CENTRO DE ASTROBIOLOGÍA

CSIC
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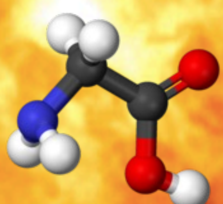
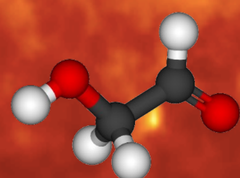
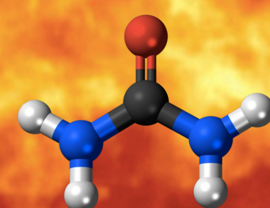
INTA Instituto Nacional de Técnica Aeroespacial

Towards prebiotic chemistry in the interstellar medium







Izaskun Jiménez-Serra
(CSIC)

XXXVIII Trobades de la Mediterrania– Institut Menorquí d'Estudis– 6th November 2023

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CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

INTA
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Carlos Briones/Jacobo Aguirre

External collaborators:

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Miguel Requena-Torres (U. Maryland)
Sergio Martin (ESO)
Arnaud Belloche (MPIfR)

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Emilio Cocinero (UPV)
J. L. Alonso, E. Alonso (UVA)
M. Melosso, L. Bizzocchi, C. Puzzarini (U. Bologna)

Materials physicists/chemists:

Belen Mate, Víctor Herrero (IEM)
Juan Garcia de la Concepcion (UEX)

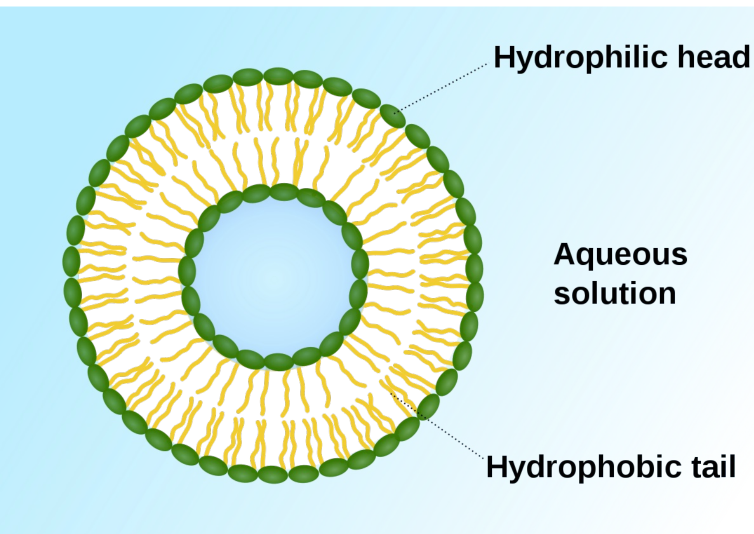
Astrochemistry as an interdisciplinary field of research

Life: definition and characteristics

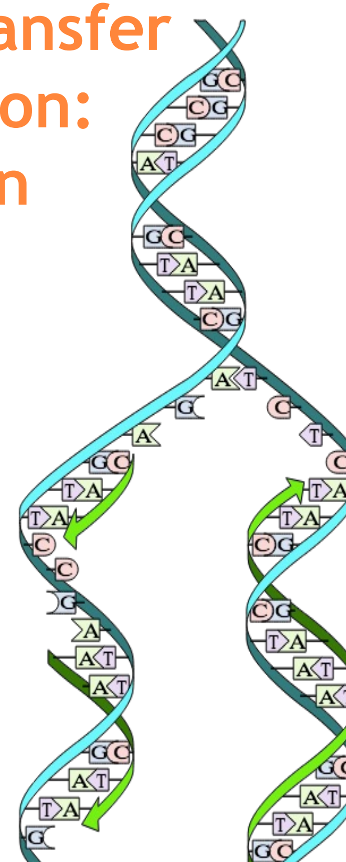
NASA's definition:

"Life is a self-sustaining chemical system capable of Darwinian evolution"

