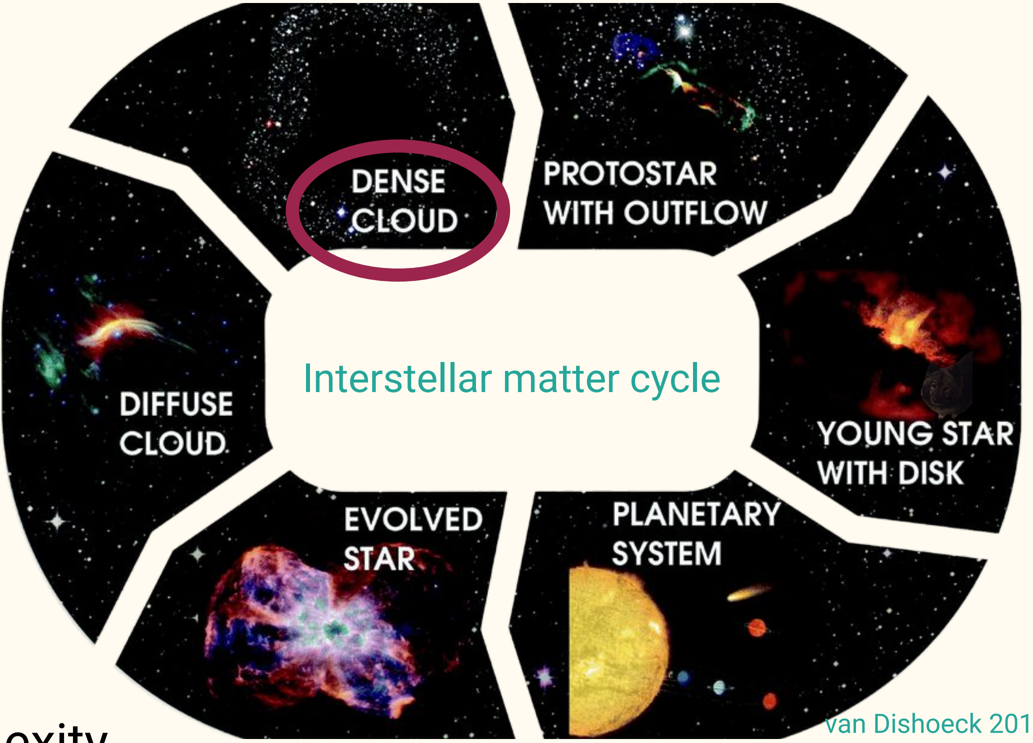


Introduction
Interstellar medium (ISM)

- Interstellar medium (ISM)
  - 99% of the mass = gas
    → 90% H + 9% He + 1% C, N, O, etc.
  - 1% of the mass = grains

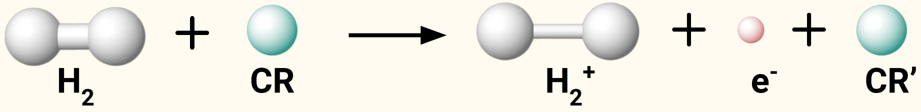
- Dense molecular clouds
  - density: from 10^4 to 10^7 cm^{-3}
  - temperature: from 8 to 20 K

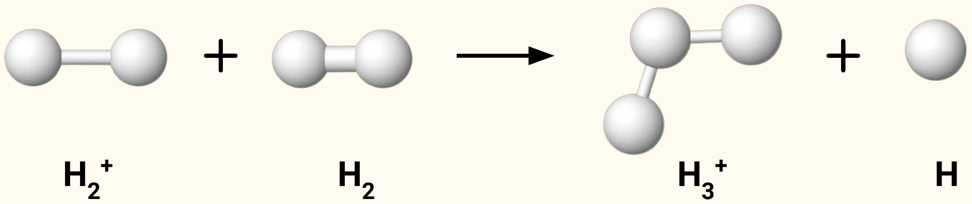
- Chemical reactions:
  - in gas phase
  - on the grain surfaces



van Dishoeck 2014

- **Cosmic-rays**: ionization → ISM molecular complexity
  → ionization of H_2 (most abundant molecule) ⇒ H_2 cosmic-ray **ionization rate ζ** (s^{-1})



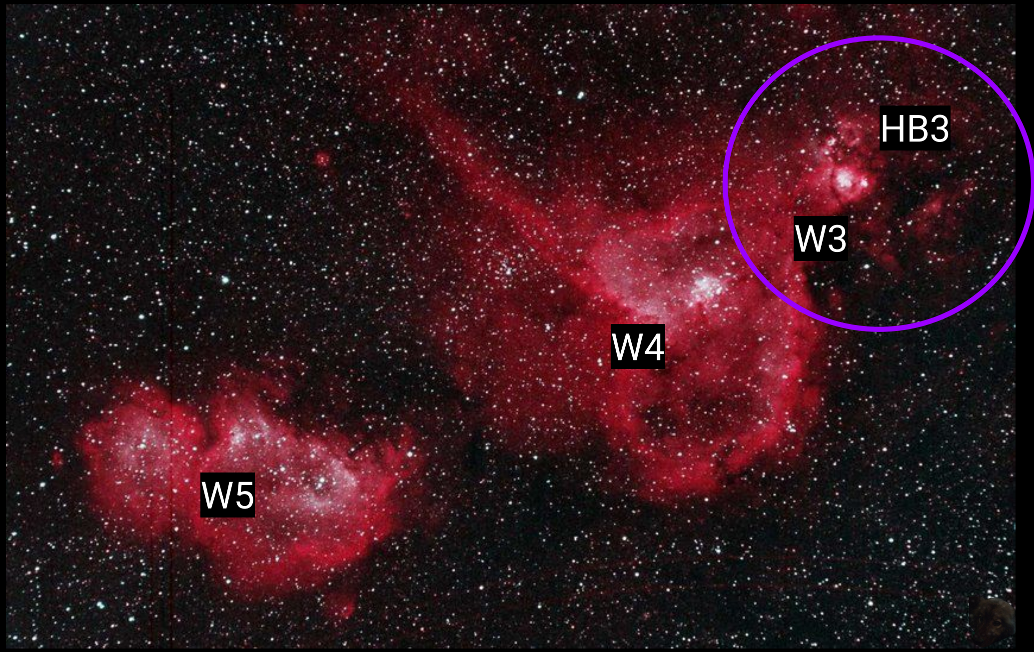


Scientific context

Studied region: the HB3/W3 complex

- ✶ Location: ~2 kpc in the northern constellation Cassiopeia, in the Heart Nebula
- ✶ W3: giant molecular cloud and HII region containing a very active factory of massive stars
- ✶ HB3 (G132.7+1.3): Supernova Remnant. Its south eastern part is adjacent to W3 (Digel et al. 1996)

