Chemistry in Star Formation

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using slides prepared by
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Astrochemistry :

Study of *formation, destruction and excitation of molecules*
in astronomical environments and their influence on
the *structure, dynamics and evolution of astronomical objects*.

Dalgarno (2008, ARA&A, 46, 1)

2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	12 atoms	>12 atoms
H_2	C_3 *	*c*-C_3H	C_5 *	C_5H	C_6H	CH_3C_3N	CH_3C_4H	CH_3C_5N	HC_9N	*c*-C_6H_6 *	$HC_{11}N$
AlF	C_2H	*l*-C_3H	C_4H	*l*-H_2C_4	CH_2CHCN	$HC(O)OCH_3$	CH_3CH_2CN	$(CH_3)_2CO$	CH_3C_6H	*n*-C_3H_7CN	C_{60} *
AlCl	C_2O	C_3N	C_4Si	C_2H_4*	CH_3C_2H	CH_3COOH	$(CH_3)_2O$	$(CH_2OH)_2$	C_2H_5OCHO	*i*-C_3H_7CN	C_{70} *
C_2**	C_2S	C_3O	*l*-C_3H_2	CH_3CN	HC_5N	C_7H	CH_3CH_2OH	CH_3CH_2CHO	$CH_3OC(O)CH_3$?	$C_2H_5OCH_3$?	C_{60}^+ *
CH	CH_2	C_3S	*c*-C_3H_2	CH_3NC	CH_3CHO	C_6H_2	HC_7N	CH_3CHCH_2O 2016			
CH^+	HCN	C_2H_2*	H_2CCN	CH_3OH	CH_3NH_2	CH_2OHCHO	C_8H				
CN	HCO	NH_3	CH_4 *	CH_3SH	*c*-C_2H_4O	*l*-HC_6H *	$CH_3C(O)NH_2$				
CO	HCO^+	HCCN	HC_3N	HC_3NH^+	H_2CCHOH	CH_2CHCHO (?)	C_8H^-				
CO^+	HCS^+	$HCNH^+$	HC_2NC	HC_2CHO	C_6H^-	CH_2CCHCN	C_3H_6				
CP	HOC^+	HNCO	HCOOH	NH_2CHO	CH_3NCO 2015	H_2NCH_2CN	CH_3CH_2SH (?)				
SiC	H_2O	HNCS	H_2CNH	C_5N		CH_3CHNH					
HCl	H_2S	$HOCO^+$	H_2C_2O	*l*-HC_4H *							
KCl	HNC	H_2CO	H_2NCN	*l*-HC_4N							
NH	HNO	H_2CN	HNC_3	*c*-H_2C_3O							
NO	MgCN	H_2CS	SiH_4 *	H_2CCNH (?)							
NS	MgNC	H_3O^+	H_2COH^+	C_5N^-							
NaCl	N_2H^+	*c*-SiC_3	C_4H^-	HNCHCN							
OH	N_2O	CH_3 *	HC(O)CN								
PN	NaCN	C_3N^-	HNCNH								
SO	OCS	PH_3	CH_3O								
SO^+	SO_2	HCNO	NH_4^+								
SiN	*c*-SiC_2	HOCN	H_2NCO^+ (?)								
SiO	CO_2 *	HSCN	$NCCNH^+$ 2015								
SiS	NH_2	H_2O_2									
CS	H_3^+ (*)	C_3H^+									
HF	SiCN	HMgNC									
HD	AlNC	HCCO 2015									
FeO ?	SiNC										
O_2	HCP										
CF^+	CCP										
SiH ?	AlOH										
PO	H_2O^+										
AlO	H_2Cl^+										
OH^+	KCN										
CN^-	FeCN										
SH^+	HO_2										
SH	TiO_2										
HCl^+	C_2N										
TiO	Si_2C 2015										
ArH^+											
NO^+ ?											

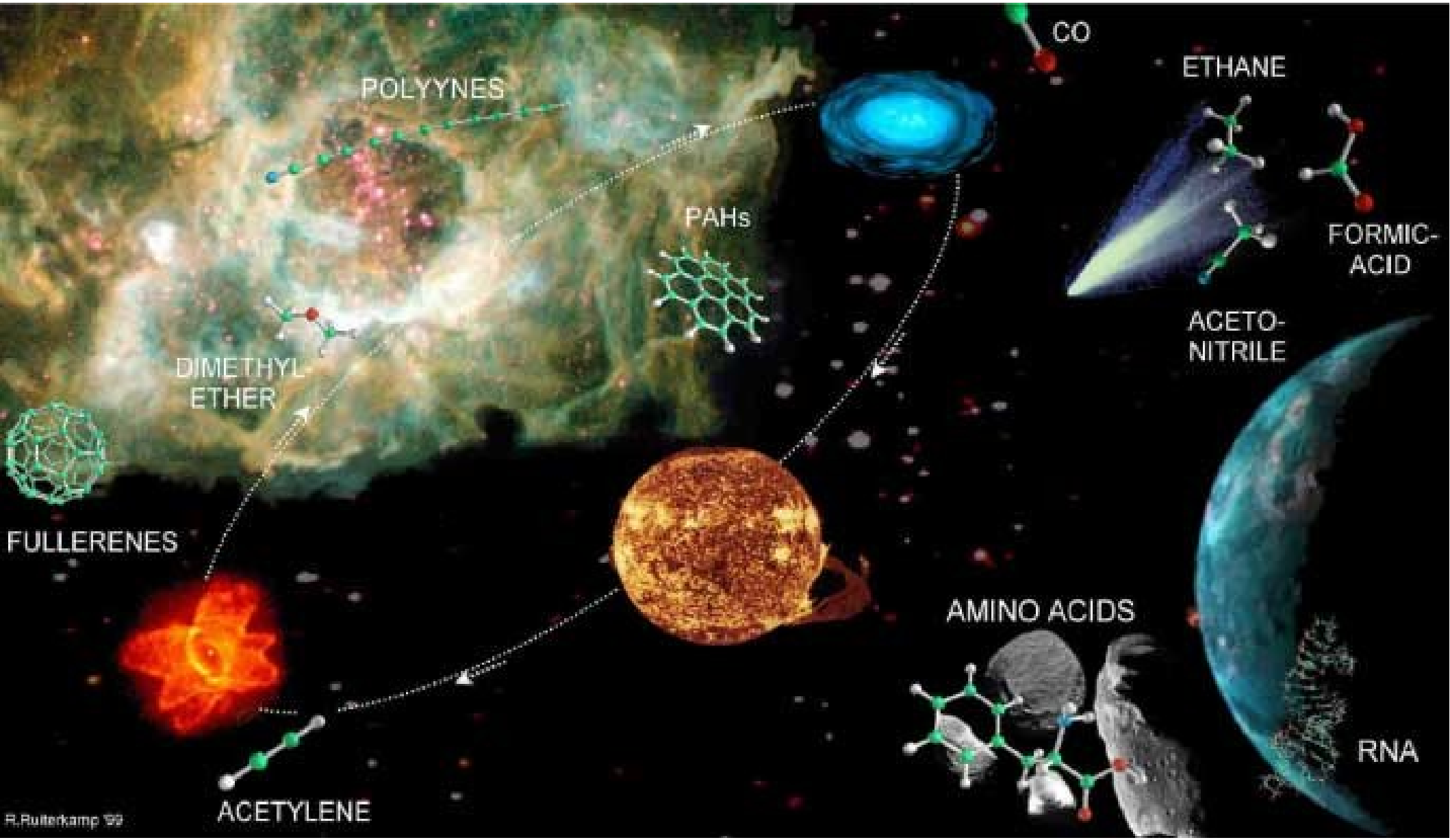
Almost **200 molecules** detected !!!

CDMS catalogue (University of Cologne)

2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	>8 atoms
OH	H_2O	H_2CO	*c*-C_3H_2	CH_3OH	CH_3CCH	HC_6H	*c*-C_6H_6 *
CO	HCN	NH_3	HC_3N	CH_3CN	CH_3NH_2		C_{60}* (?)
H_2 *	HCO^+	HNCO	CH_2NH	HC_4H *	CH_3CHO		
CH	C_2H	C_2H_2 *	NH_2CN	$HC(O)NH_2$			
CS	HNC	H_2CS ?	*l*-C_3H_2				
CH^+ **	N_2H^+	$HOCO^+$	H_2CCN				
CN	OCS	*c*-C_3H	H_2CCO				
SO	HCO	H_3O^+	C_4H				
SiO	H_2S	*l*-C_3H					
CO^+	SO_2						
NO	HOC^+						
NS	C_2S						
NH	H_2O^+						
OH^+	HCS^+						
HF	H_2Cl^+						
SO^+	NH_2						
ArH^+ 2015							
CF^+ 2016							

Galactic chemistry

Extragalactic chemistry


CO
ETHANE
POLYYNES
PAHs
FORMIC-
ACID
ACETO-
NITRILE
DIMETHYL
ETHER
FULLERENES
AMINO ACIDS
RNA
ACETYLENE
R.Rutterkamp '99

Goals

Astrochemistry

- Uses not excitation, but abundances of molecules as tracers of past and present physical conditions, source ages, feedback by outflows, shocks, UV...
- The more, the merrier
  - **More** lines – more reliable identification and characterization
    - Handle on opacities, blending
    - Constraints on physical conditions
  - **More** species – more constraints on chemical models

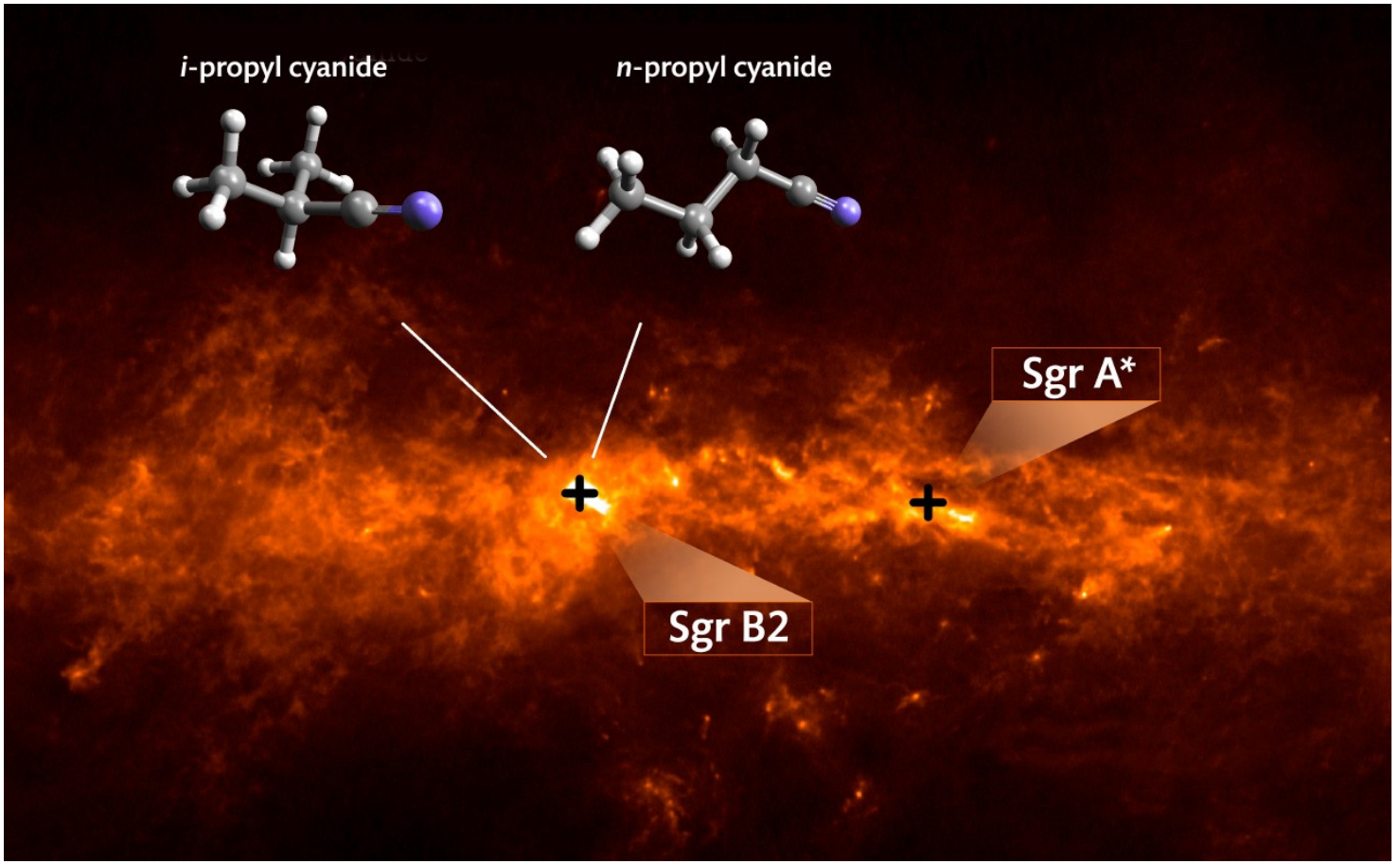
Large bandwidths are good

Examples of Chemistry in Star Formation

Example results

SgrB2

ALMA spectral scans to search for **new molecular species**



- Iso-propyl cyanide
- Alkanethiols and alkanols
- ^{13}C-substituted ethyl cyanide
- Deuterated complex organic molecules
- Vibrationally excited n-propyl cyanide
- …

Belloche et al. (2014, Science, 345, 1584) ; Belloche et al. (2016, A&A, 587, 91) ;
Müller et al. (2016, A&A, 587, 92) ; Müller et al. (2016, A&A, arXiv 1608.08129 ; and many more