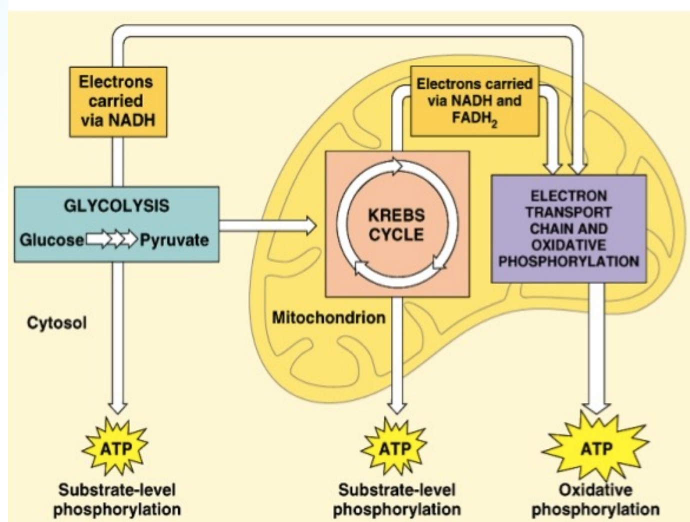
Compartmentalized



Storage and transfer of information: replication

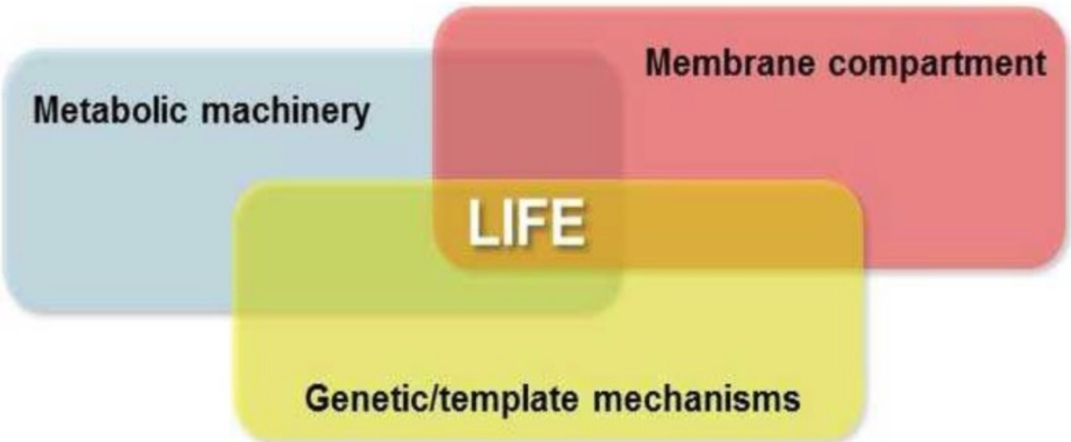


Metabolism

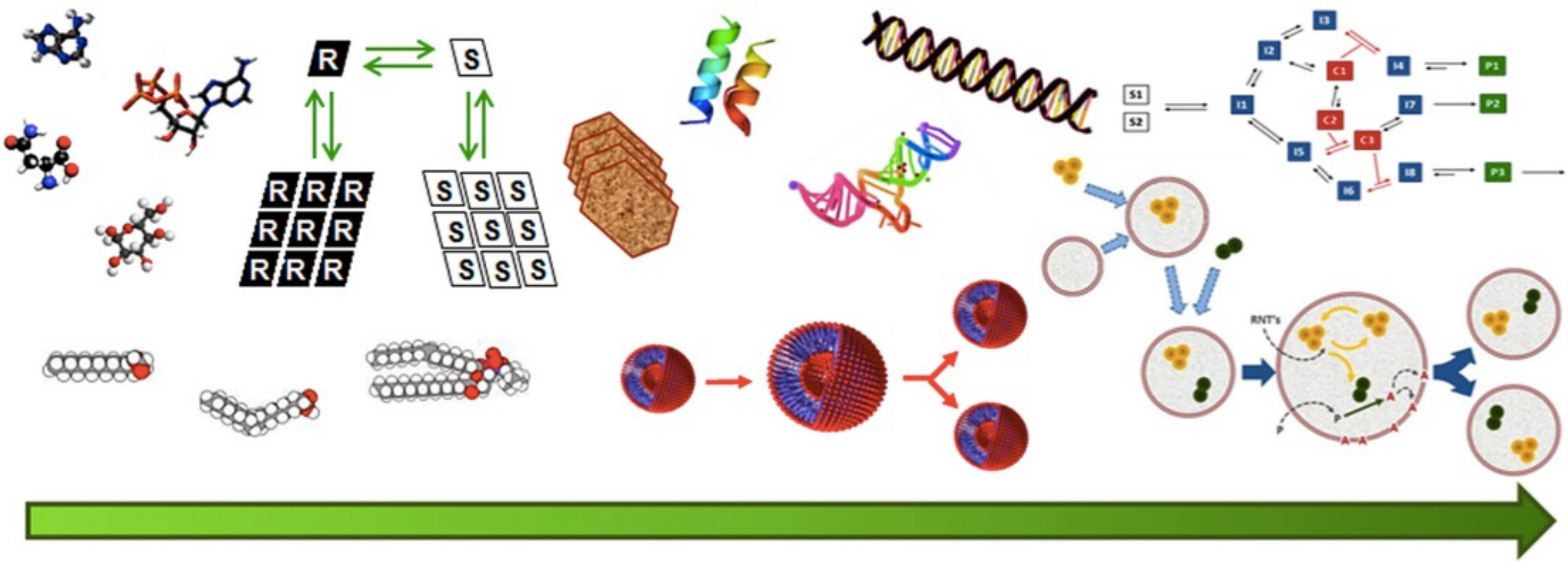


Prebiotic Systems Chemistry