- ✶ Age of the SNR: ~ 20-30 kyr
- ✶ Explosion energy: ~ 10^{51} erg



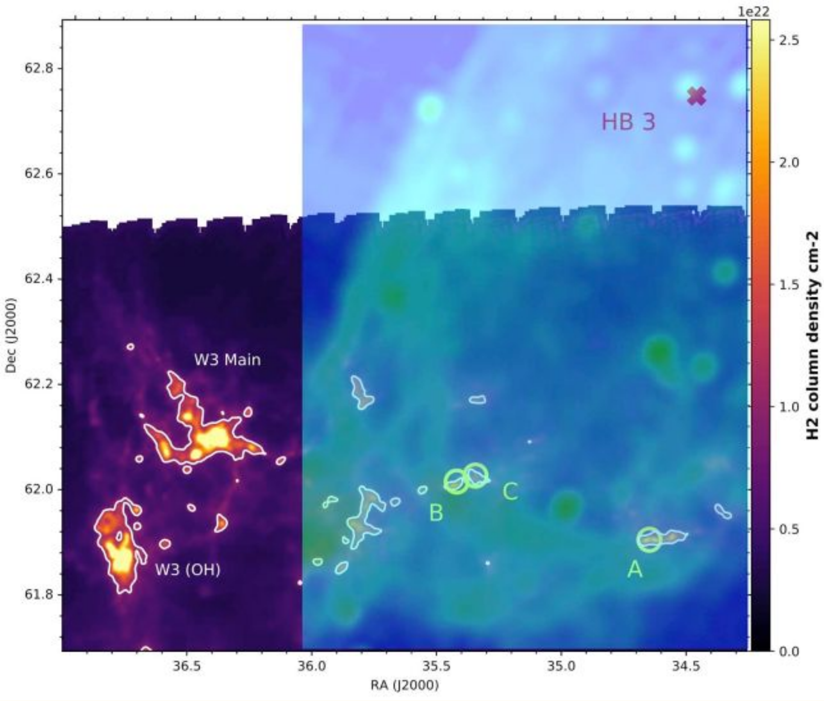
The Heart Nebula

Context

Astrochemistry - Cosmic-rays (CRs)

- ✶ Cosmic-rays: ionization → impact on the chemistry
  → H_2 ionization rate ζ (s^{-1}) : typical value ζ_{H2} = ~ 10^{-17} s^{-1}

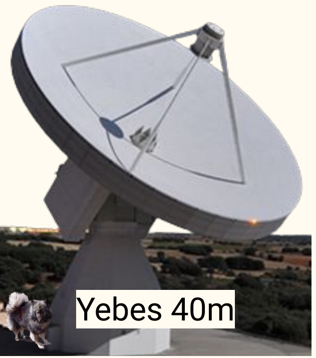
- ✶ Goal: use several direct and indirect chemical tracers of the ionization in order to constrain the CR ionization rate in the HB3/W3 complex to better understand the processes responsible for the acceleration and propagation of CRs in the Galaxy



- ✶ Chemical modeling with Nautilus: identification of the most sensitive species to the ionization rate ζ

- ✶ Radio observations:
  - ○ 2 campaigns already done with the IRAM 30m before the beginning of my PhD (single pointings)
  - ○ 1 with the Yebes 40m in 2022 (P. I., single pointings)
  - ○ 1 with the IRAM 30m in 2024 (P. I., on-the-fly map)

on A and B



Methods
3-phase Nautilus gas-grain model (Ruaud et al. 2016, Wakelam et al. 2024)

✶ Nautilus uses:

- 1141 chemical species, including 548 on the grains
- different types of reactions:

→ in the gas phase, on the grain surfaces and gas-grain interactions

✶ Based on the resolution of chemical kinetics differential equations

✶ Computes the gas and ice composition as a function of time for a set of physical conditions (such as T_{gas}, T_{dust}, A_V, n_H, ζ), either static or time-dependent, starting from an initial gas-phase composition

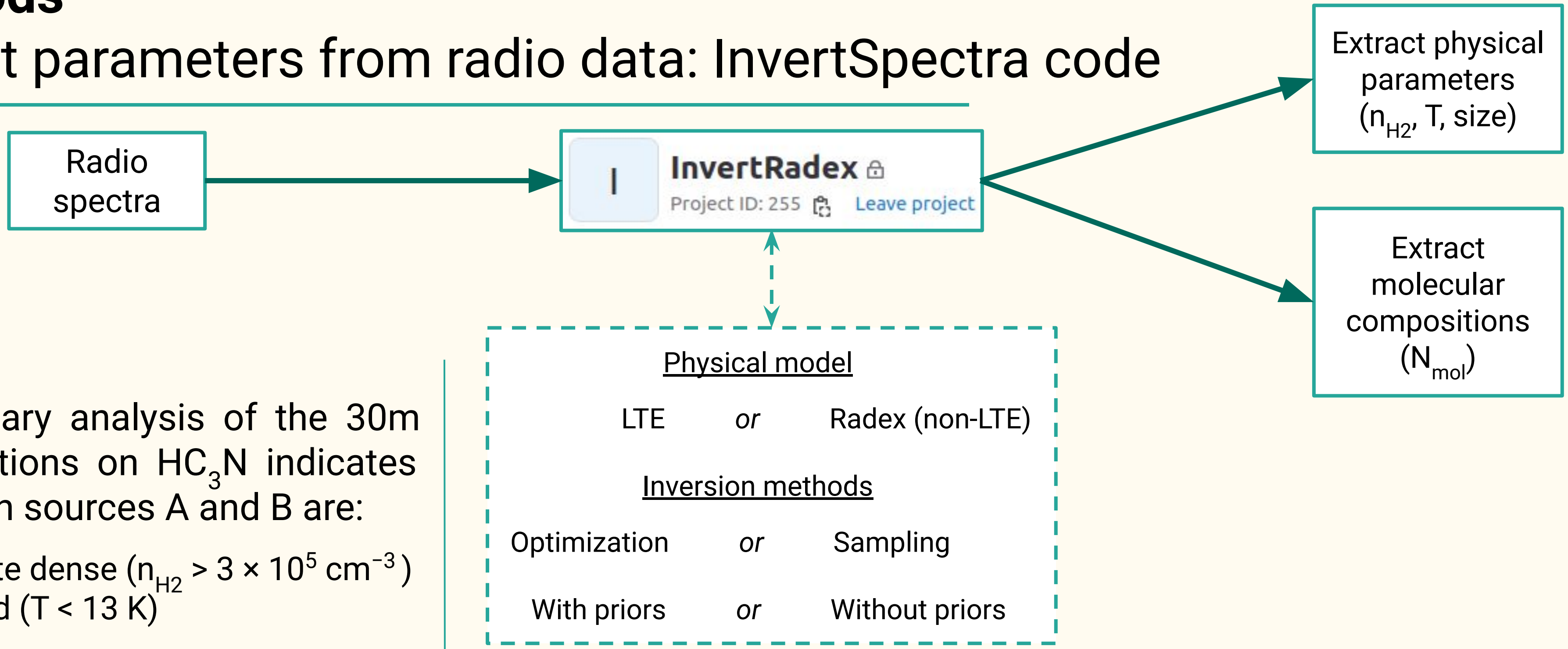
⇒ Outputs: time-dependent abundances of the molecules (gas + ice)

Developed at the LAB by Valentine Wakelam

Goal: reproduce the observed molecular column densities to constrain ζ

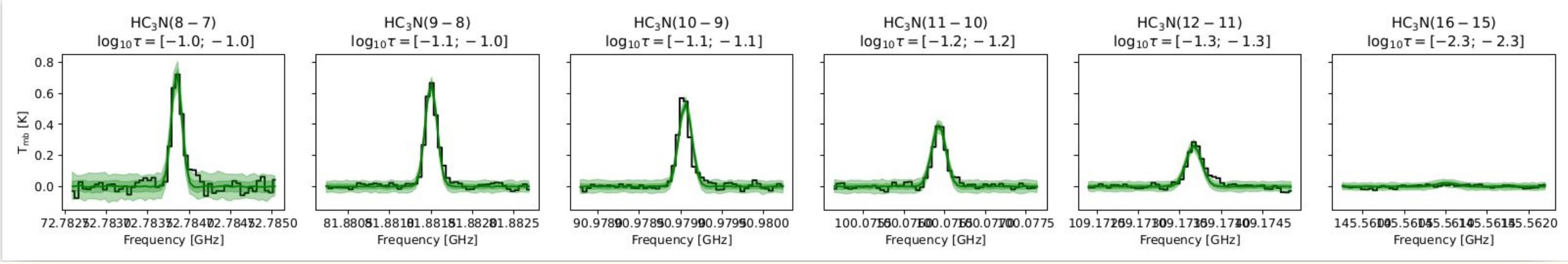
Methods

Extract parameters from radio data: InvertSpectra code



- ✶ Preliminary analysis of the 30m observations on HC_3N indicates that both sources A and B are:
  - ○ quite dense ($n_{H2} > 3 \times 10^5$ cm^{-3})
  - ○ cold (T < 13 K)