Example results

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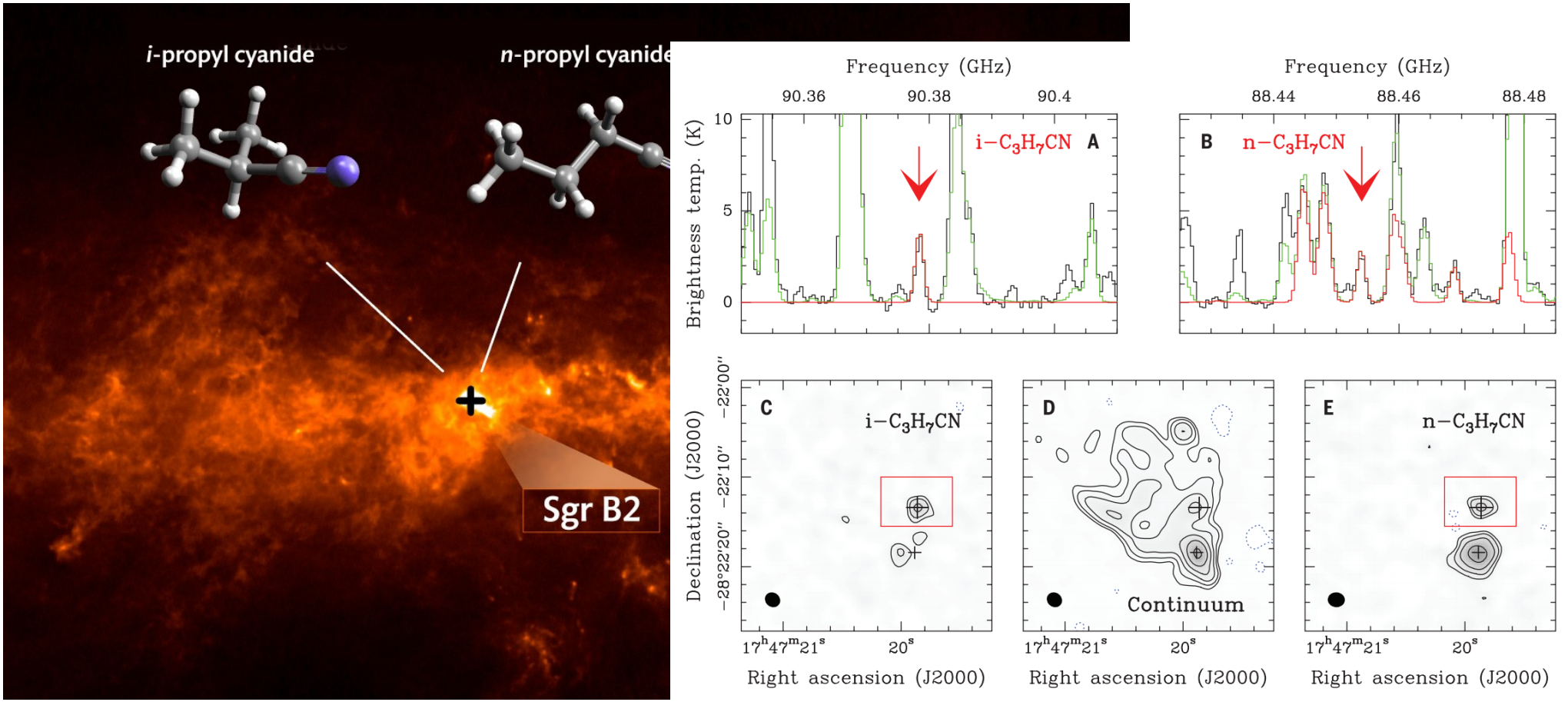

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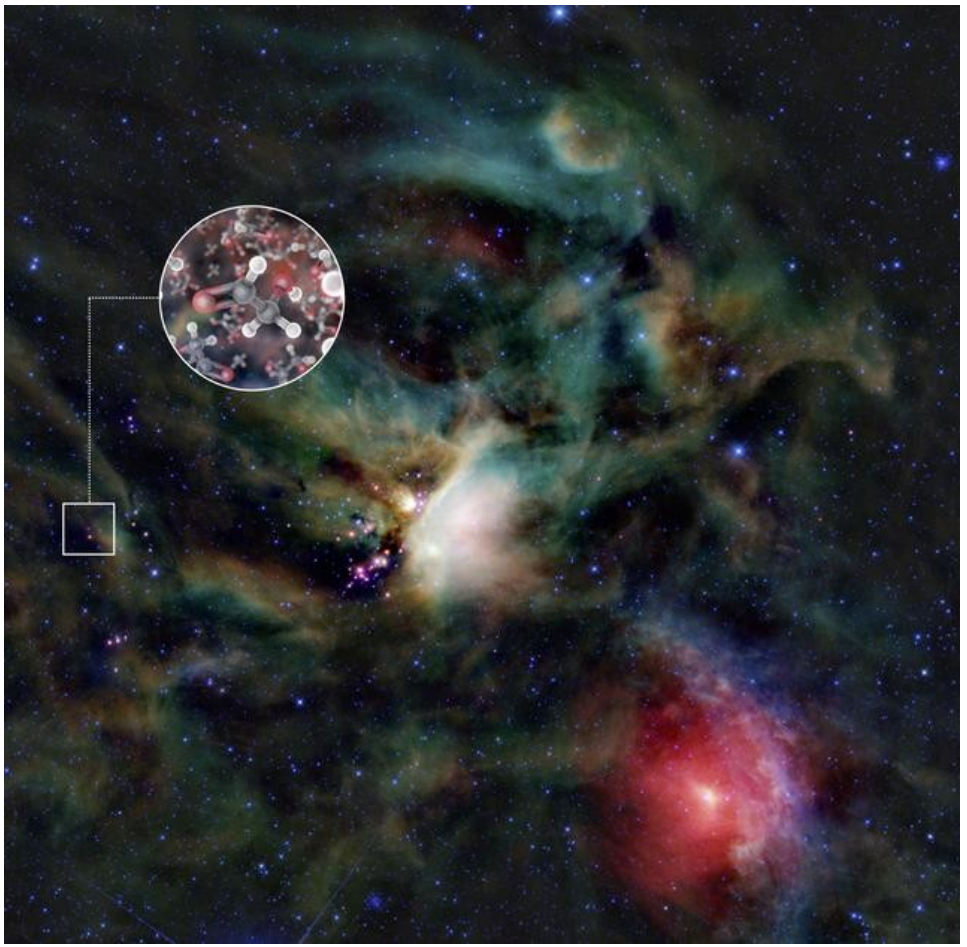
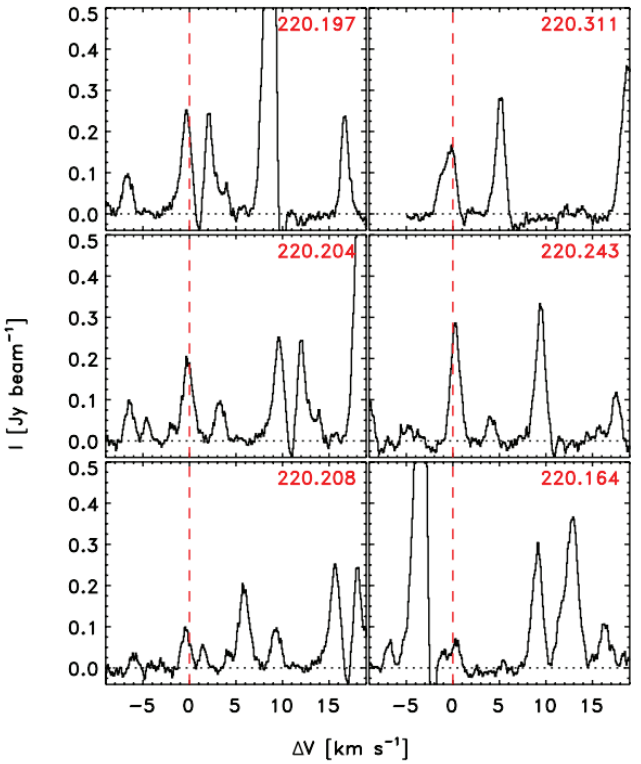
Example results

IRAS 16293-2422 (solar type star)

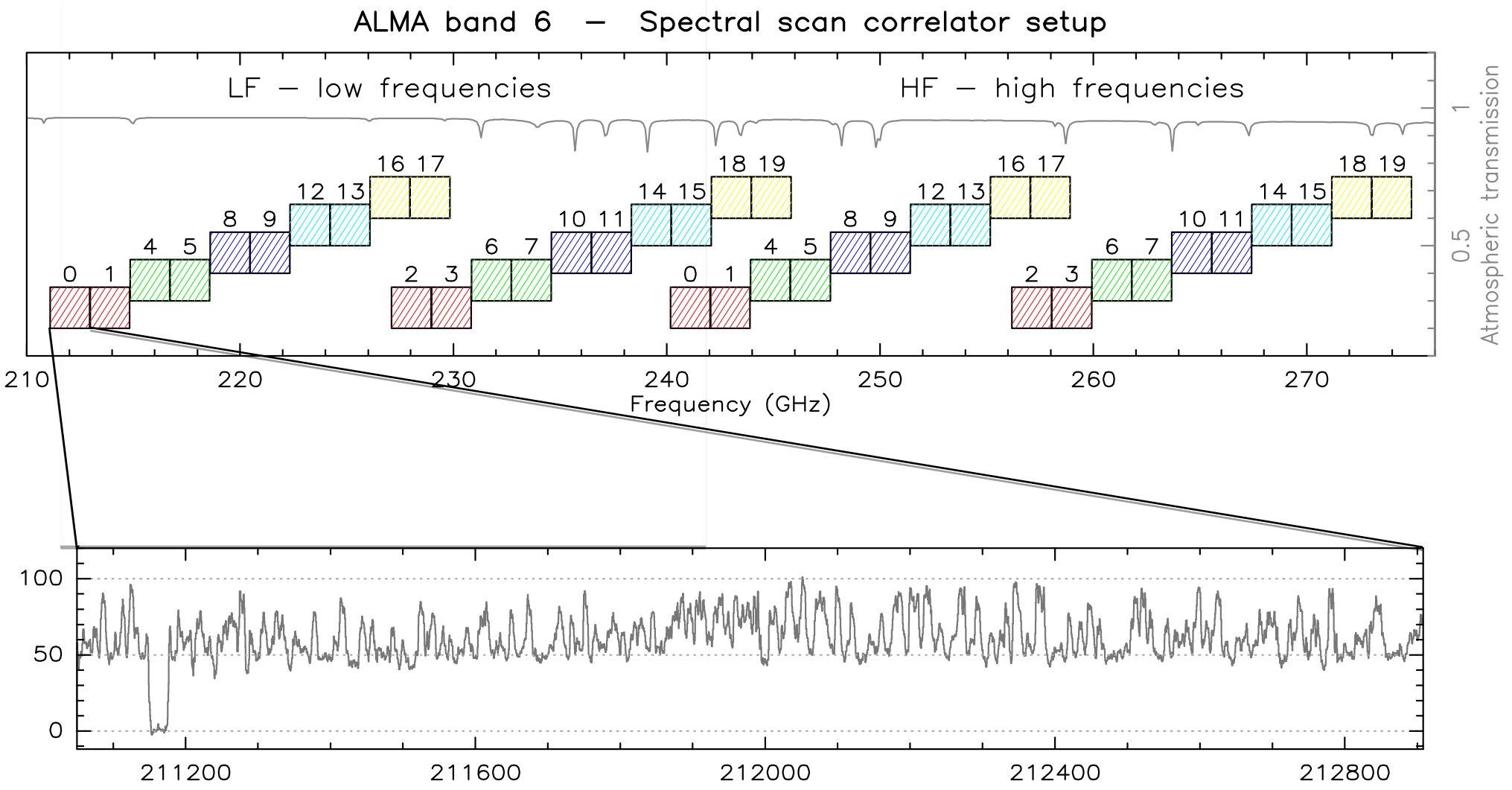


Detection of the simplest sugar in a solar-type protostar: Glycolaldehyde ($HCOCH_2OH$)

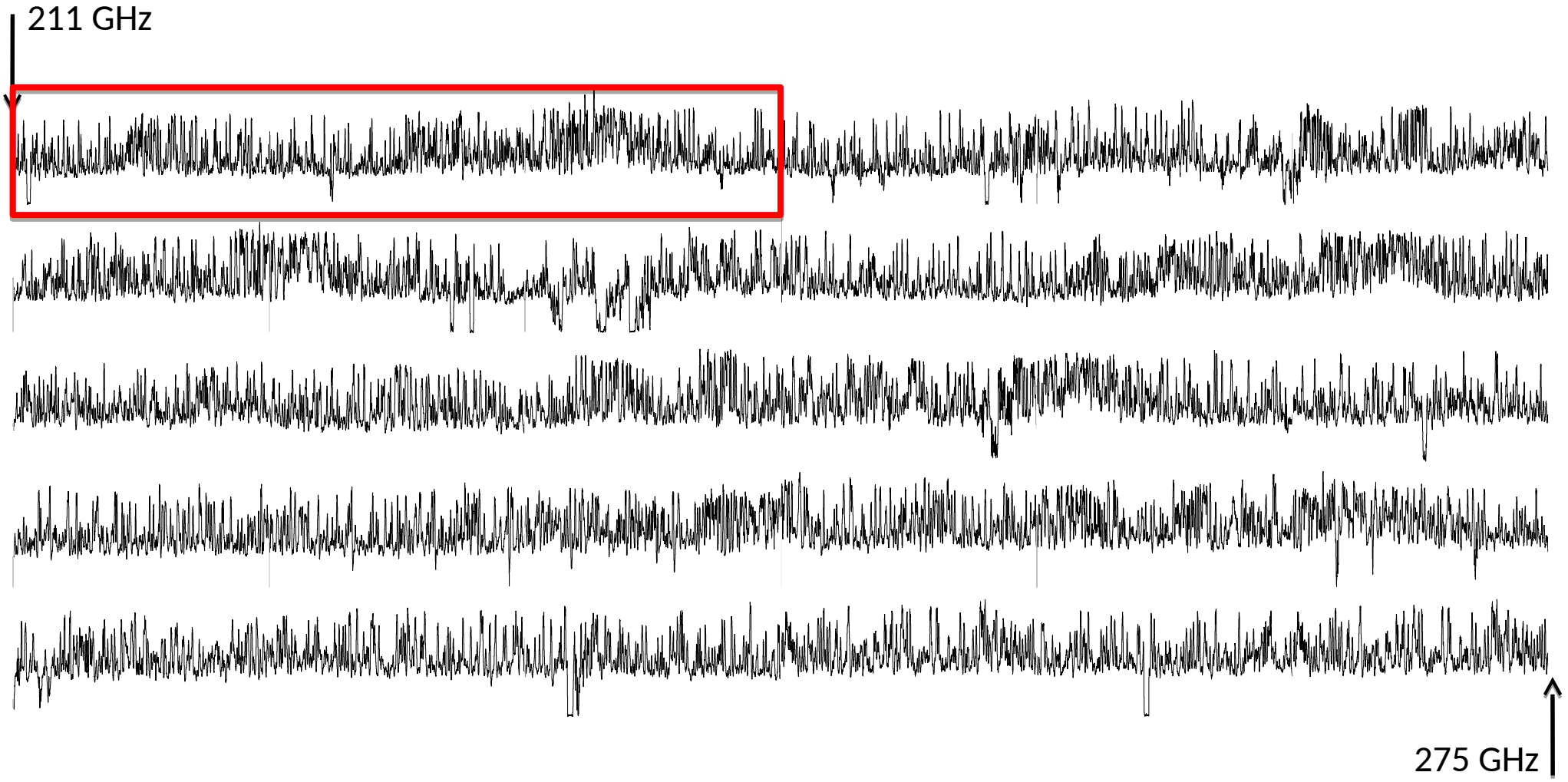


Jørgensen et al. (2012, ApJL, 757, L4) ; Jørgensen et al. (2016, A&A arXiv1607.08733)

Example results: ALMA line survey of SgrB2 (M) and (N)