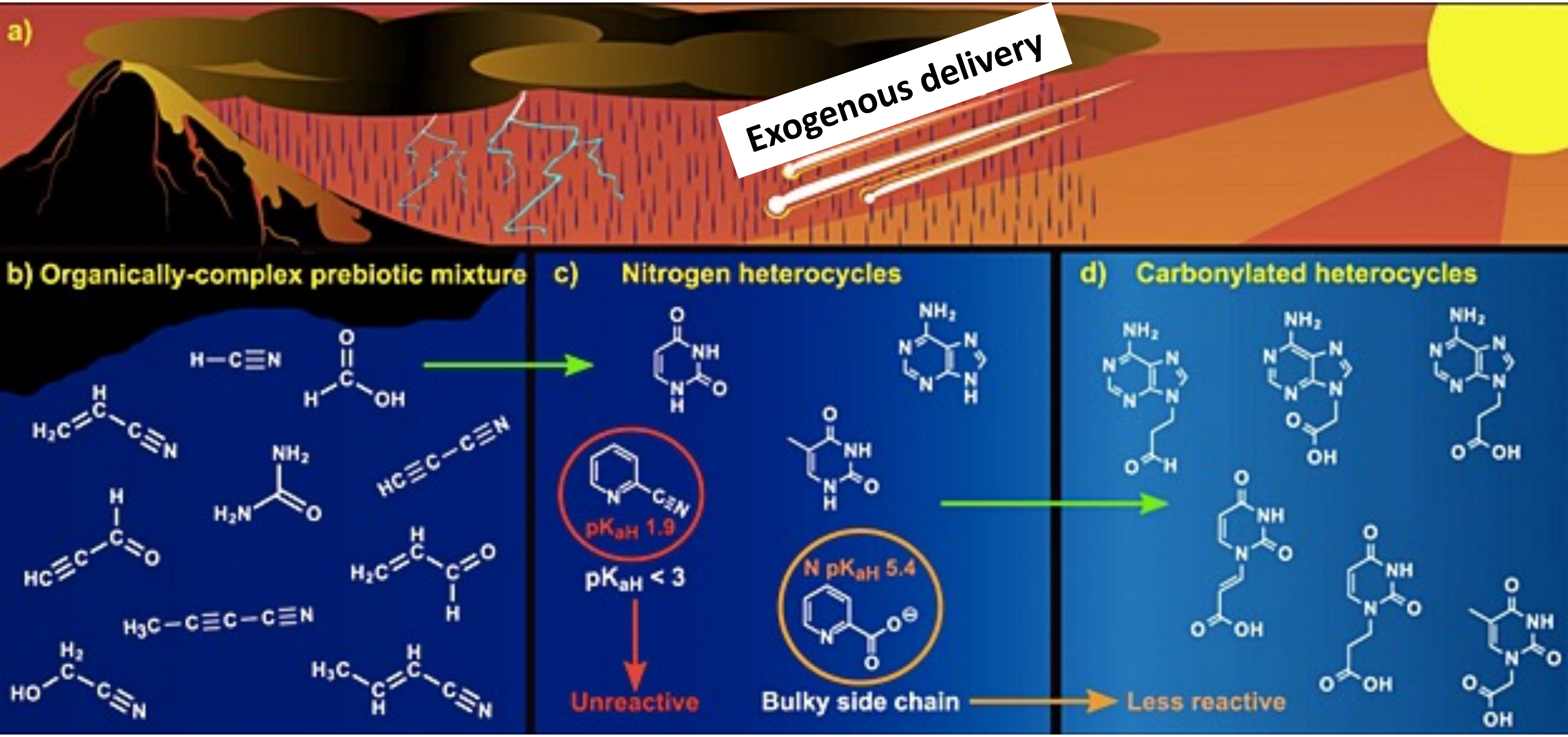
(Ruiz-Mirazo et al. 2014)



"a high diversity of precursor components was available on the prebiotic Earth and that these components could progressively turn into primordial metabolic, self-replicating, and membrane-bounded subsystems"