- ✶ Physical parameters determined for HC_3N then used as prior distributions to help the fit for the other species

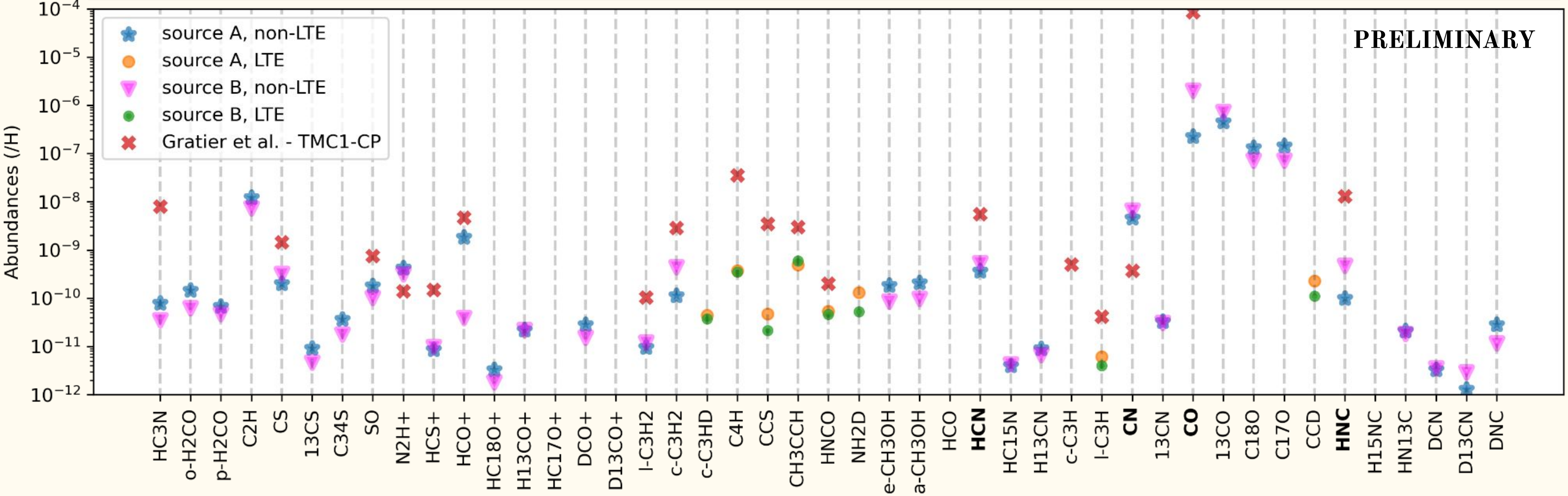


→ allows to extract N_{mol} for all the molecules in LTE + in Radex when the collision rates are available

Results

Comparison of the molecular abundances

Abundances of the molecules extracted from the IRAM 30m, in non-LTE when the collision rates are available, or in LTE if not. The **bold** font is used for species presenting optically thick lines.



- 38 molecules detected, including some isotopologues in the 30m data
- Comparison with TMC-1: very similar for some species (SO, N_2H^+, etc.), very different for others (HC_3N, CCS, etc.)

Constraining ζ_{H2} with chemistry?
Using Nautilus and simulated data

- Exploration on a grid of parameters (size 50x50x64):
  - n_H → between 10^4 and 10^7 cm^{-3}
  - ζ_{H2} → between 10^{-18} and 10^{-15} s^{-1}
  - time → between ~100 and 10^7 years

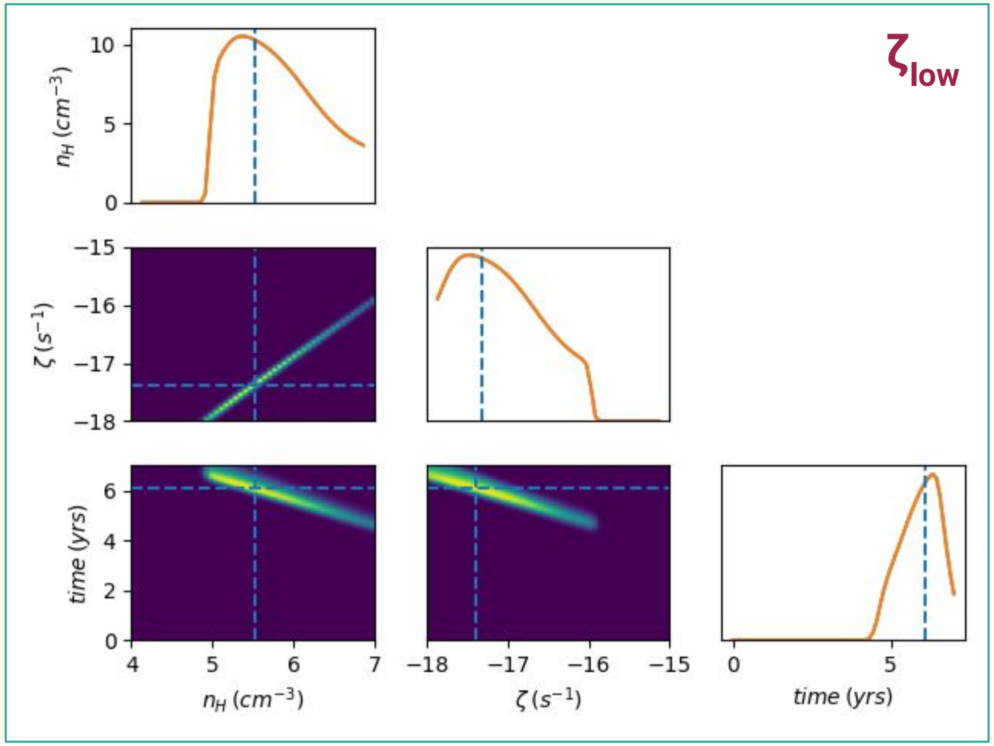
- Simulated data: as a first attempt
  - for the set of observed molecules
  - for a given value of the uncertainty on the abundances
  - for a given time and n_H → check if we can differentiate two ≠ ζ_{H2} values (ζ_{high} vs ζ_{low})