Spectrum (211-275 GHz) towards 1 single pixel



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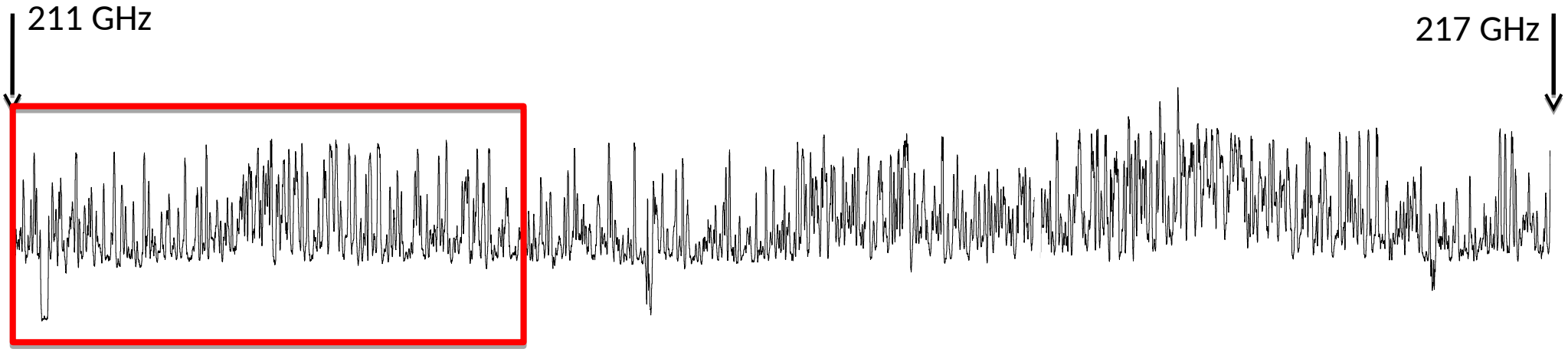

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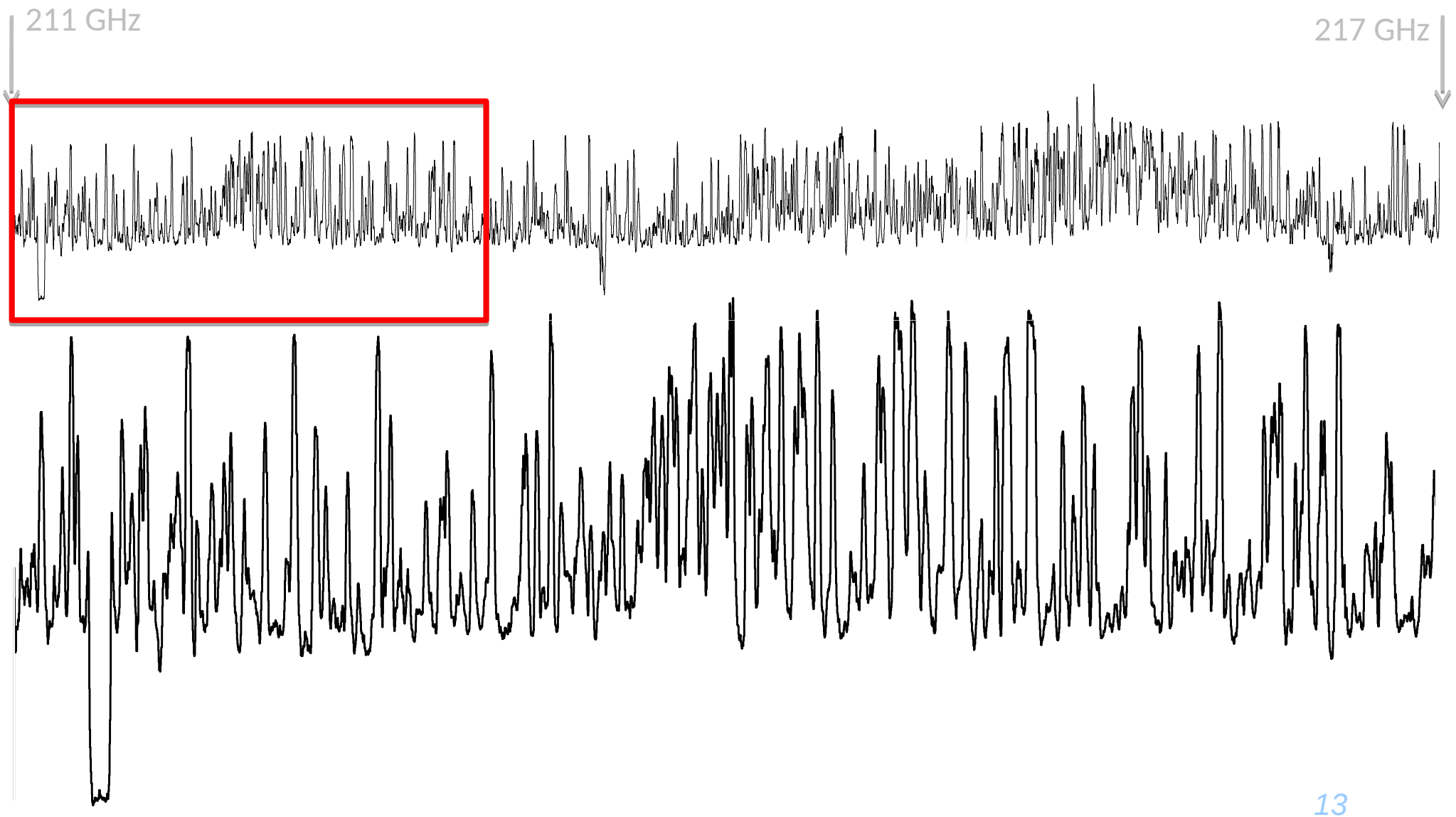
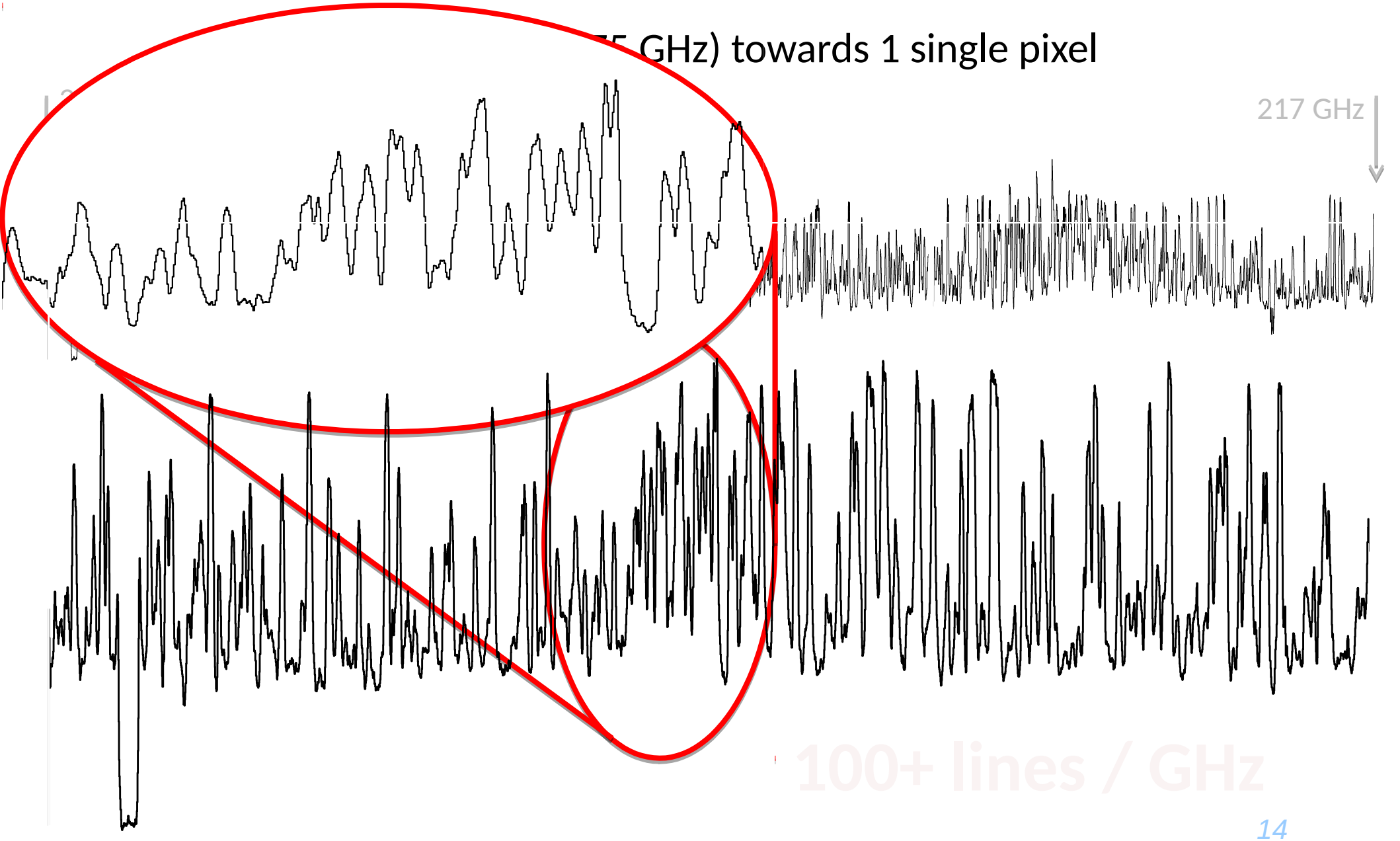
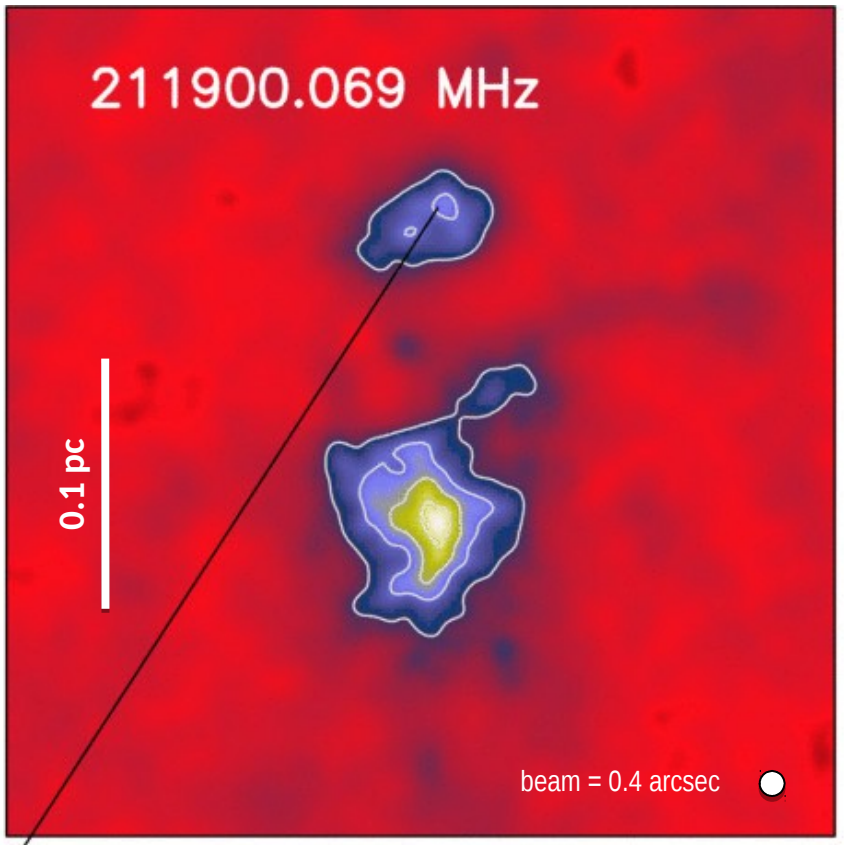


GHz) towards 1 single pixel

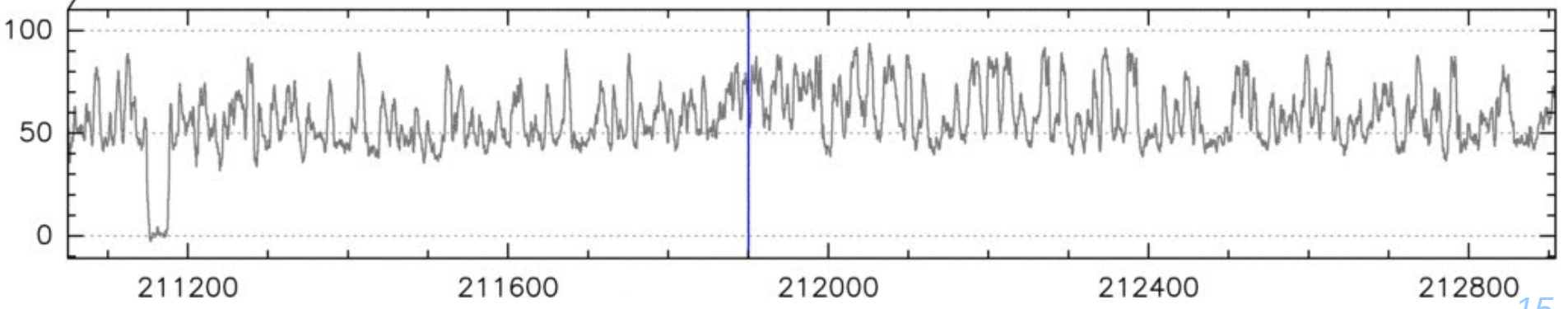


100+ lines / GHz



Chemically rich spectra !