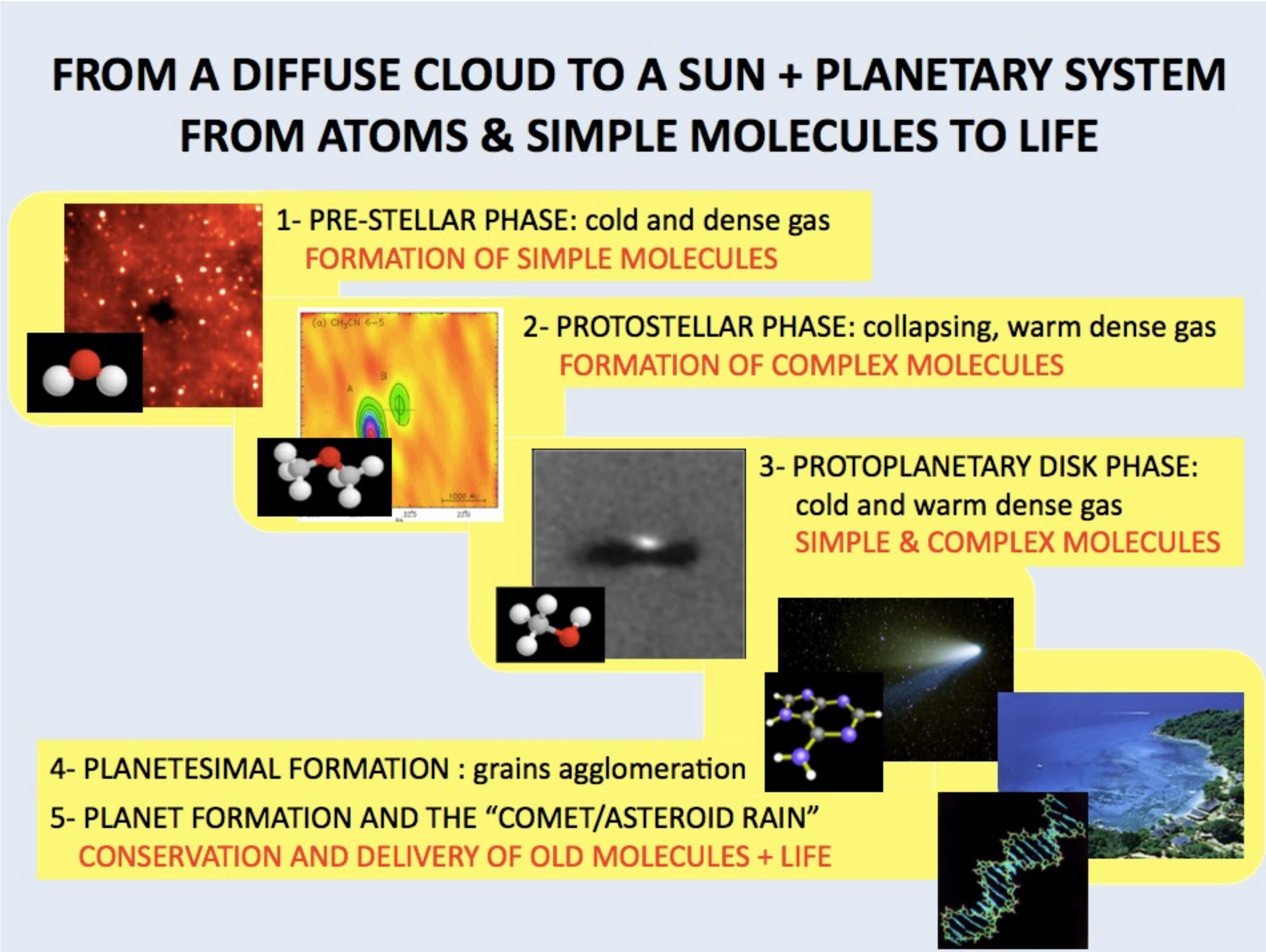


Work hypothesis:
Prebiotic precursors could form already in the ISM



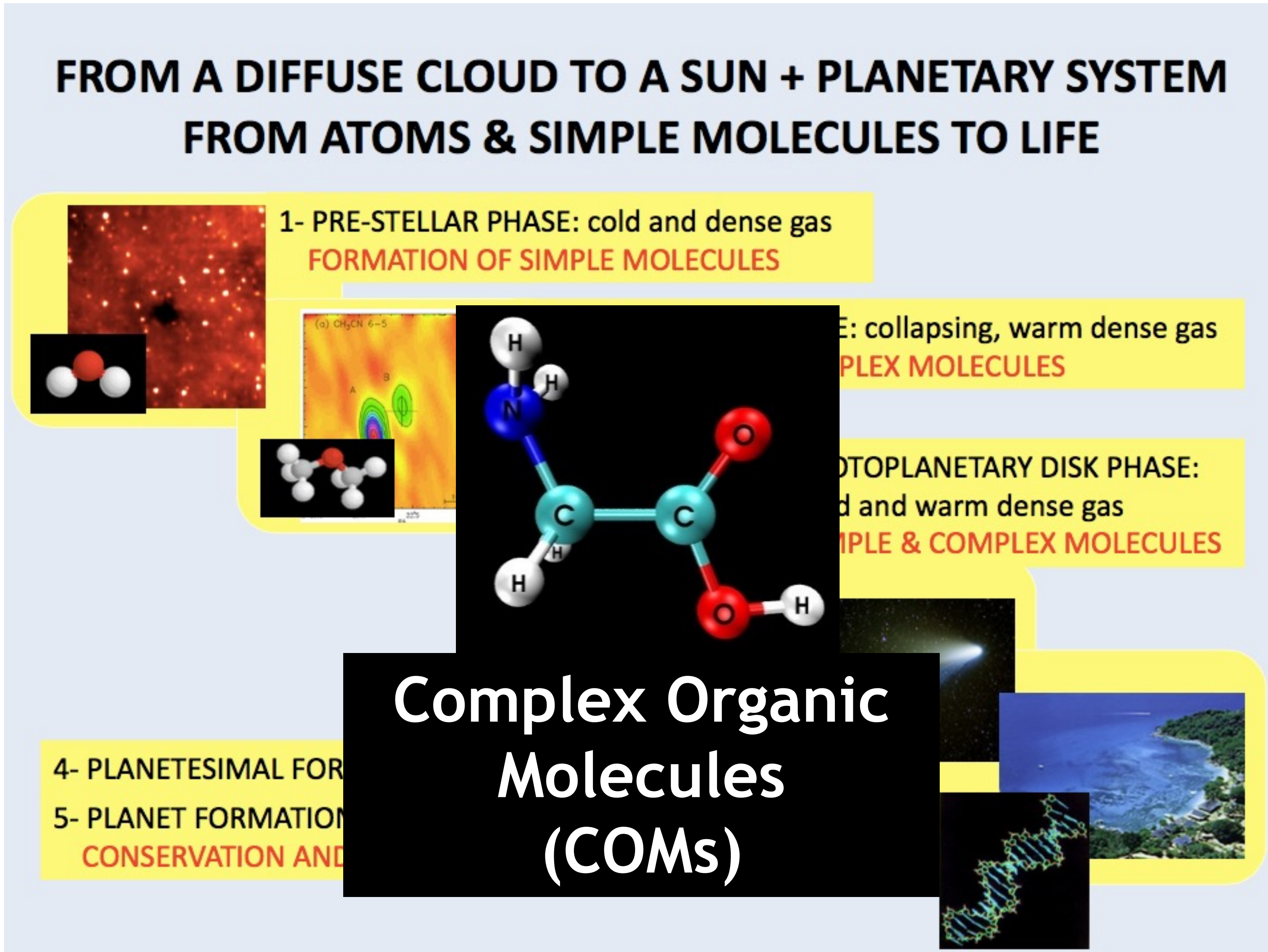
Survival of organic prebiotic material after meteor impact possible
(Chyba & Sagan 1992; Pierazzo & Chyba 2006; McCaffrey et al. 2014)

From the ISM to the Origin of Life



Caselli & Ceccarelli (2012)

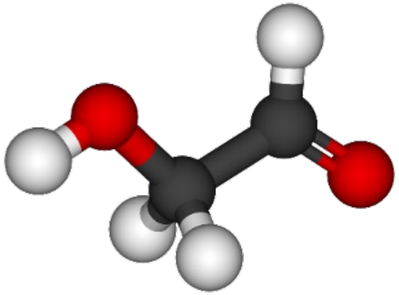
From the ISM to the Origin of Life



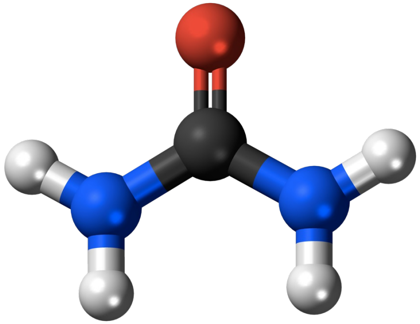
Caselli & Ceccarelli (2012)

Precursors of prebiotic compounds: Complex Organic Molecules (COMs)