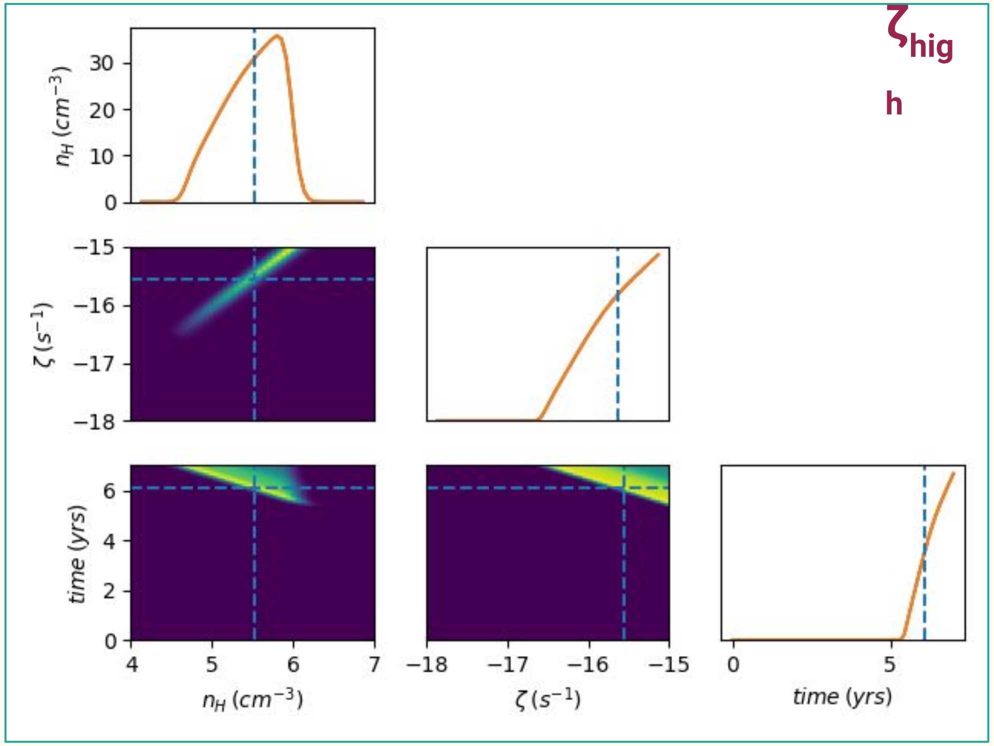
⇒ Goal: get the posterior probability distributions of the 3 parameters for a given observation

Constraining ζ_{H2} with chemistry?

A first test: likelihood only, no prior

Code developed by **Lydie Roosens** during her M1 internship at the LAB

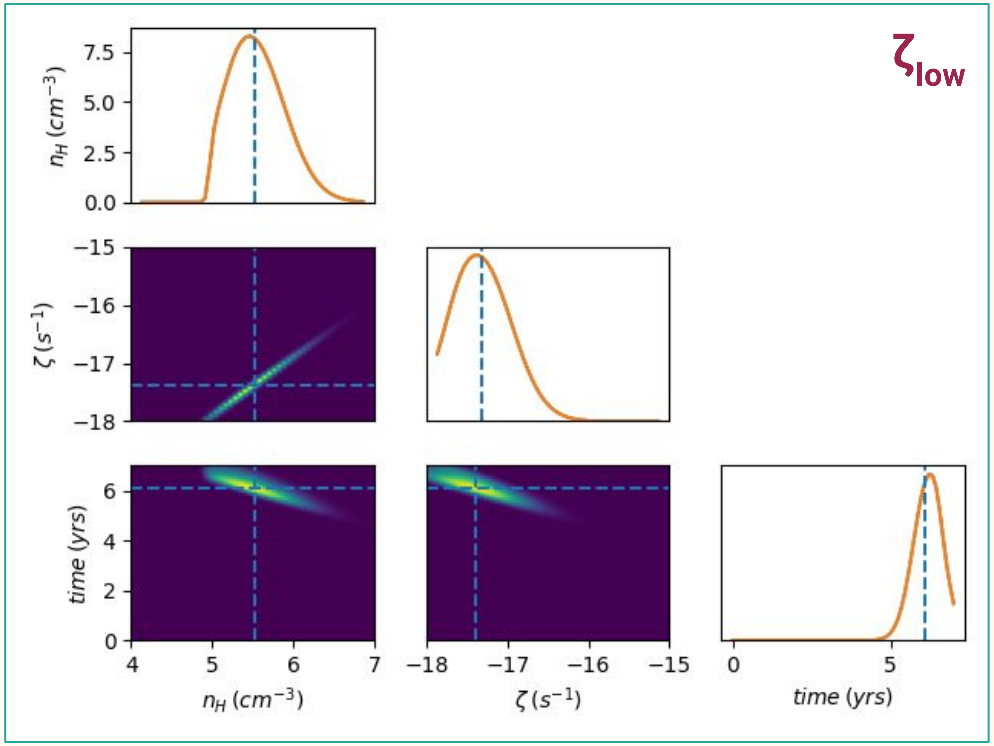


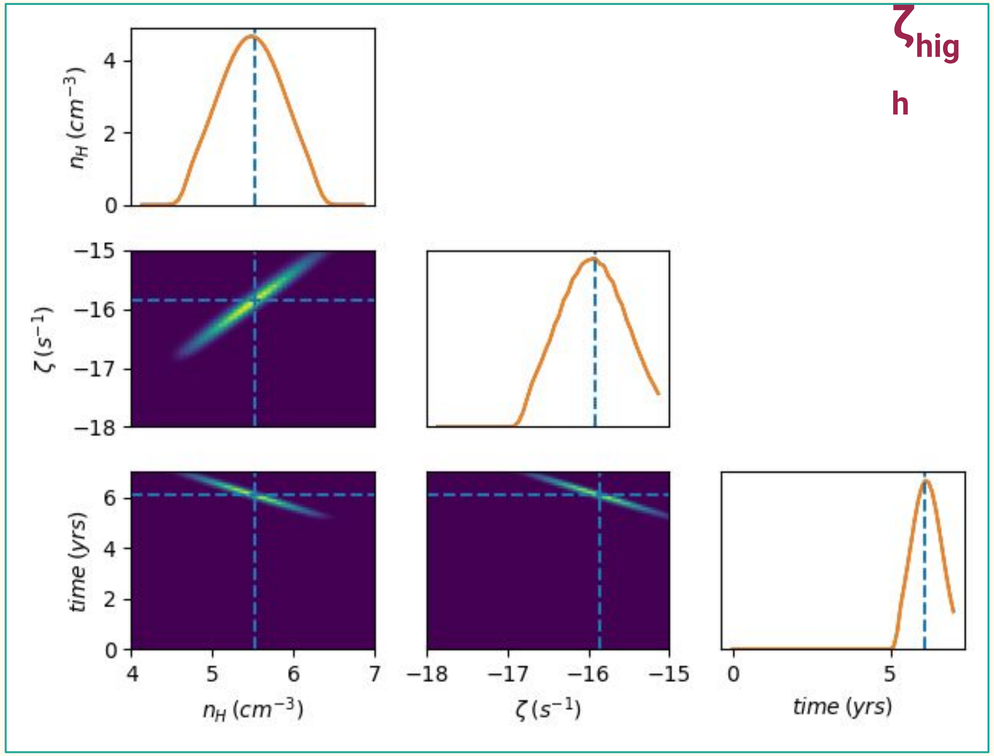


→ As it is, we can already roughly discriminate between high and low ζ_{H2}

Constraining ζ_{H2} with chemistry?