First Problem: **continuum determination**



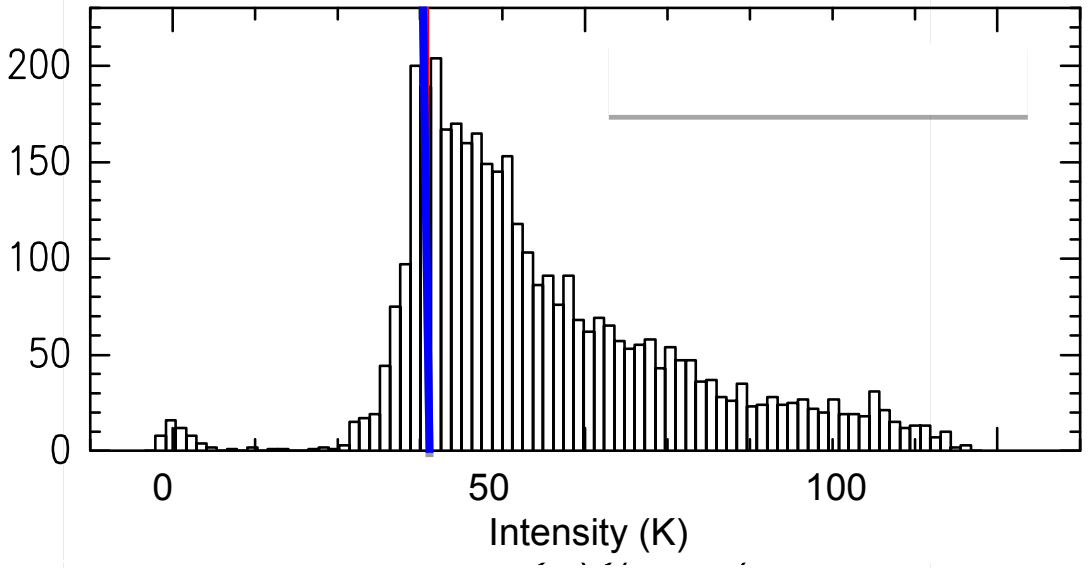
Sánchez-Monge et al. (2016, in prep)

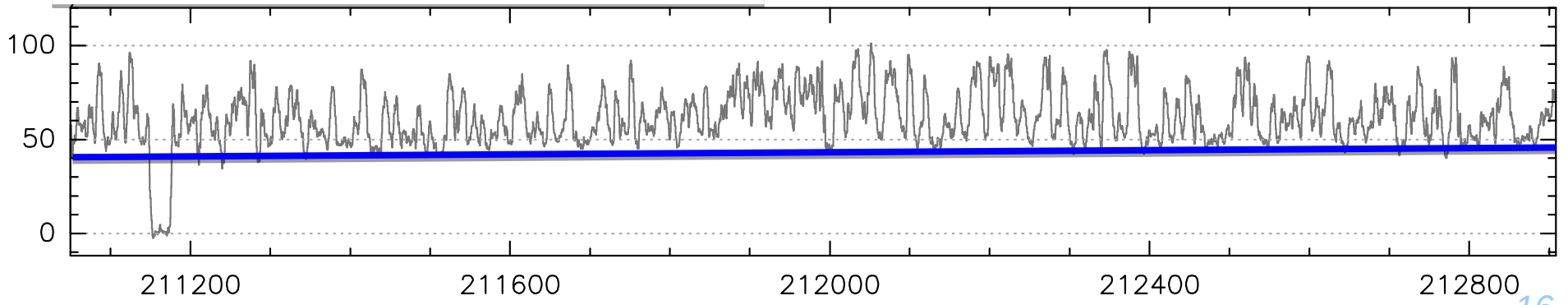
Continuum level determination

'subcont' : a new statistical method

Statistical analysis pixel by pixel

1. Extraction of the spectrum for each pixel
   (over a given frequency range)
2. Sigma-clipping method
   (discarding the outliers)
3. Determination of the continuum level after convergence





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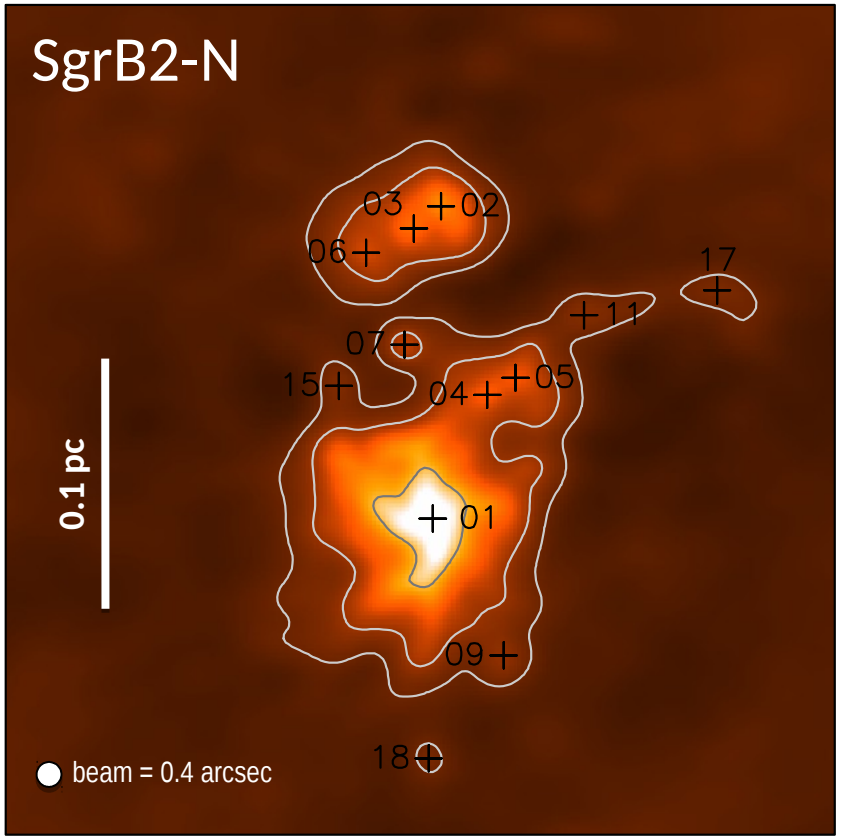
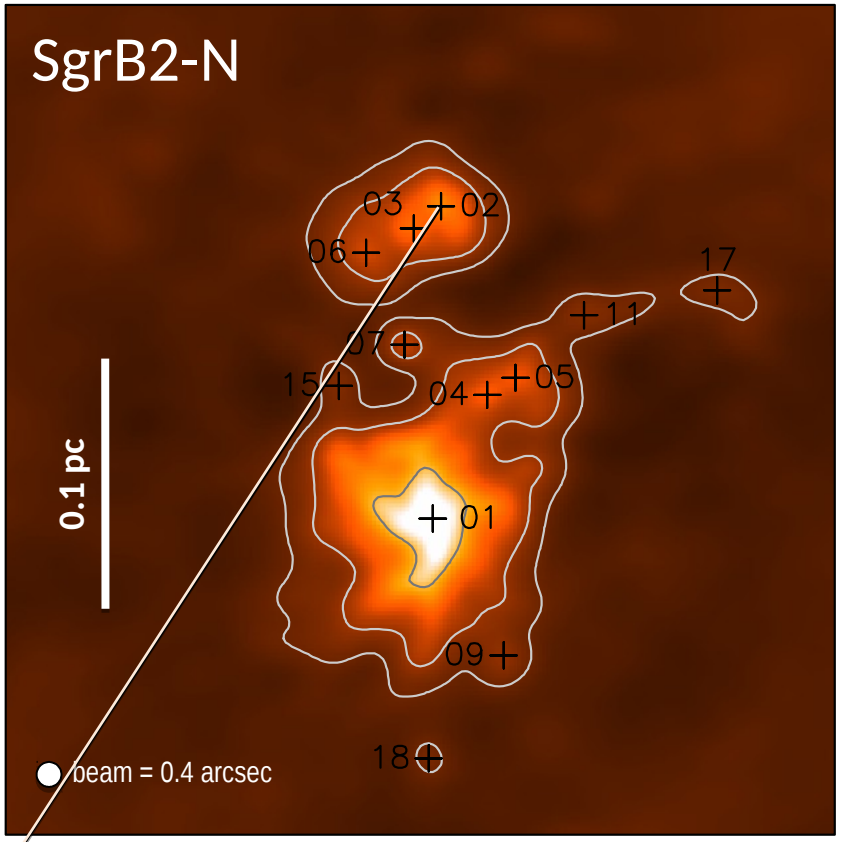


SgrB2-N continuum

- Main core:
  4600 $M_{\odot}$, 0.06 pc and 10^8 cm^{-3}
- Monolithic structure,
  opacity effect ?, superposition of cores in 3D ?
  contains HII regions (must fragment)
- Spiraling structure converging to the center

- Several small condensations,
  with multiple hot molecular cores

Sánchez-Monge et al. (2016, in prep)



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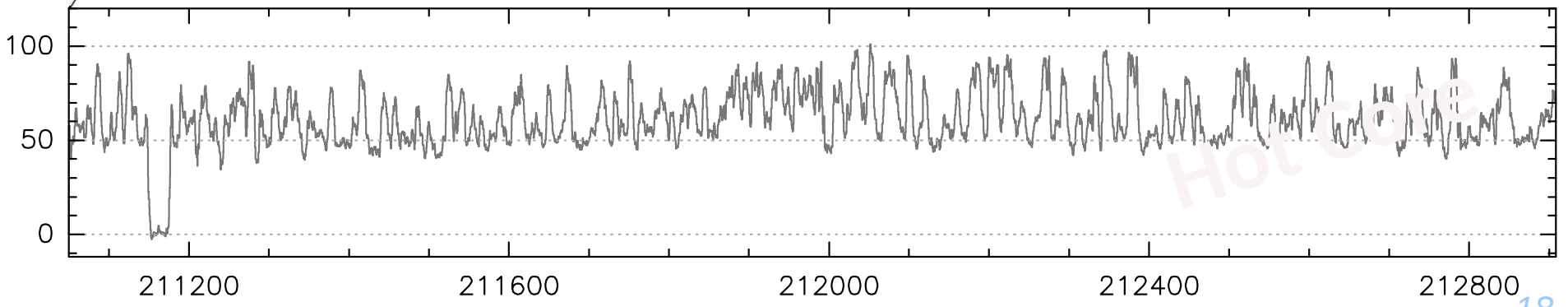
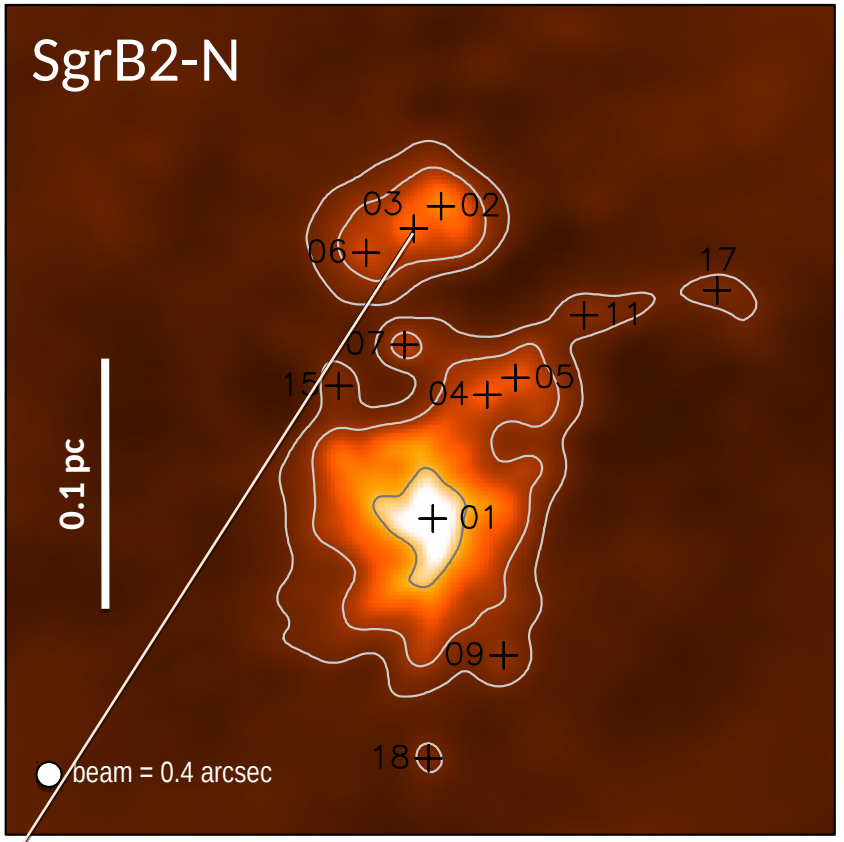


Sánchez-Monge et al. (2016, in prep)



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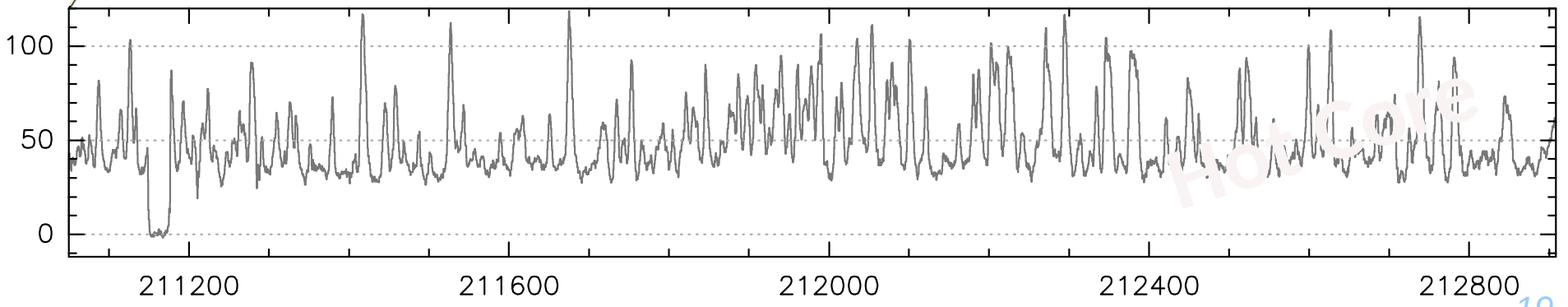

Sánchez-Monge et al. (2016, in prep)

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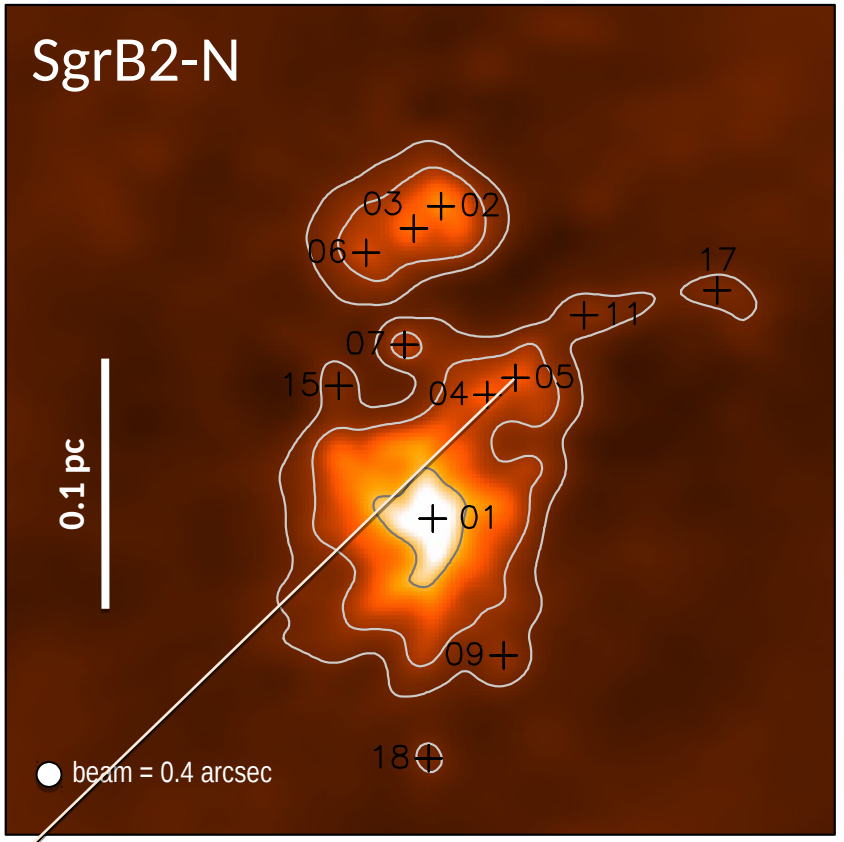