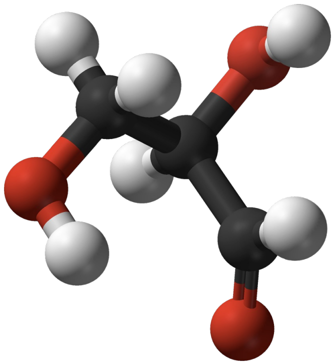
COMs are carbon-based compounds with ≥6 atoms
(Herbst & van Dishoeck 2009)



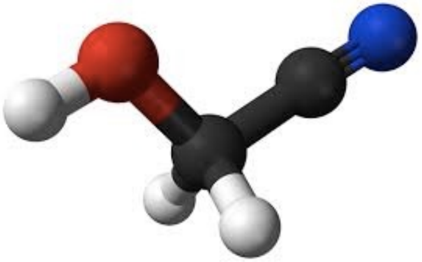
Glycolaldehyde
(CH_2OHCHO)



Urea
(NH_2CONH_2)



Glyceraldehyde
($CH_2OHCH(OH)CHO$)



Glycolonitrile
($HOCH_2CN$)

Outline:

- Complex Organic Molecules (COMs): How do they form and where are they found?
- Search of COMs of prebiotic interest in the ISM
- Emergence of interstellar chemical complexity explained by Complex Network Theory

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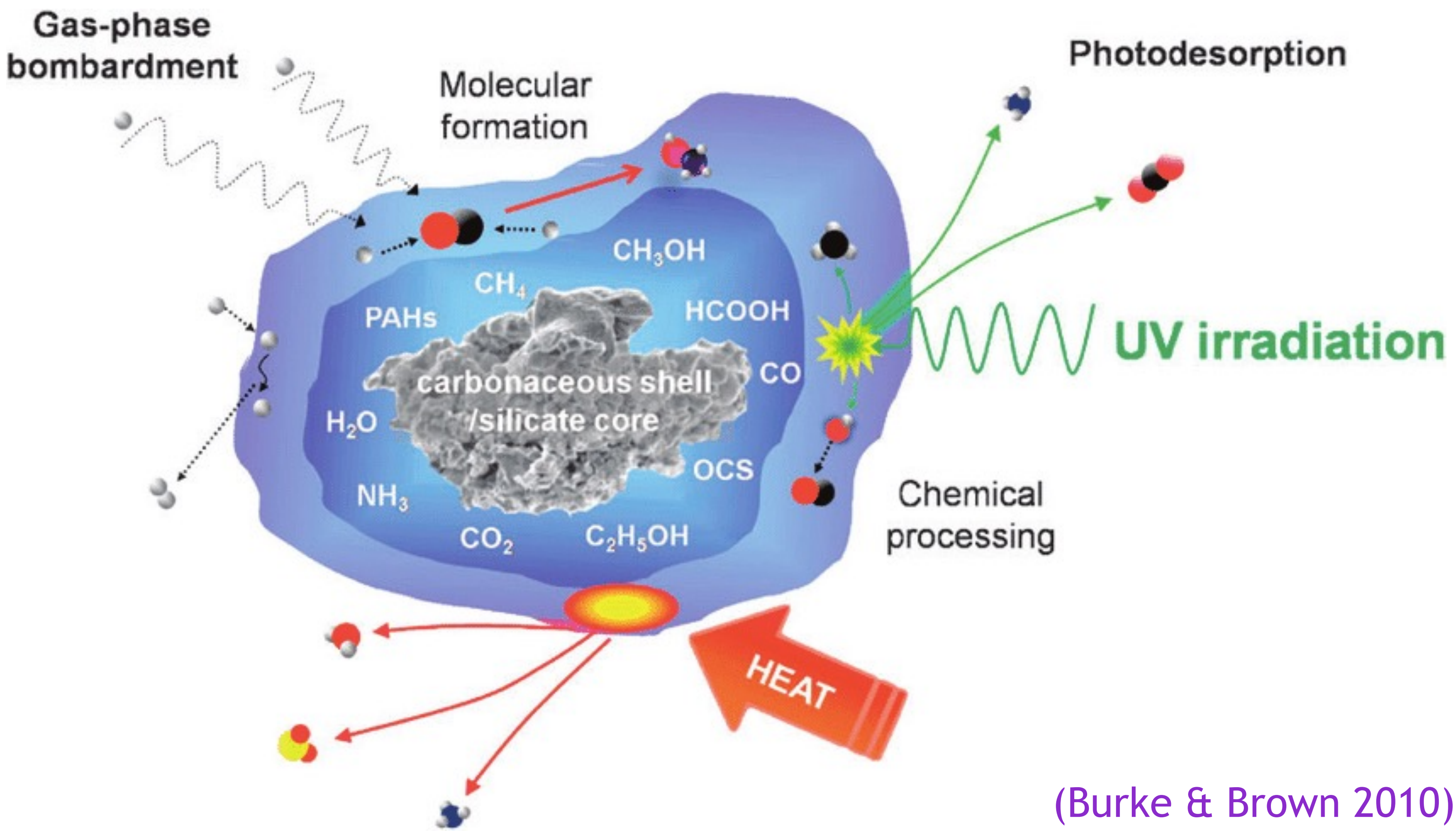
COM formation on dust grains

COMs formed mainly via:

1. Hydrogenation (H addition; Charnley et al. 1997, 2001)
2. Radical-radical surface reactions (efficient at T>30 K; Garrod et al. 2008)