Adding a prior on n_H

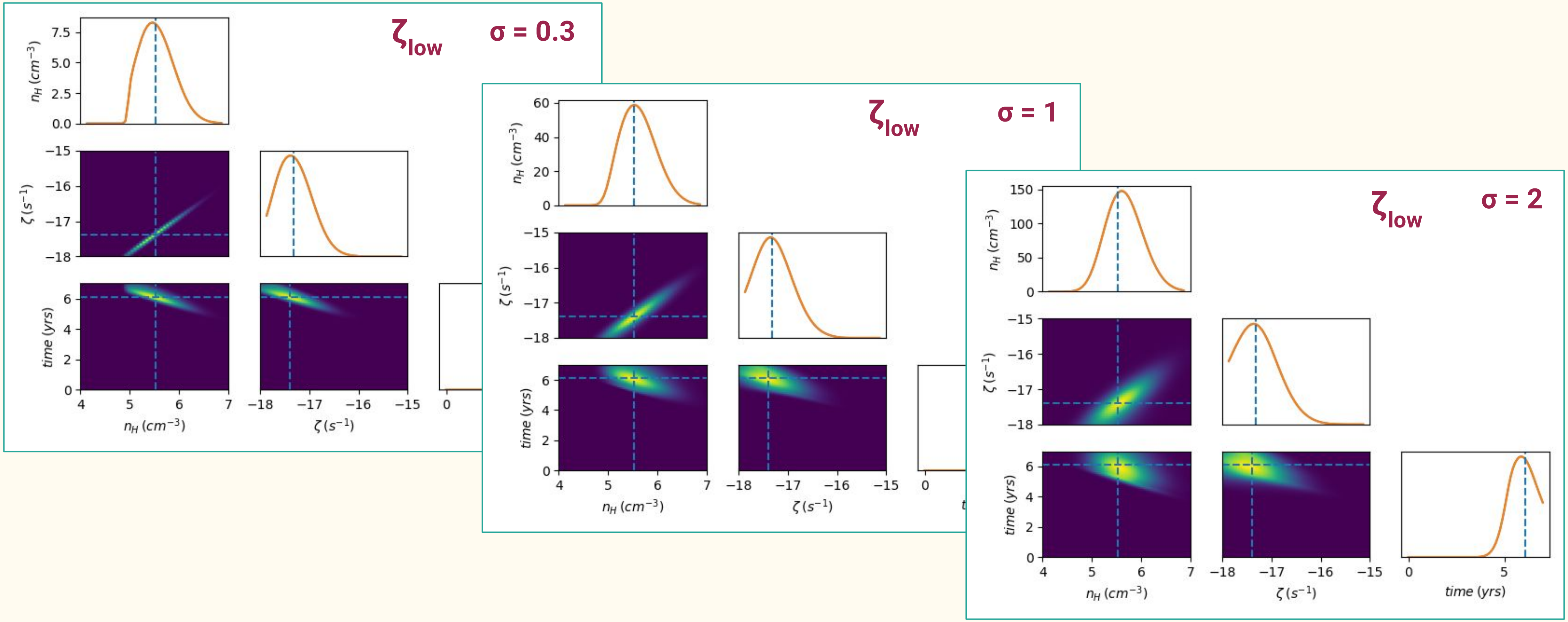




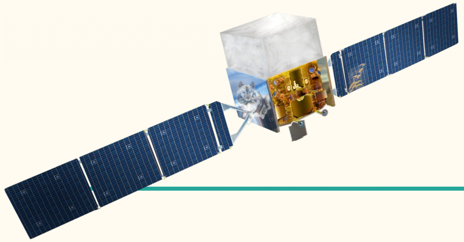
→ Adding a prior on the density reduces the uncertainty on the other parameters

Constraining ζ_{H2} with chemistry?

→ We can discriminate high and low ζ_{H2} when working on simulated data
→ Tests with increasing σ still allow us to discriminate ζ_{H2} (until a factor of >100 on the abundances)

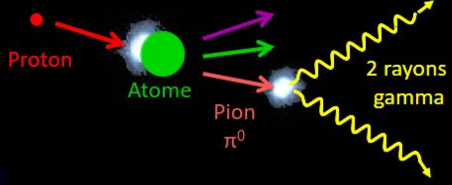


→ Next step: same work on our real observational data



Gamma-ray astronomy and astrochemistry

Link between the two parts

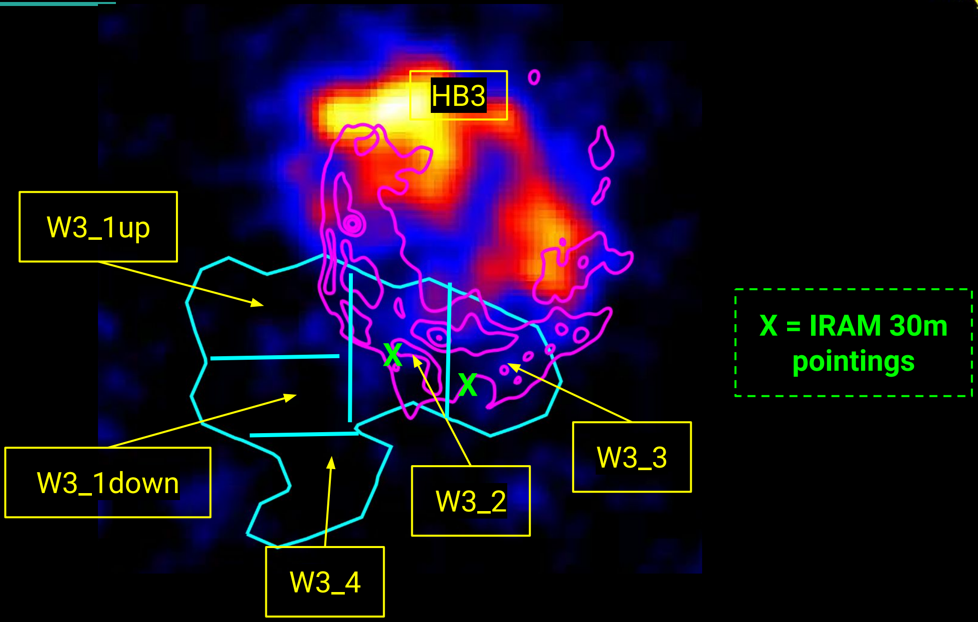


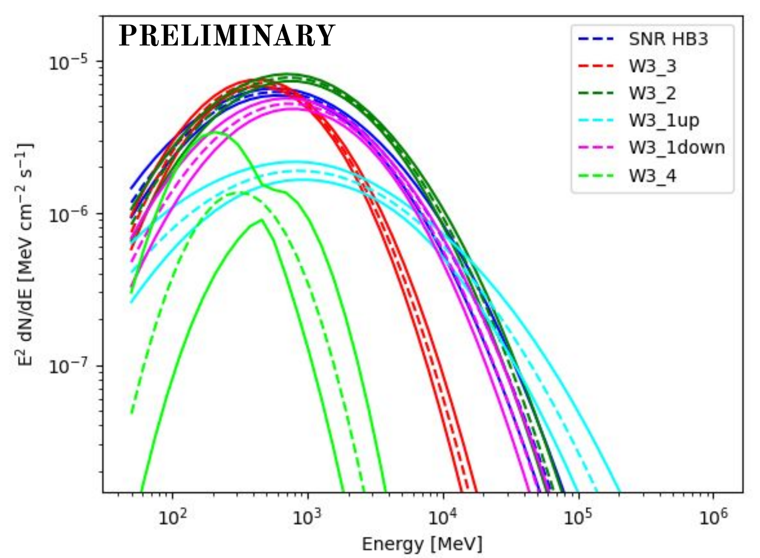
- ✶ Analysis of 14 years of Fermi-LAT data
- ✶ Morphological analysis results after multiple tests:
  - ○ for W3: Dame ^{12}CO template iteratively divided into 5 parts
  - ○ for HB3: uniform disk

- ✶ The two 30m pointings are in two different parts of W3 : W3_2 and W3_3

- ✶ These two parts have significantly different gamma-ray spectra, thus different cosmic-ray spectra

⇒ we expect to find two different H_2 cosmic-ray ionization rates!