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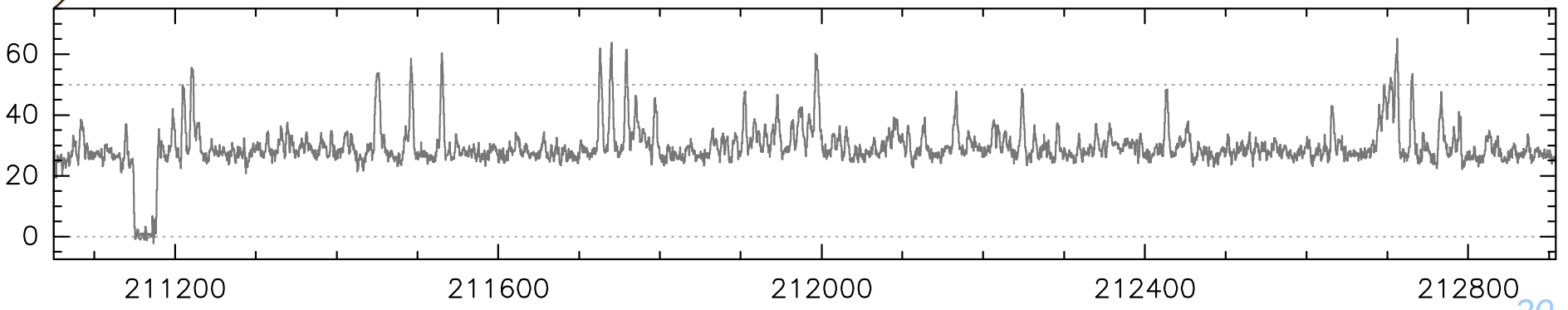

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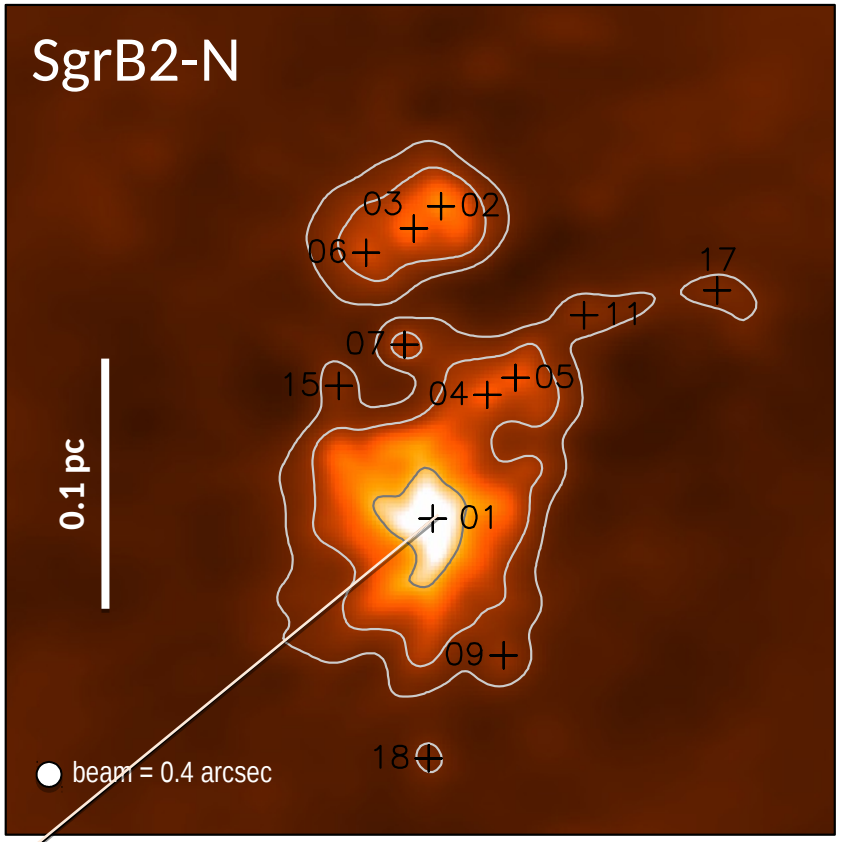

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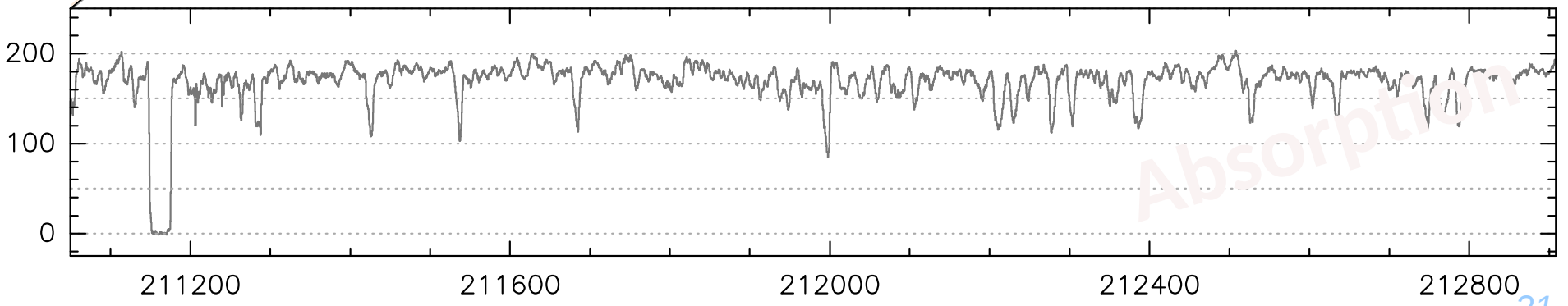

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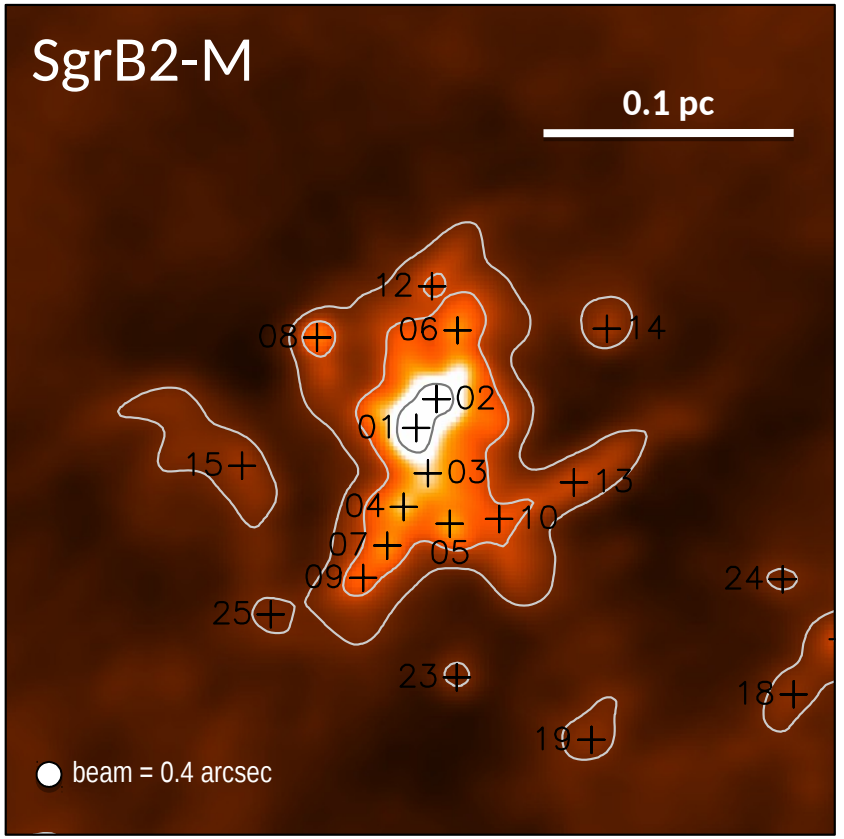
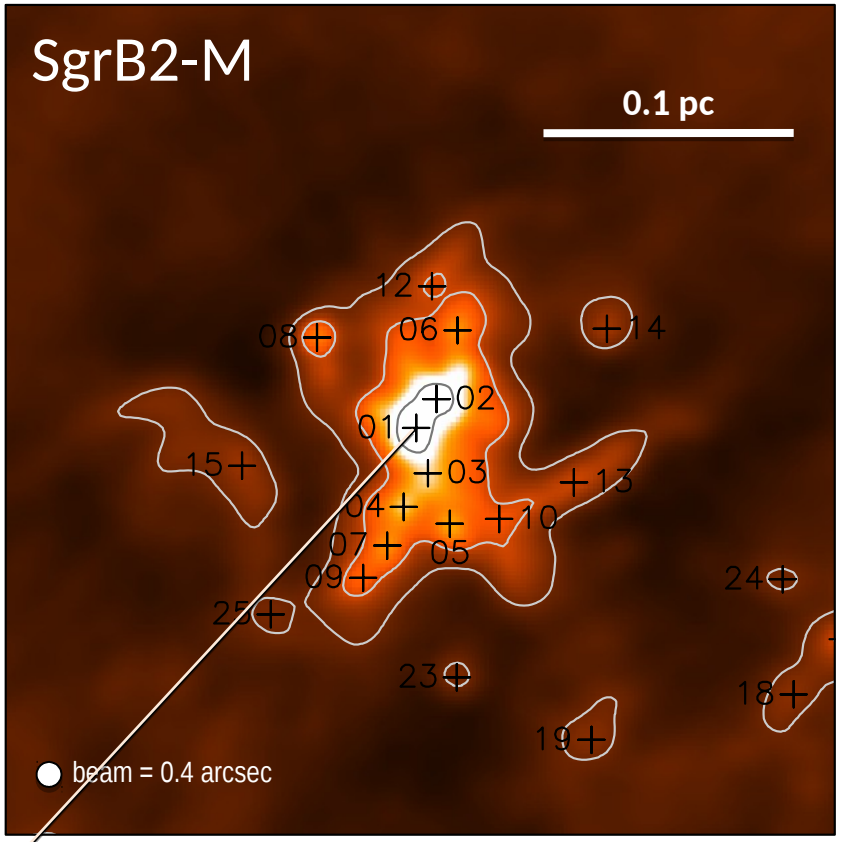


SgrB2-M continuum

- Two main (central) cores:
  1100 $M_{\odot}$, 0.02 pc and 5×10^8 cm^{-3}
- Highly fragmented, with elongated structures
- 1 mm continuum heavily affected by free-free (ionized gas) emission

- Deep absorptions towards condensations, due to bright hypercompact HII regions

Sánchez-Monge et al. (2016, in prep)



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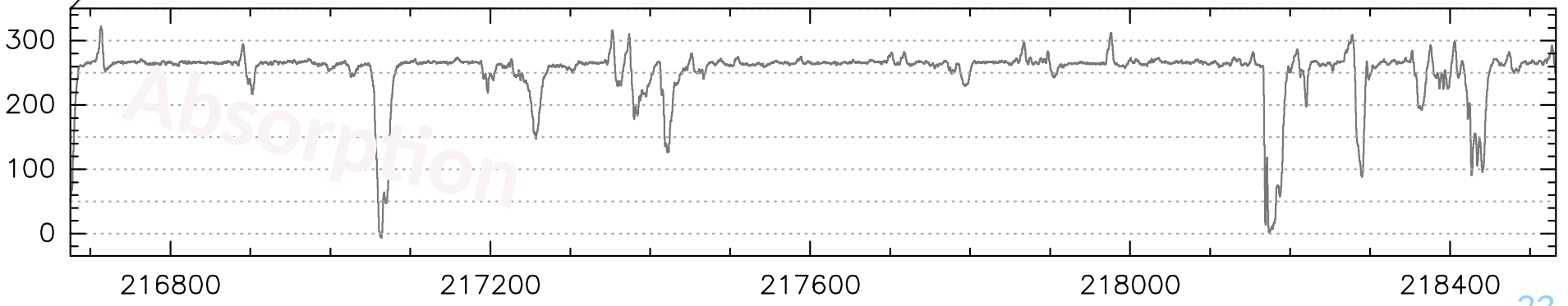

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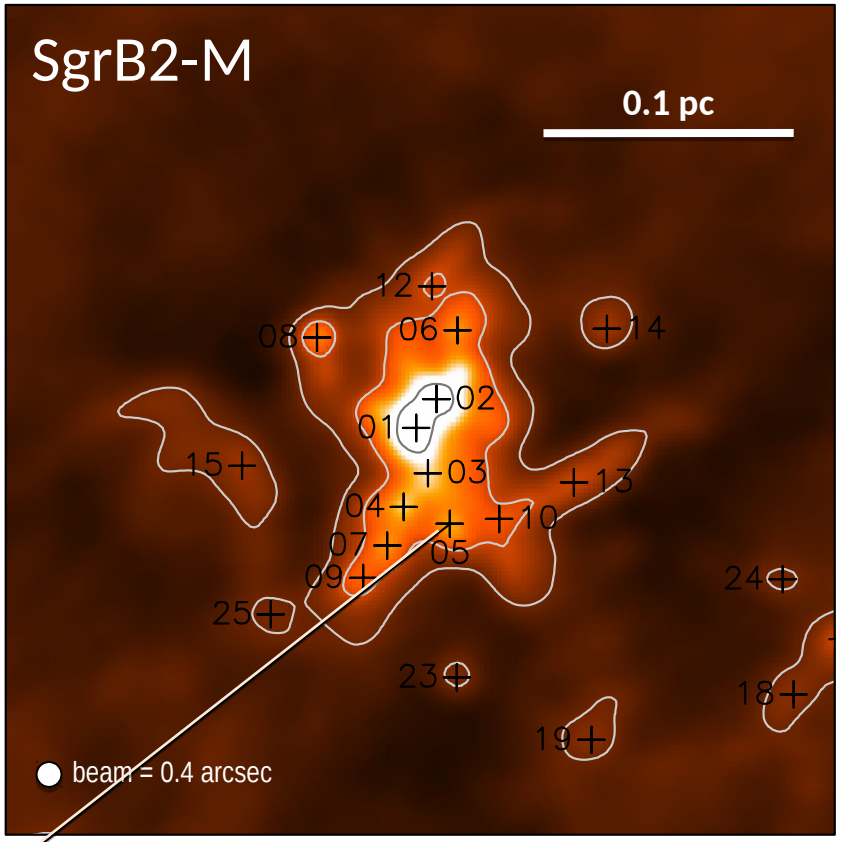