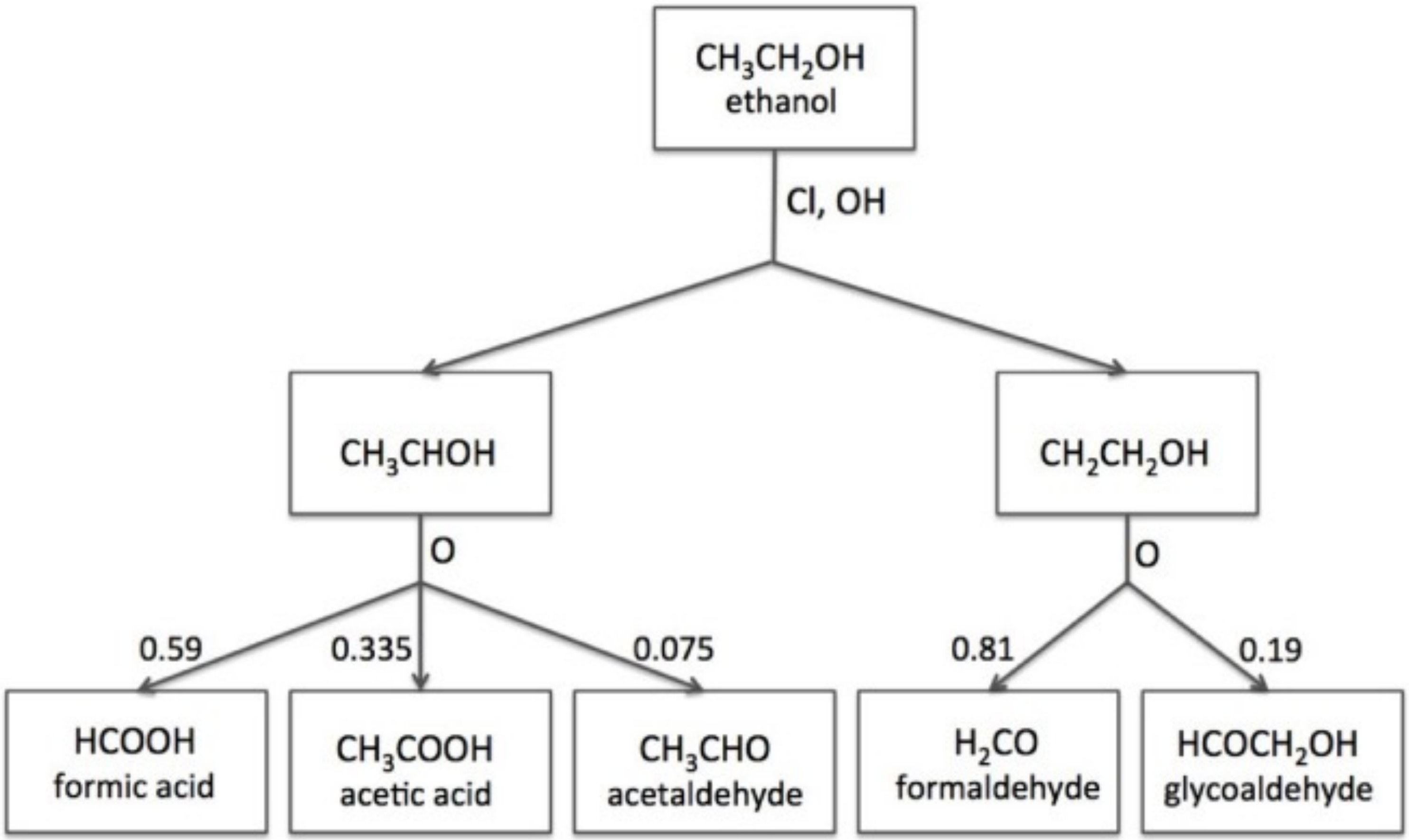


(Burke & Brown 2010)

COM formation for T<30 K

Gas phase reactions A + B → C + D

(Charnley et al. 1995; Vasyunin & Herbst 2013; Barone et al. 2015; Balucani et al. 2015; Vasyunin et al. 2017; Skouteris et al. 2017; 2018; 2019)