Conclusions

- Study of the impact of cosmic-rays on the chemistry of W3 (the molecular cloud interacting with the SNR HB3)

- Observations:
  - Radio data (IRAM 30m and Yebes 40m)

- Methods:
  - Nautilus (chemical modeling)

- Goal: Reproduce the observed molecular column densities with Nautilus to constrain ζ_{H2} (the H_2 ionization rate)
  - Tests on a parameter grid (n_H, ζ_{H2}, time)
  - Discriminate high and low ζ_{H2} with simulated data

- Perspectives:
  - Discriminate high and low ζ_{H2} on real observational data
  - Link the astrochemistry and gamma-ray studies

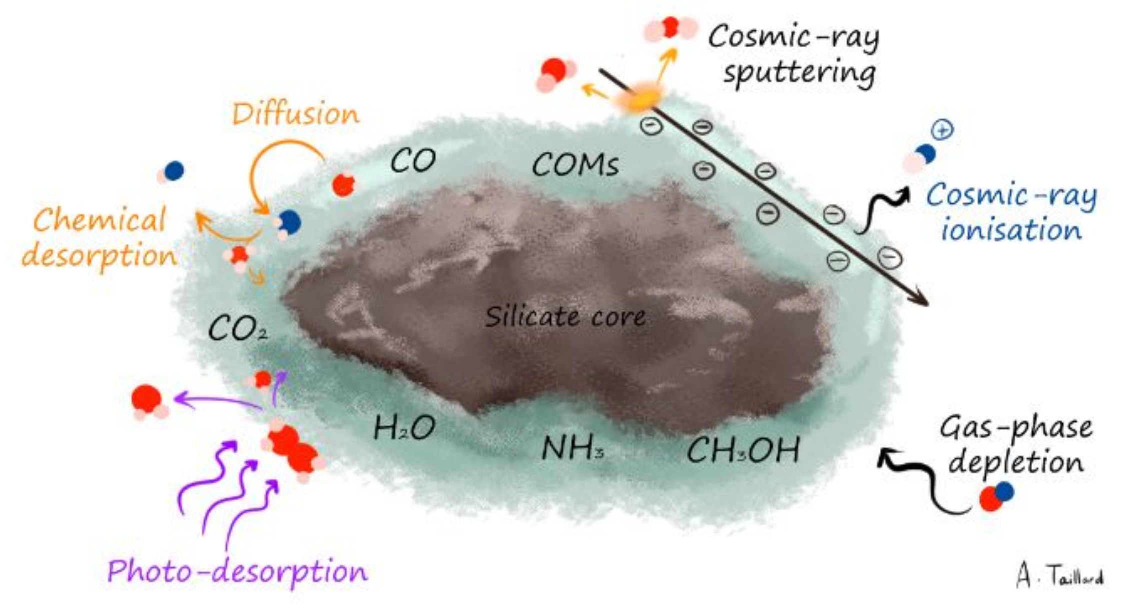
⇒ constrain ζ_{H2} and understand better the cosmic-rays in the HB3/W3 region

BACK-UP

Methods

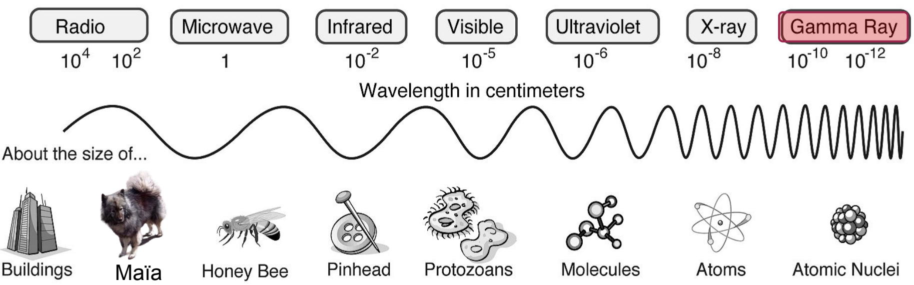
Cosmic-rays related processes in Nautilus (Ruaud et al. 2016, Wakelam et al. 2024)

- ✶ Photodissociation/ionization with cosmic ray
- ✶ Gas phase photodissociations/ionizations by secondary UV photons generated by CR
- ✶ Desorption induced by cosmic-ray stochastic heating
- ✶ Photodissociations by cosmic rays induced UV photons on grain surface
- ✶ Photodesorption by UV induced by cosmic rays
- ✶ Cosmic-ray sputtering (see Wakelam et al. 2021)



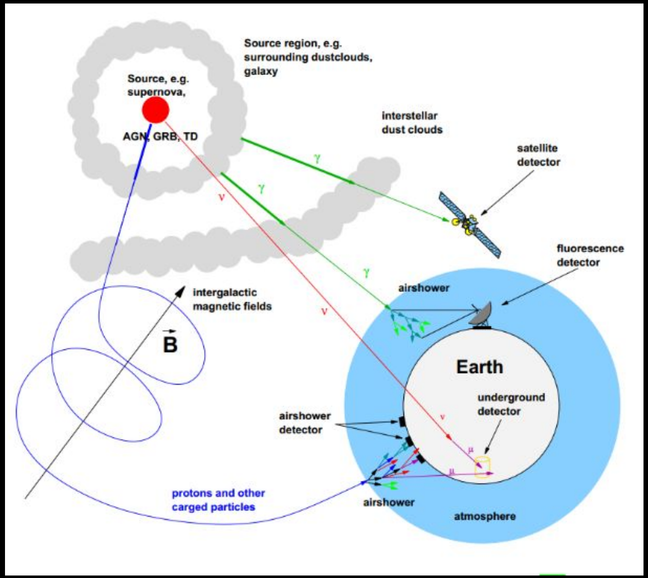
Scientific context

γ-ray astronomy - Cosmic-rays (CRs)



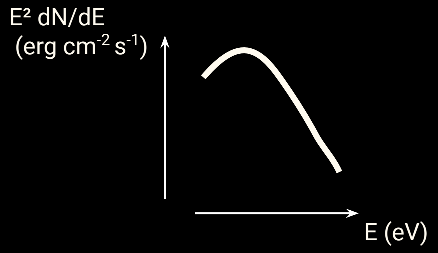
- ✶ γ-rays = photons with E > 100 keV
- ✶ γ-ray astronomy → fundamental tool to observe the Universe using deep penetrating γ-ray photons
- ✶ Image ~~the Universe~~ with CRs → CRs are deflected by the magnetic field!