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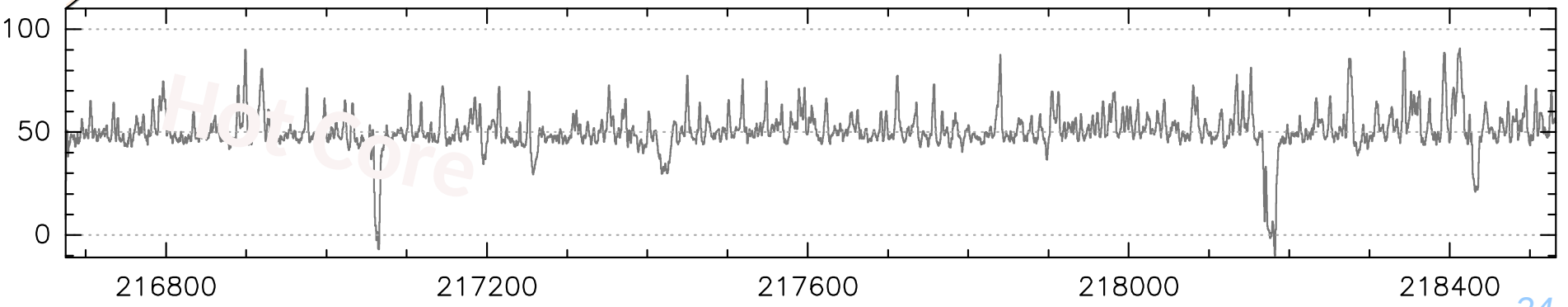
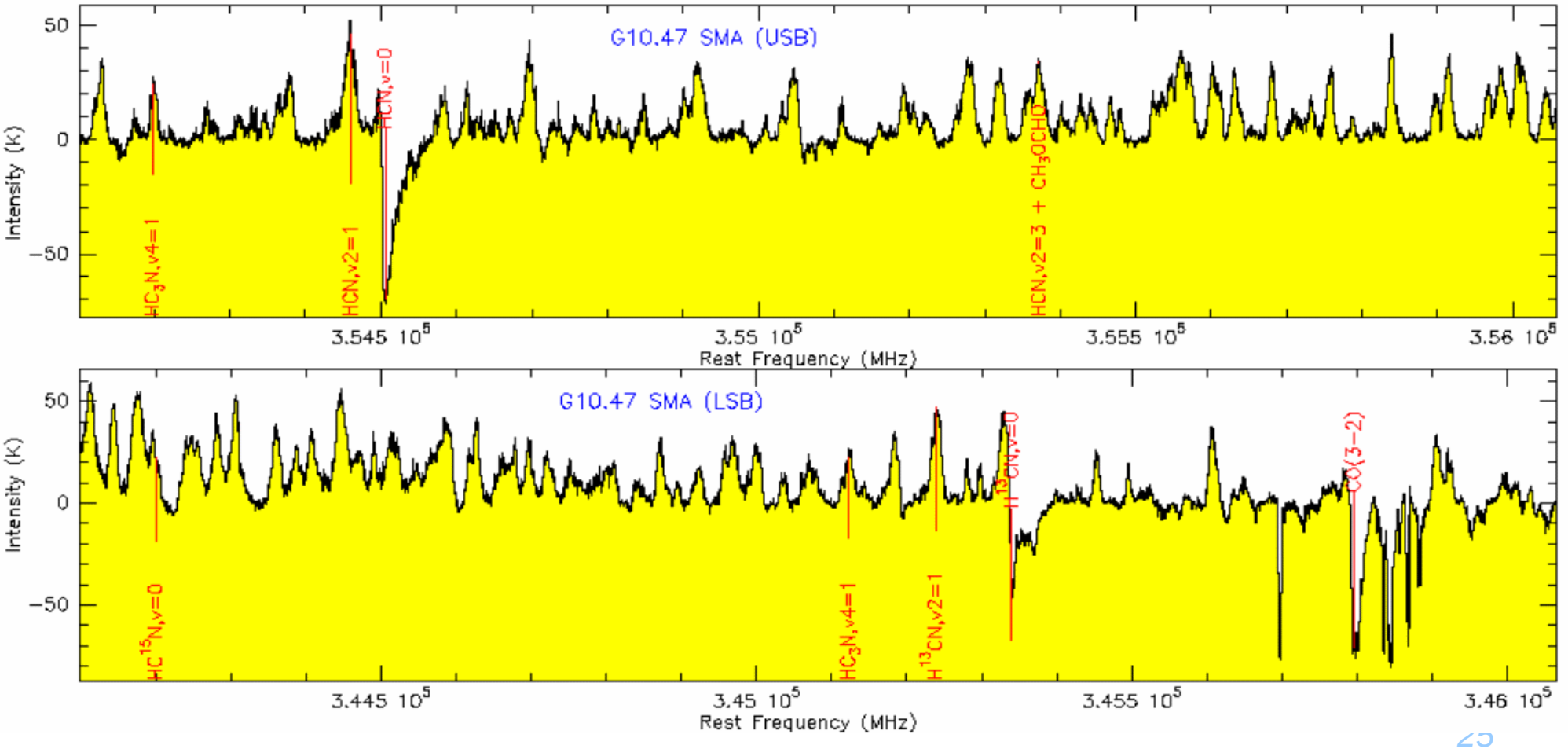


Sánchez-Monge et al. (2016, in prep)

Not only ALMA
SMA spectra toward the central position of G10.47



What do we need?

- Identify as many lines as possible **fast**
- Determine physical parameters **fast**
- We have maps: need to do this for all pixels – **fast**
- … to allow astrophysicists to spend their time to do a scientific analysis

How do we do this?

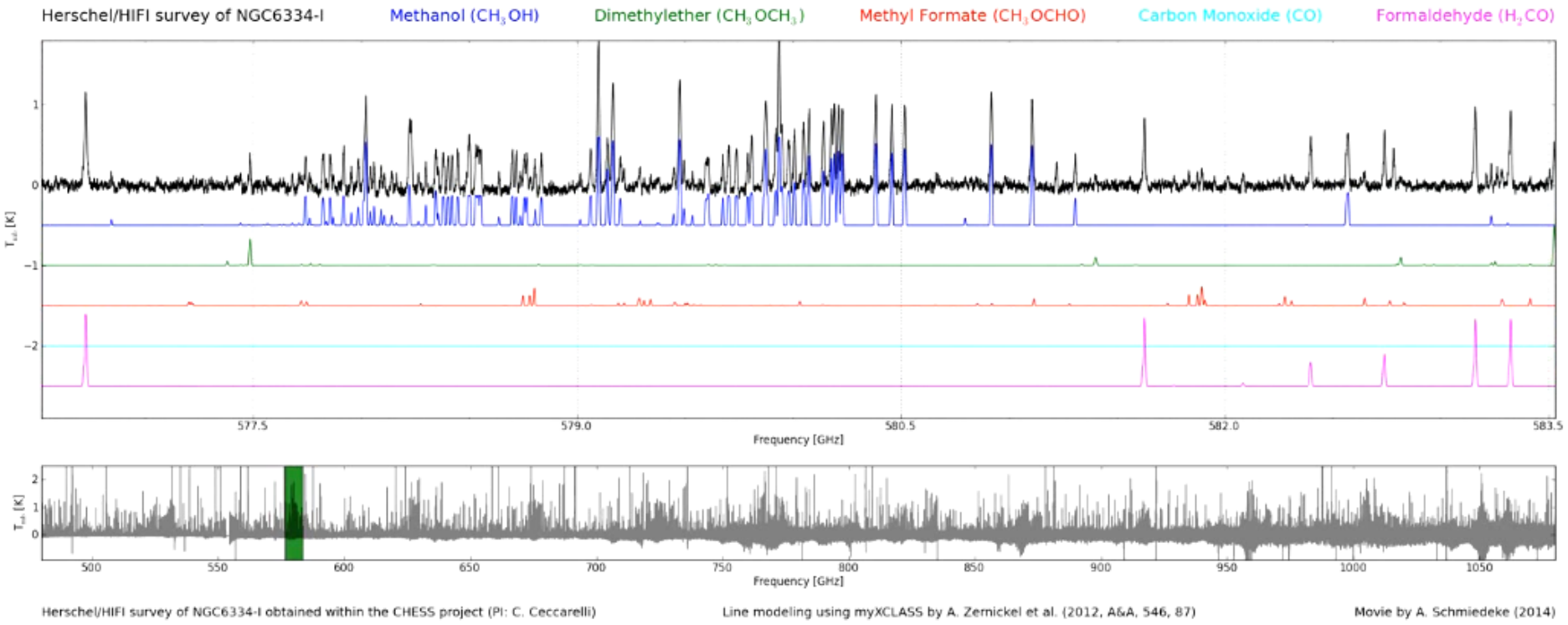
- Option A

How do we do this?

- Option B

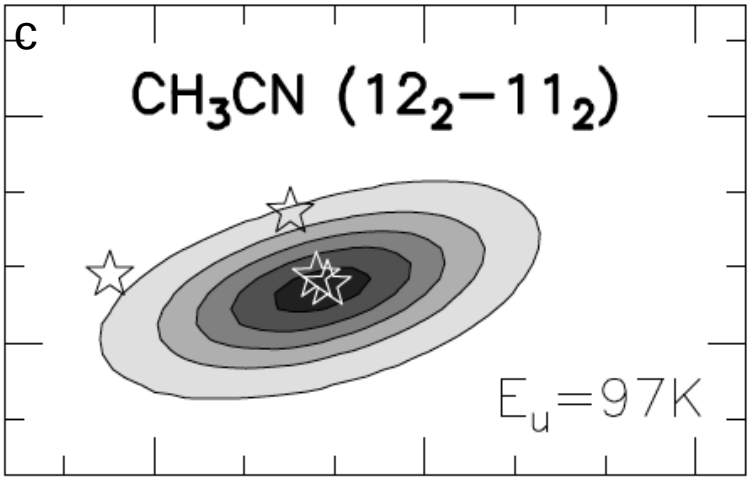
Option B: XCLASS

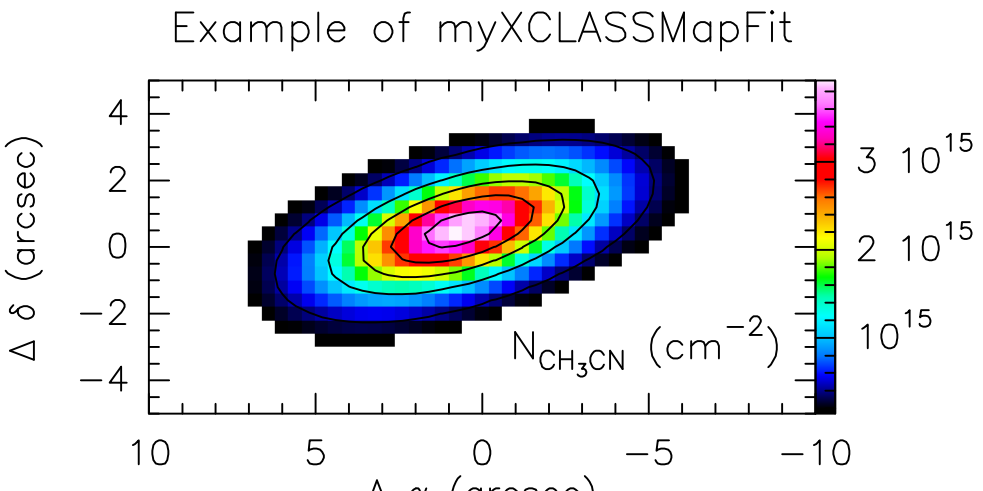
XCLASS generates **synthetic spectra** in LTE approximation
Automatic optimization of parameters using many different algorithms
MPI parallelized
Using CDMS/VAMDC data bases

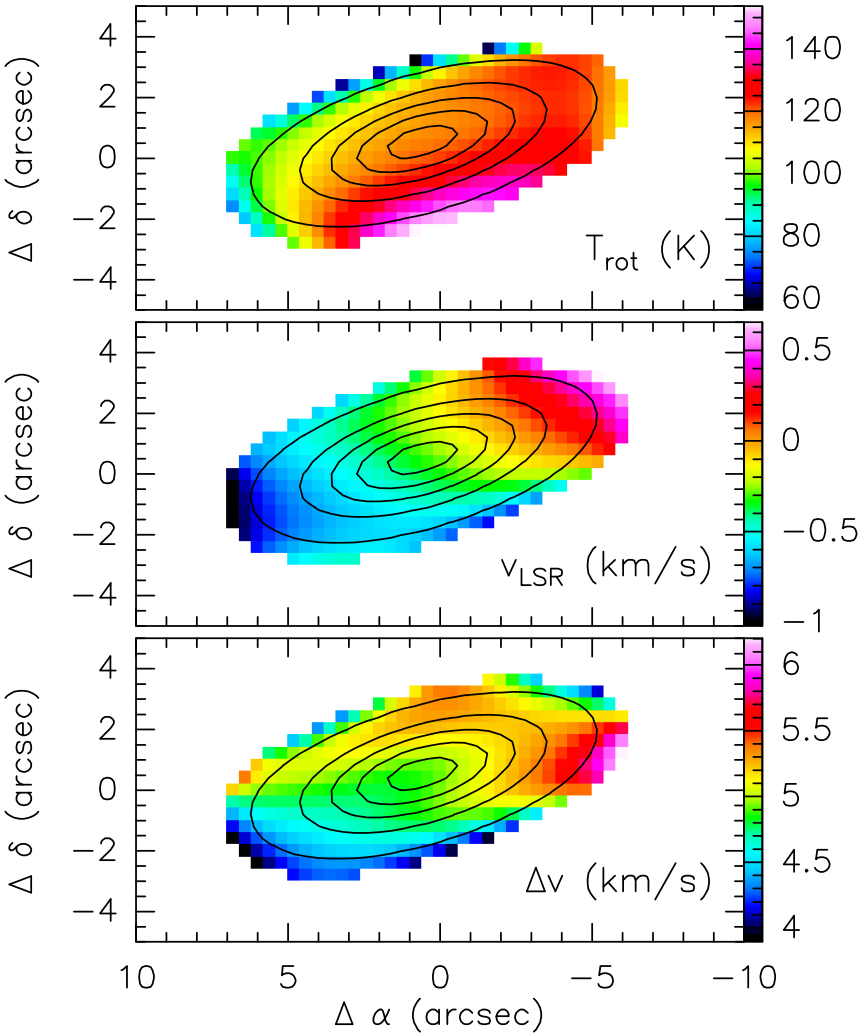


Option B: XCLASS

example of **myXCLASSMapFit**:
- from CH_3CN line fitting







Option C: more sophisticated RT

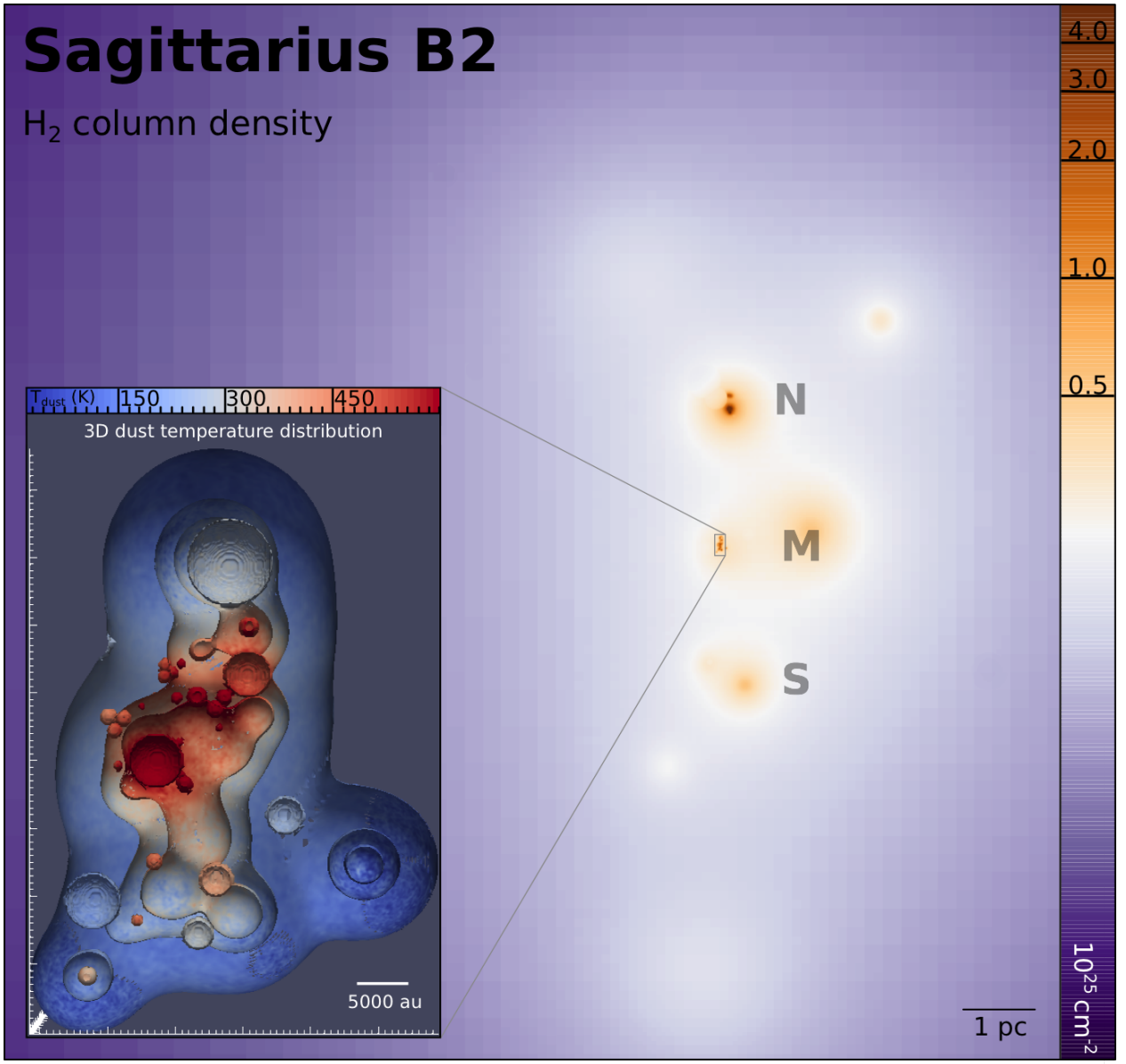
Pandora

Python framework, versatile
3D radiative transfer modeling
[Schmiedeke et al. 2016]