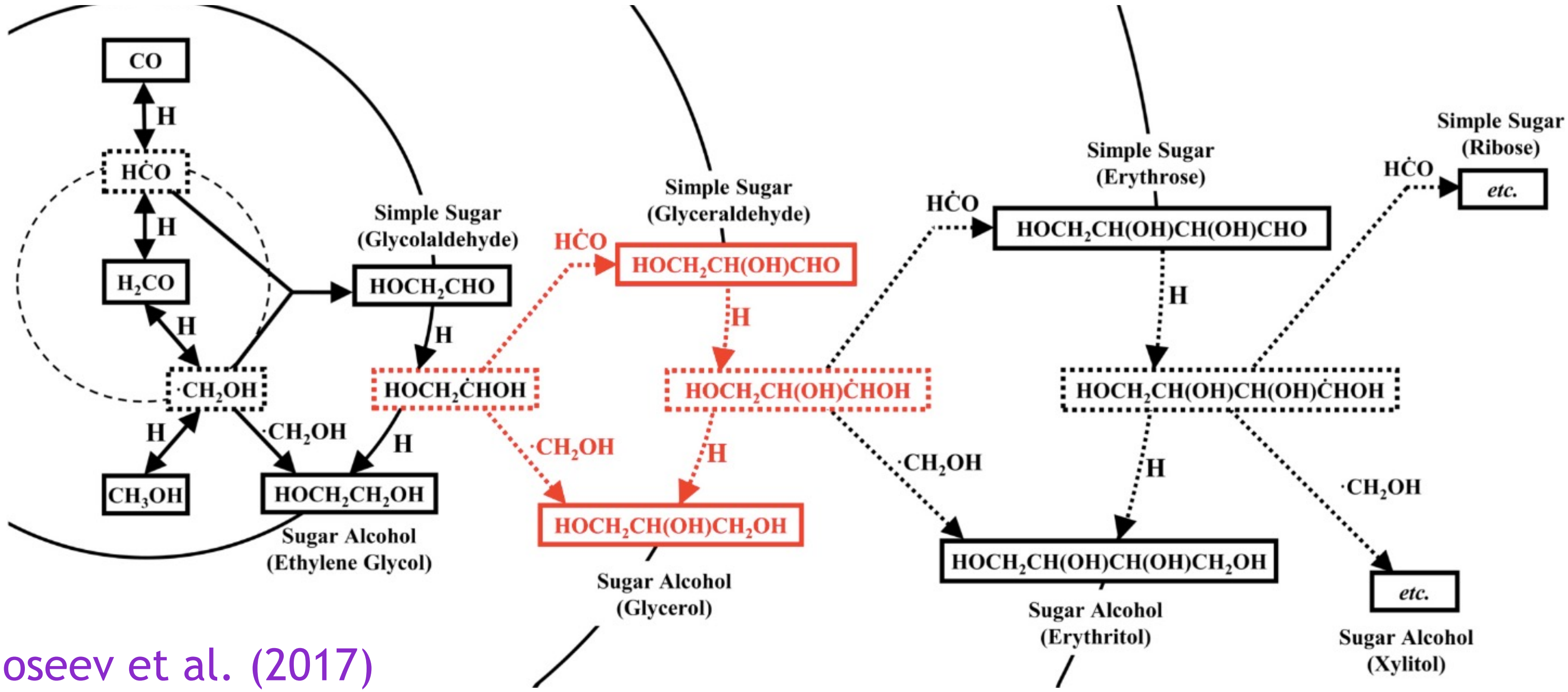


Skouteris et al. (2018)

COM formation for T<30 K

Additional mechanisms proposed:

1. Non-canonical explosions on grains (Rawlings+13; Holdship+19)
2. Cosmic-ray induced radical diffusion (Reboussin+2014)
3. Impulsive spot heating on grains by CRs (Ivlev+2015)
4. Sputtering of grains by CRs (Dartois+20; Wakelam+21)
5. Non-diffusive "in-situ" formation on grains (Chuang+20; Qasim+19; Garrod+22)



Fedoseev et al. (2017)

Complex Organic Molecules (COMs) ubiquitous in the ISM

- Star forming regions: Hot Cores and Hot Corinos
  (Hollis+2000,2004; Beltran+2009; Belloche+2016; Jorgensen+2012; Lykke+2017)

- Molecular Outflows
  (Arce+2008; Codella+2015; 2017; 2020)

- Photon-Dominated Regions
  (Guzman+2013)

- Cold Clouds Cores and Pre-stellar Cores
  (Marcelino+2007; Bacmann+2012; Vastel+2014; Jimenez-Serra+2016; Taquet+2017; Agundez+2019;McGuire+2018,2021; Cernicharo+2021)

- Galactic Center GMCs
  (Martin-Pintado+2001;Requena-Torres+2006,2008;Widicus-Weaver+2017;Zeng+2018)

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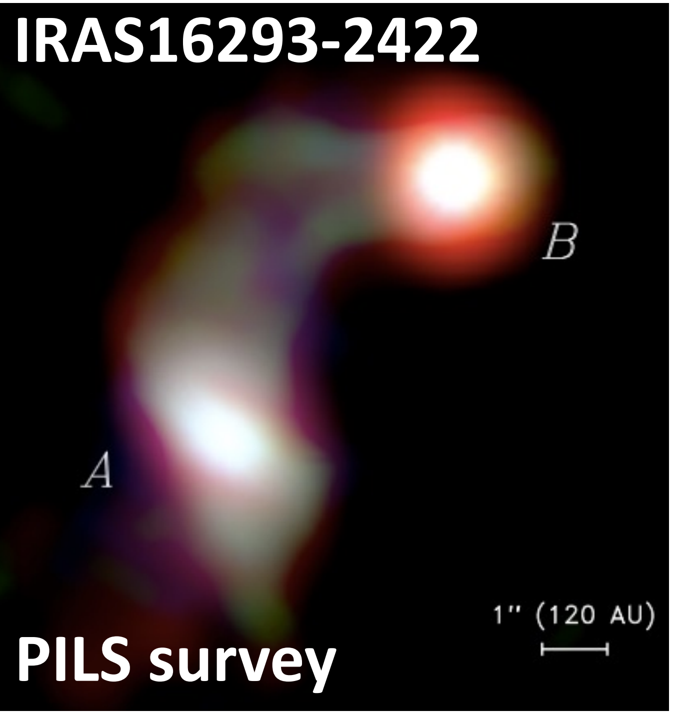
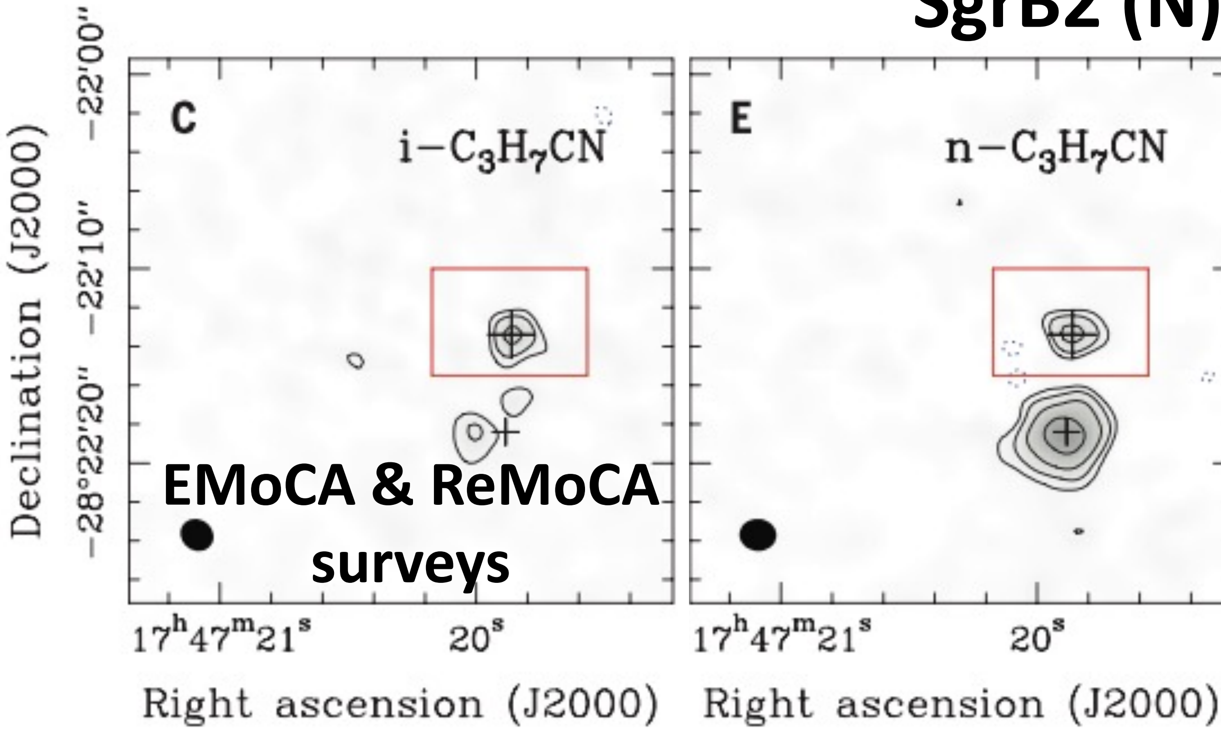
Prebiotic COMs in Hot Corinos and Hot cores (ALMA)