CR ions and electrons can interact with target particles to make γ-rays through secondary nuclear production and bremsstrahlung



- ✶ A distinctive γ-ray signature of CRs → interactions of CR protons and ions with gas and dust → characteristic $\pi^0 \rightarrow 2\gamma$ emission feature (Stecker 1971)

⇒ pion-decay bump → uniquely identifies proton acceleration



Sensitive species to the ionization rate ζ

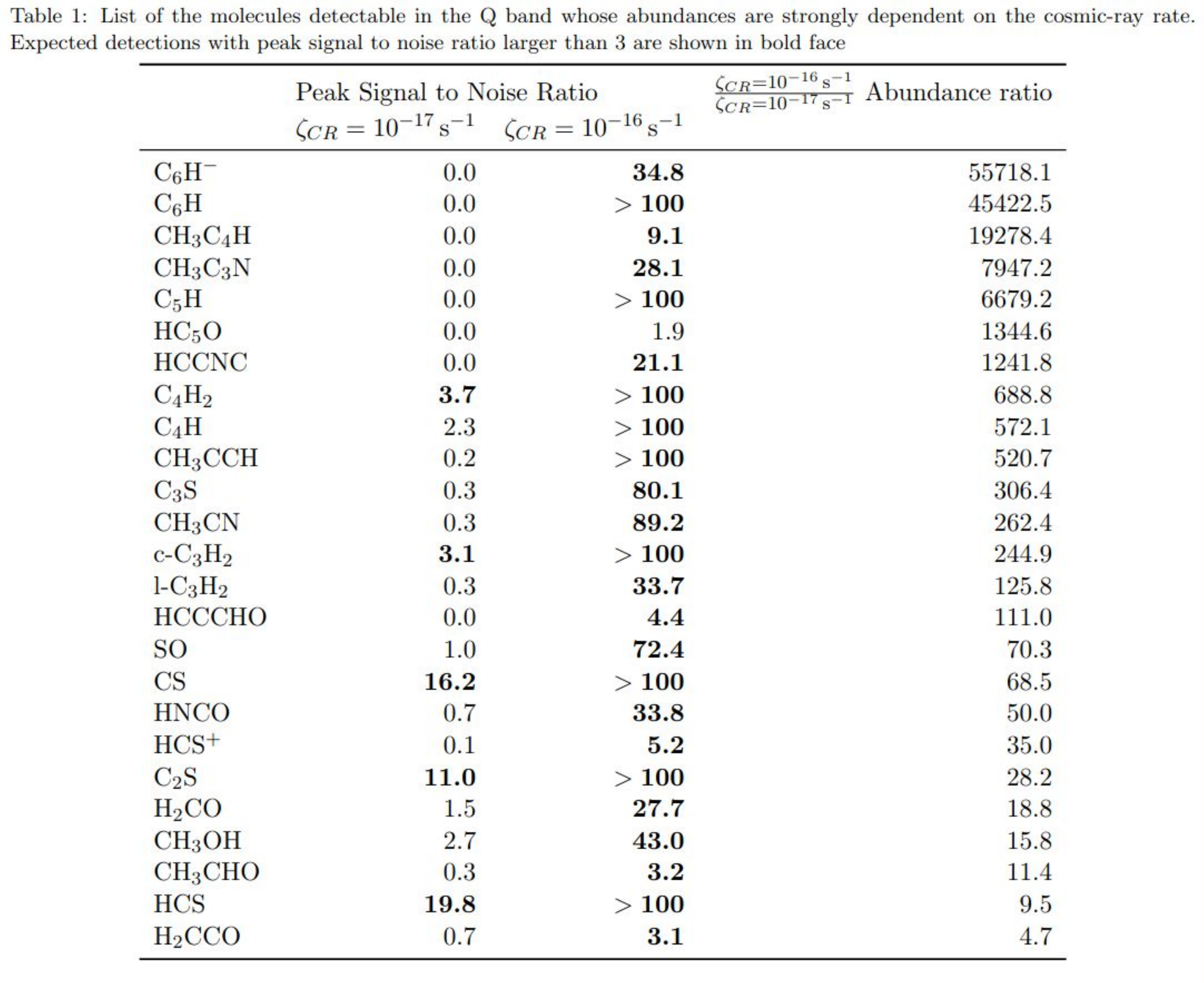
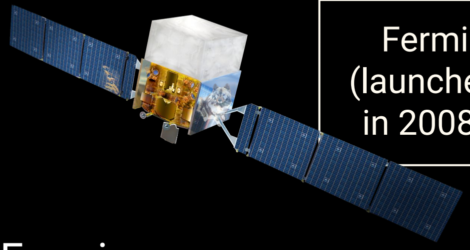


Table 1: List of the molecules detectable in the Q band whose abundances are strongly dependent on the cosmic-ray rate. Expected detections with peak signal to noise ratio larger than 3 are shown in bold face

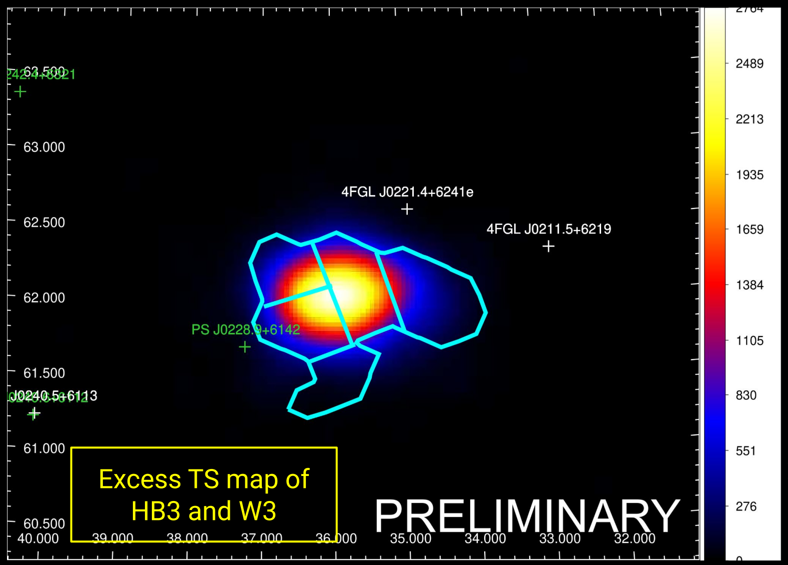
	Peak Signal to Noise Ratio		$\frac{\zeta_{CR}=10^{-16}\,\mathrm{s}^{-1}}{\zeta_{CR}=10^{-17}\,\mathrm{s}^{-1}}$ Abundance ratio
	$\zeta_{CR} = 10^{-17}\,\mathrm{s}^{-1}$	$\zeta_{CR} = 10^{-16}\,\mathrm{s}^{-1}$	
C_6H^-	0.0	**34.8**	55718.1
C_6H	0.0	$>$ **100**	45422.5
CH_3C_4H	0.0	**9.1**	19278.4
CH_3C_3N	0.0	**28.1**	7947.2
C_5H	0.0	$>$ **100**	6679.2
HC_5O	0.0	1.9	1344.6
HCCNC	0.0	**21.1**	1241.8
C_4H_2	**3.7**	$>$ **100**	688.8
C_4H	2.3	$>$ **100**	572.1
CH_3CCH	0.2	$>$ **100**	520.7
C_3S	0.3	**80.1**	306.4
CH_3CN	0.3	**89.2**	262.4
c-C_3H_2	**3.1**	$>$ **100**	244.9
l-C_3H_2	0.3	**33.7**	125.8
HCCCHO	0.0	**4.4**	111.0
SO	1.0	**72.4**	70.3
CS	**16.2**	$>$ **100**	68.5
HNCO	0.7	**33.8**	50.0
HCS^+	0.1	**5.2**	35.0
C_2S	**11.0**	$>$ **100**	28.2
H_2CO	1.5	**27.7**	18.8
CH_3OH	2.7	**43.0**	15.8
CH_3CHO	0.3	**3.2**	11.4
HCS	**19.8**	$>$ **100**	9.5
H_2CCO	0.7	**3.1**	4.7