- Uses RADMC-3D and LIME to model dust continuum and line emission

- Input parameters:
  - dense cores
  - HII regions

- Kinematics included:
  - infall (free-fall)
  - rotation (Keplerian)
  - outflow



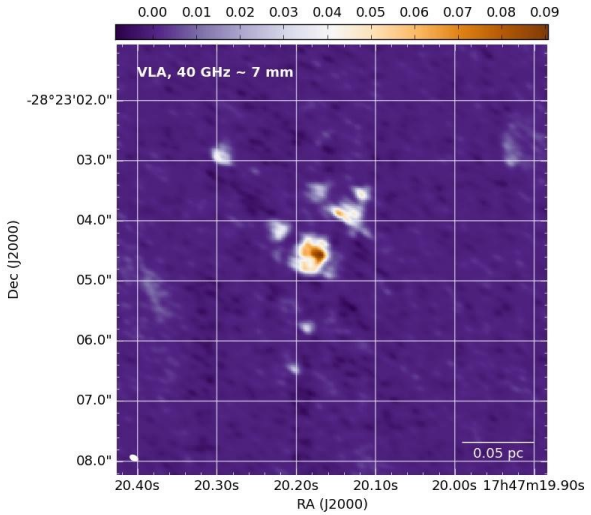
Schmiedeke et al. (2016)

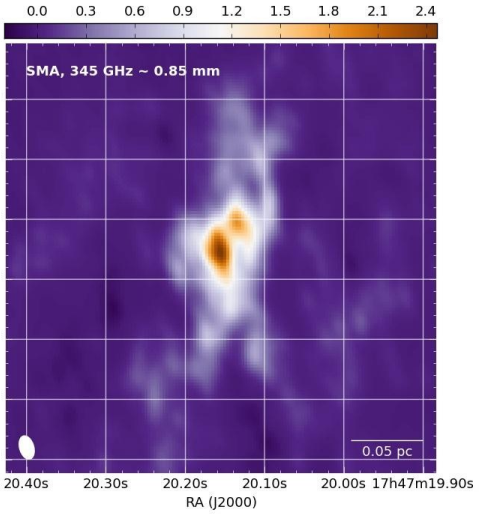
VLA @40GHz

@245GHz

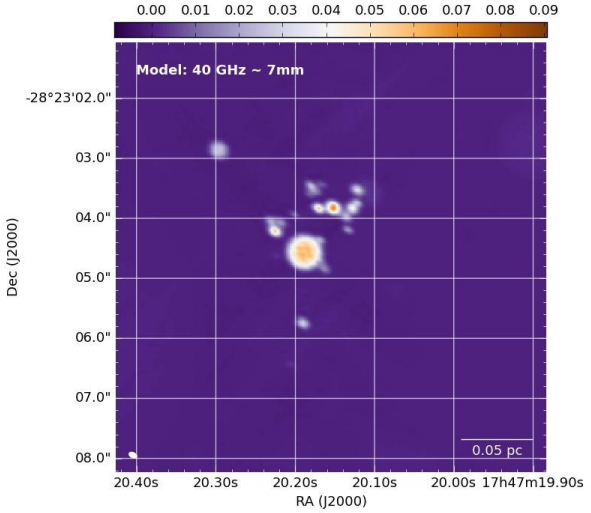
SMA @345GHz

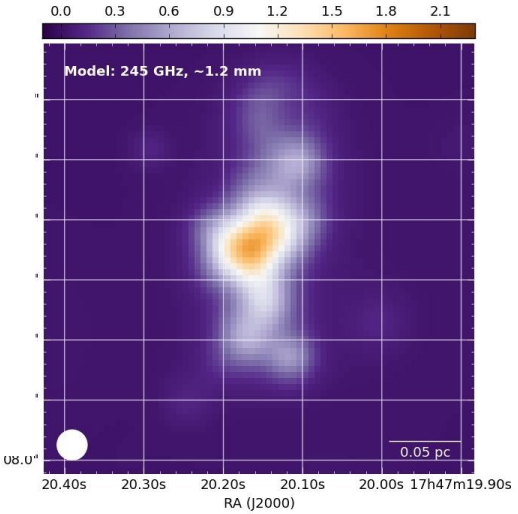
DATA

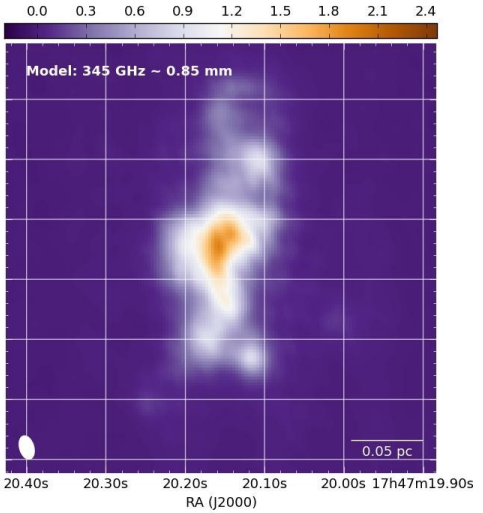




MODEL







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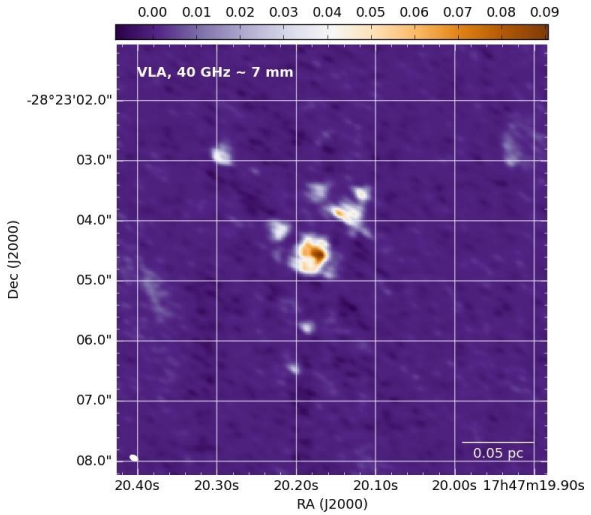

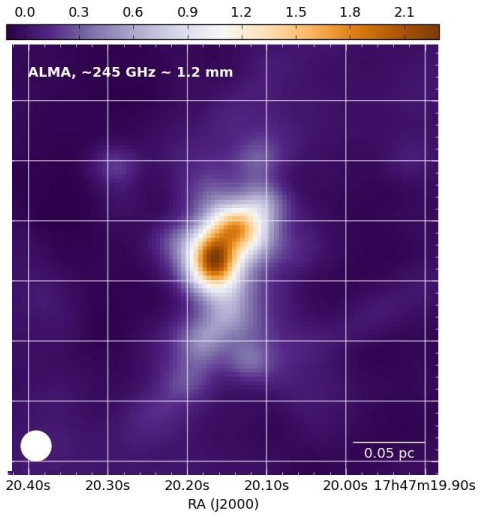

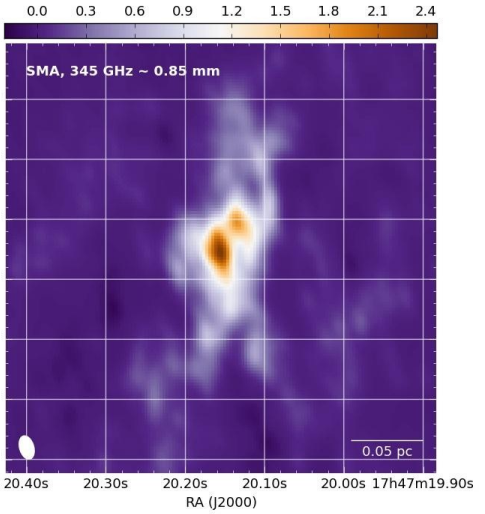

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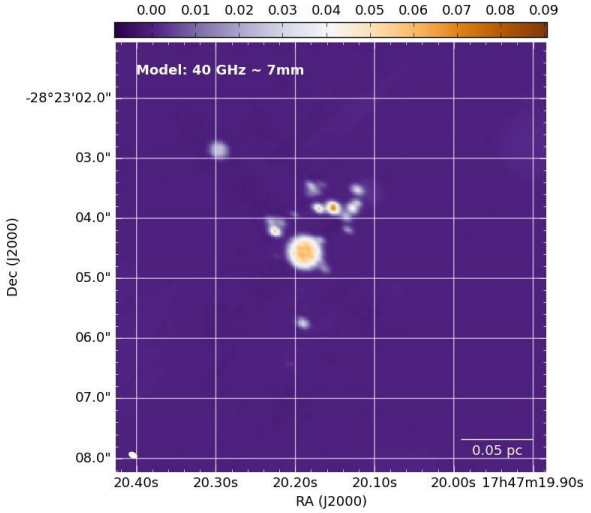

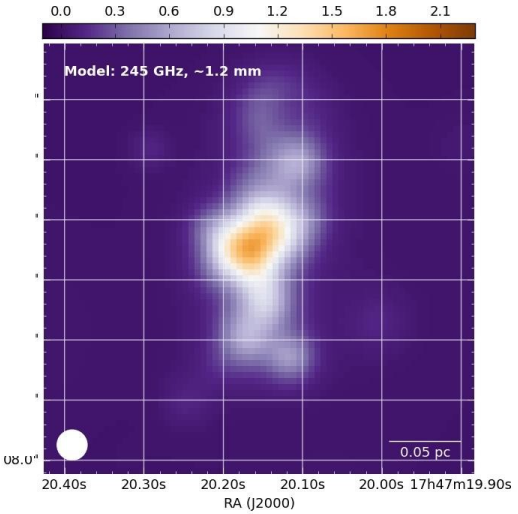

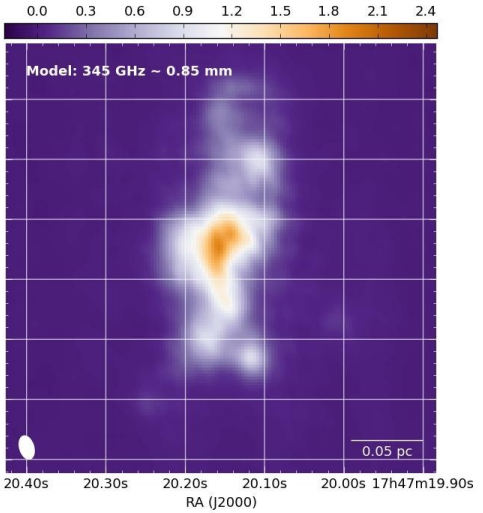

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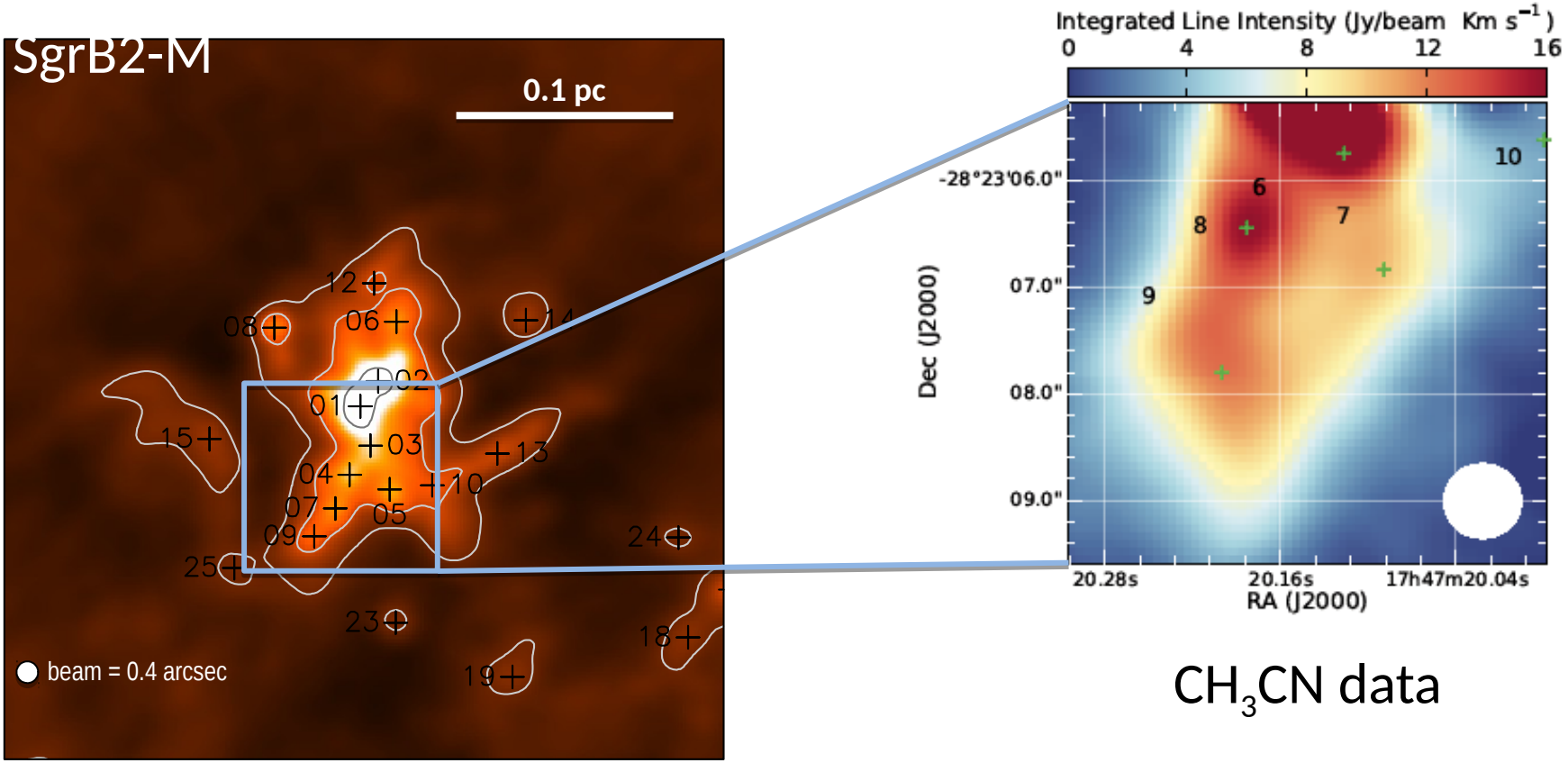
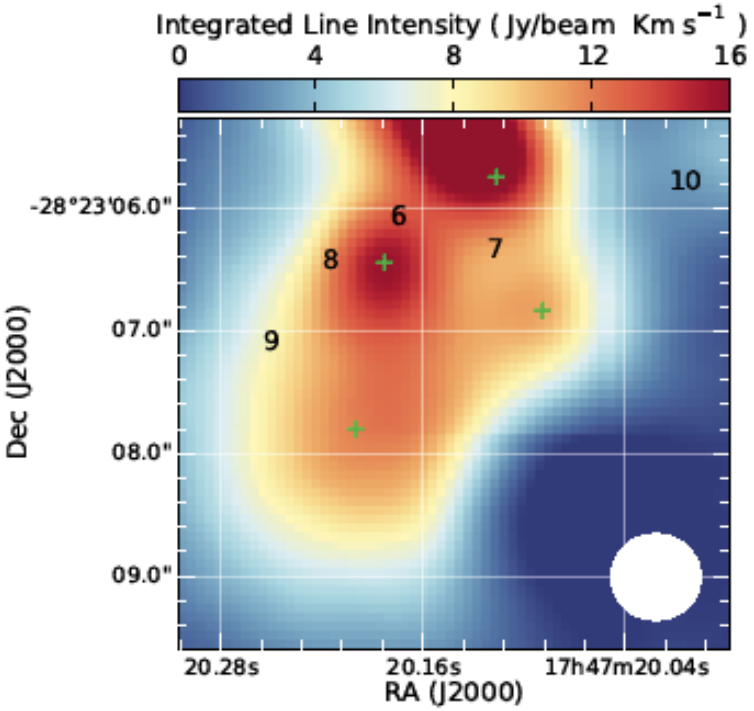


CH_3CN data

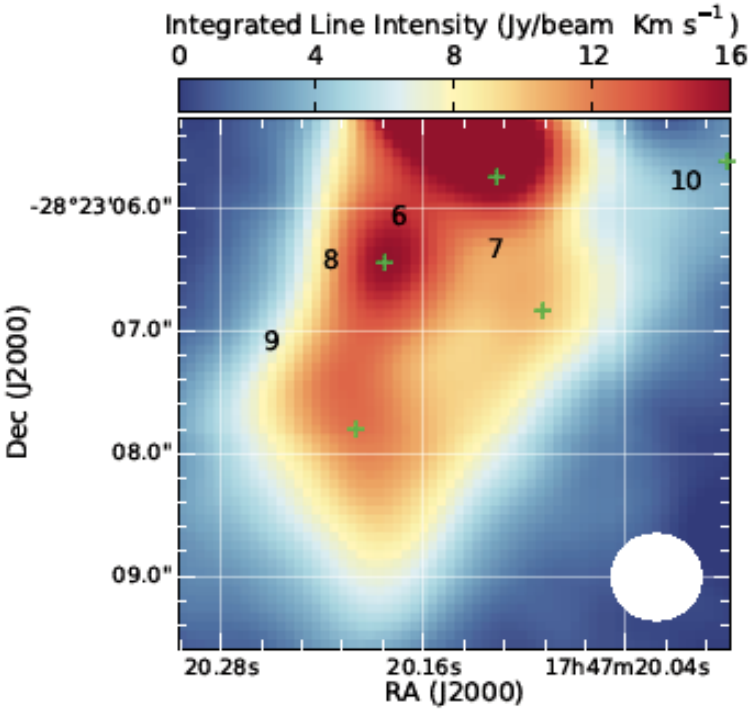
MODELING of Spectral Lines

- 3D radiative transfer model (using Pandora)

Stefan Pols (2016, Master Thesis)



CH_3CN model



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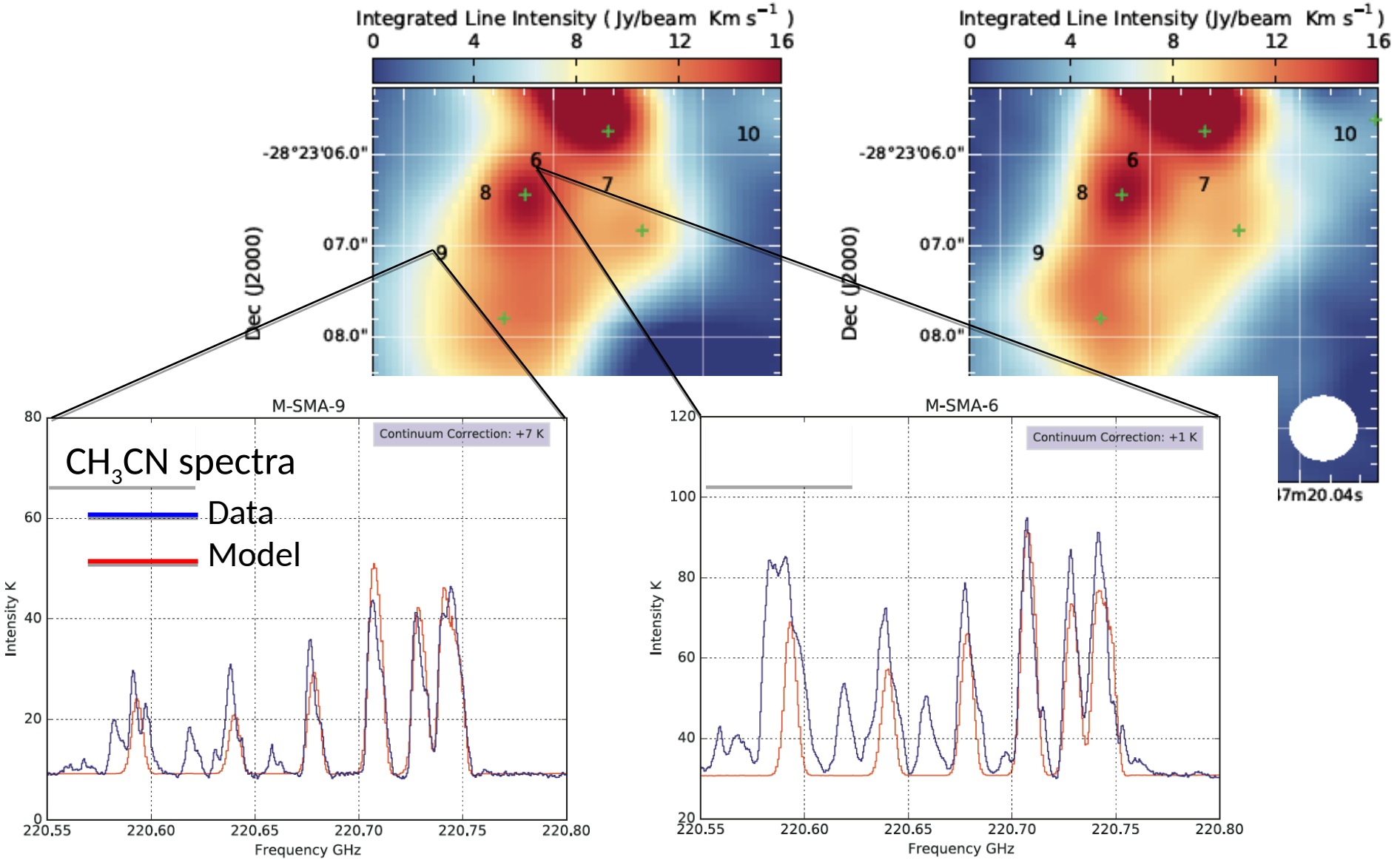

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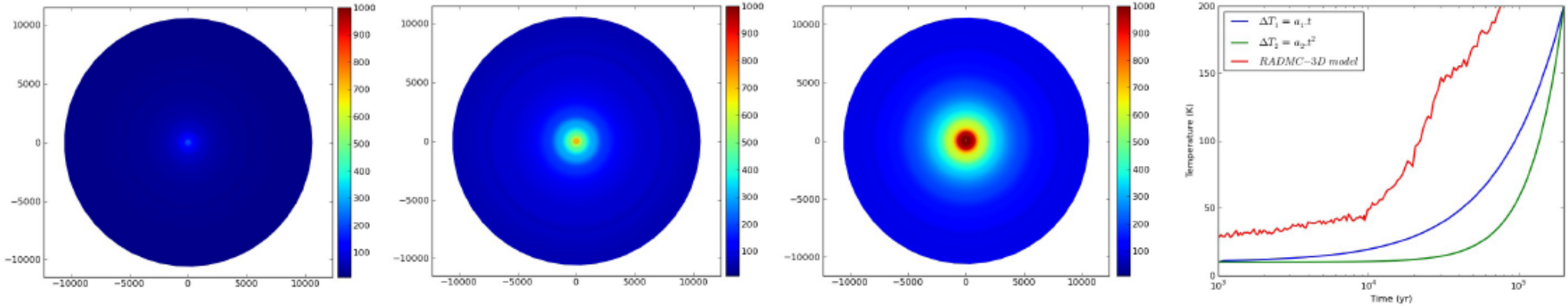
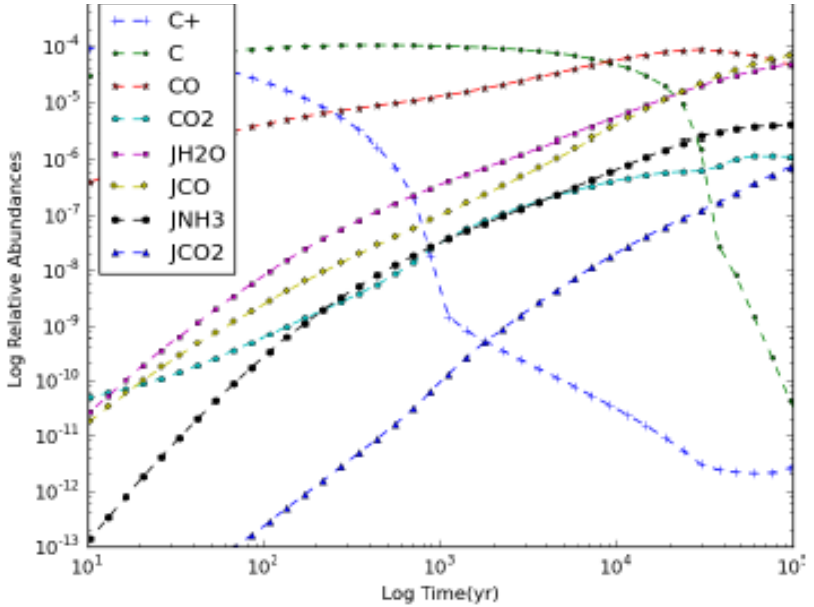
Needs integrated chemical models for interpretation

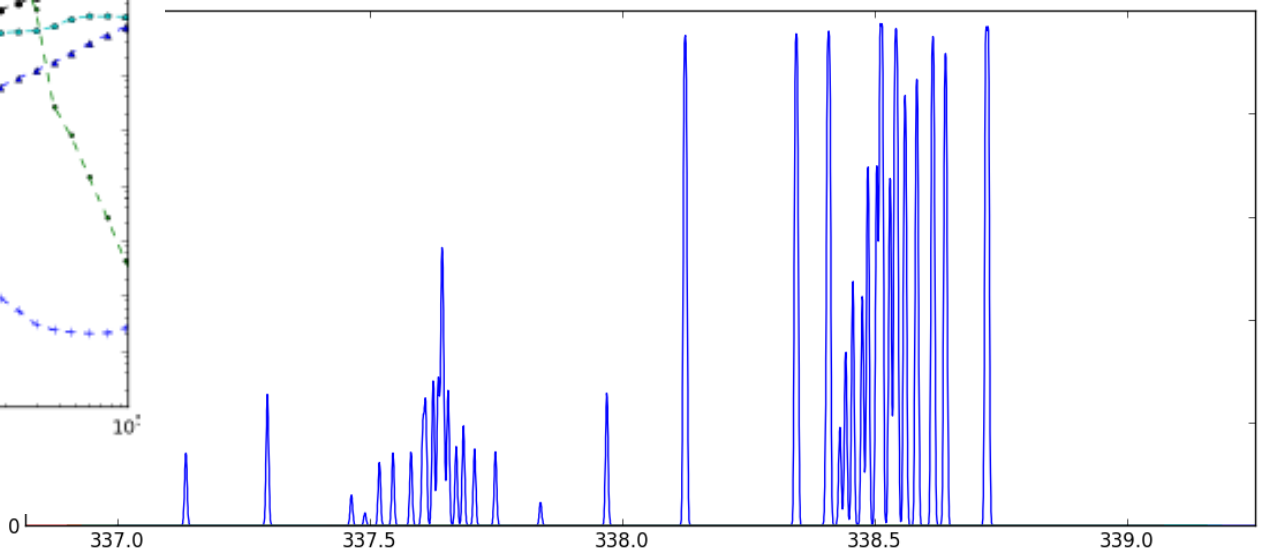
Example:

Saptarsy (Choudhury et al. 2015, Stéphan et al. 2017)

needed: thermal evolution, dynamics, initial conditions







Summary

- Chemistry in Star Formation is a powerful tool
  - To determine past and present physical parameters
  - Ages (chemical clock), feedback effects, ...
  - Requires fast, automatic data analysis and classification
  - Comparison with chemical models producing spectra
  - Needs good statistics, also in number of sources
    - For wSMA, I recommend large, coherent programs for maximum impact

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Paradigm change
(partly based on thoughts by Felix Stoehr)

- Past:
  - Observers had to struggle to get data ("Proposals")
  - Few data: small bandwidths, low sensitivity, low resolution (low spatial dynamic range, blobs)
  - Easy analysis, fast publication
- Now:
  - SMA, ALMA and JVLA produce vast amounts of data, available through archives
  - Many data: large bandwidths, high sensitivity, high resolution (high spatial dynamic range)
  - Difficult analysis, slow publication

Paradigm change
(partly based on thoughts by Felix Stoehr)

- Past:
  - Demand driven economy
  - Observatories had to deliver some data, in some format and leave the rest to the users
  - Enough to survive as observatory
- Now:
  - Supply driven economy
  - Observatories have to help observers by delivering calibrated images and providing analysis tools to ensure high enough publication rates and thus, survivial