C_3S, C_4H_2, C_8H, CCH, CCS, CH, CH_3CCH, CH_3CN, CN, CS, HC_7N, HCCNC, HCN, HCNH+, HNC, c-C_3H_2

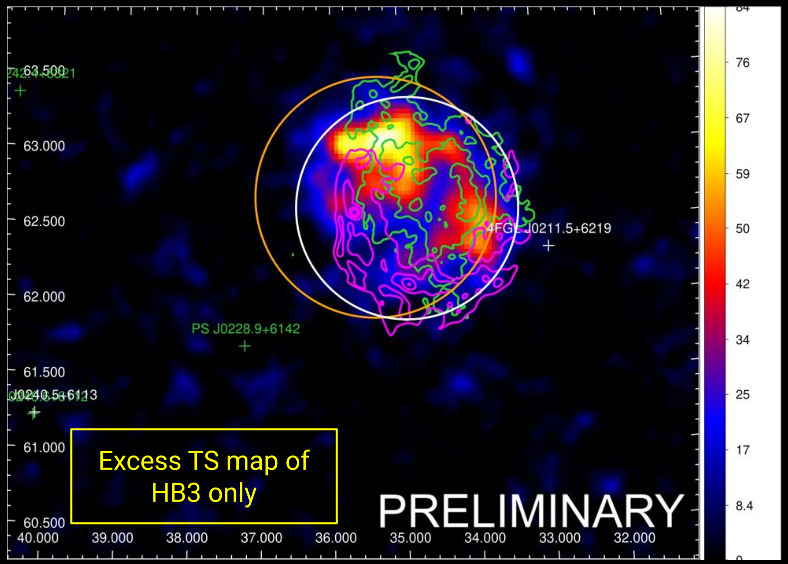
Gamma-ray analysis
Quick method & morphological analysis



Fermi
(launched
in 2008)



Excess TS map of HB3 and W3

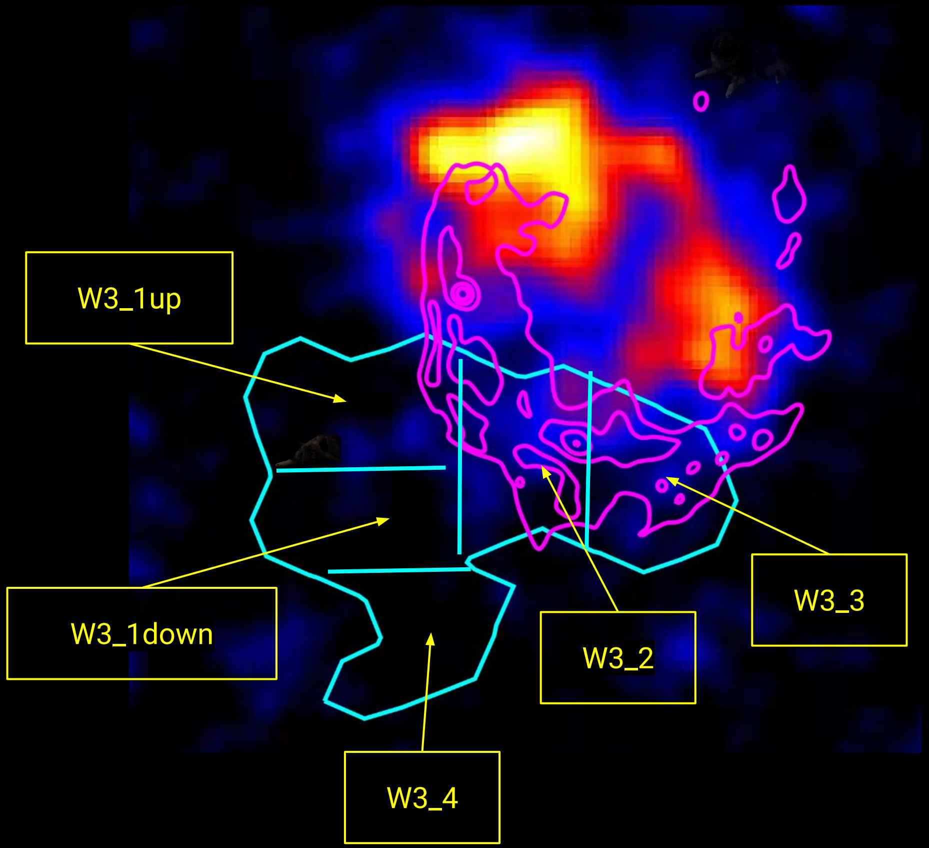


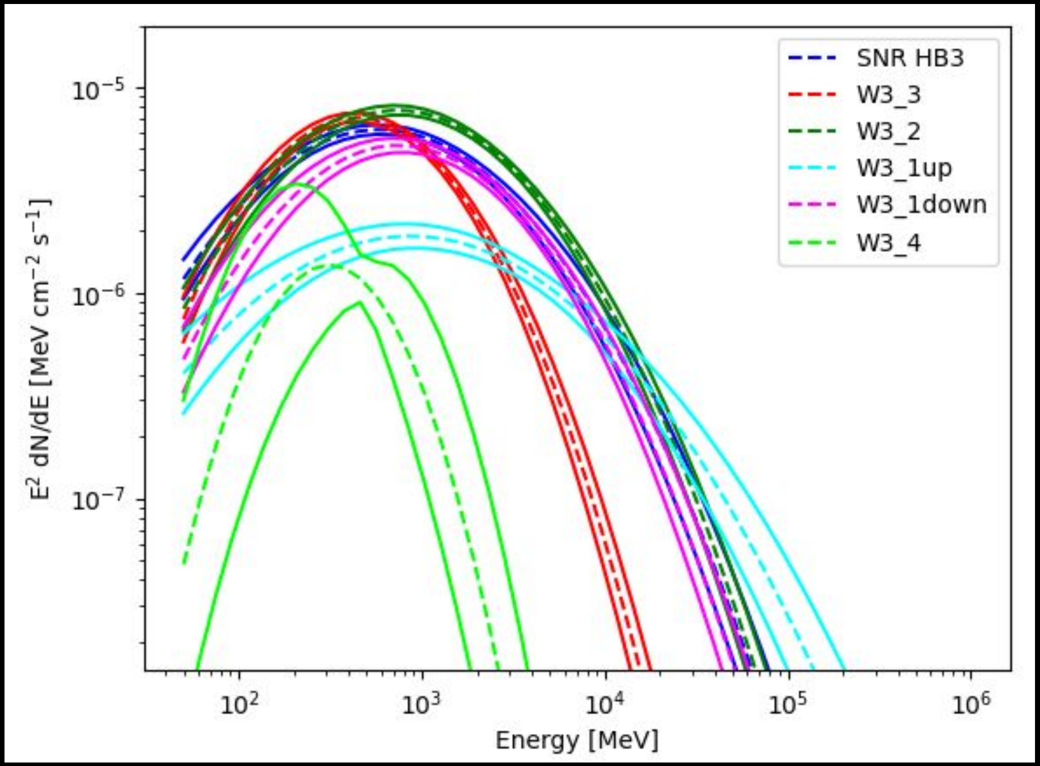
Excess TS map of HB3 only

- ✶ Analysis of 14 years of Fermi-LAT data using Fermipy (vs 6 years of data in a previous analysis by Katagiri et al. 2016)
- ✶ Maximum likelihood method: probability of obtaining the data given an input model of the sources from a region
- ✶ Templates tested to reproduce the gamma-ray emission:
  - ○ spatial templates that trace the interstellar matter distribution for W3
  - ○ multi-wavelength templates + disks (extension fit) for HB3
- ✶ W3 is 10 times brighter than HB3 → importance of the template choice for W3
- ✶ Morphological analysis results after multiple tests:
  - ○ for W3: Dame 12CO template iteratively divided into 5 parts
  - ○ for HB3: uniform disk

Gamma-ray analysis

Spectral analysis: with Dame divided into 5 parts





Comparison between the different parts of W3 and HB3 ⇒ they seem different !