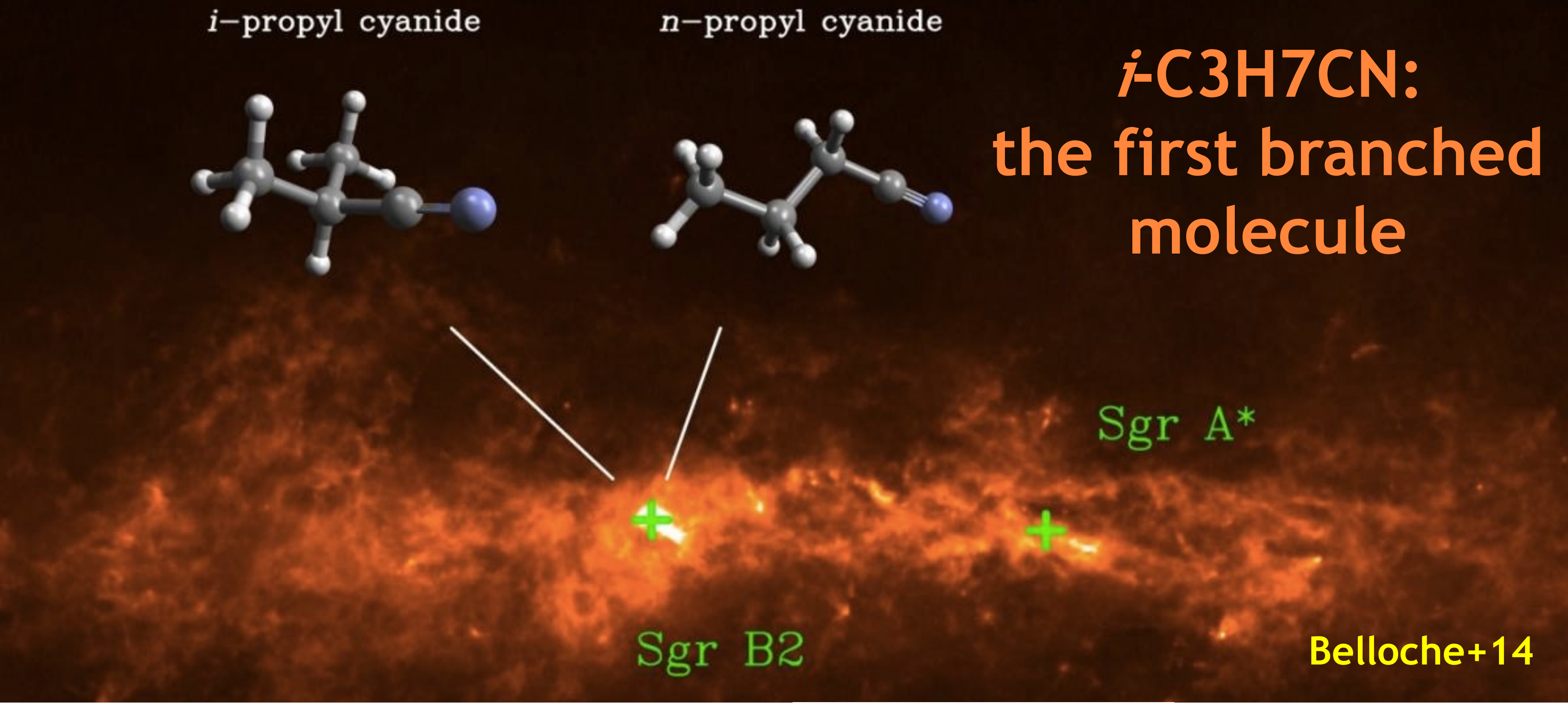
SgrB2 (N)



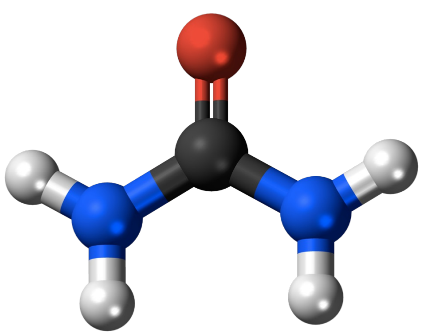
Glycolaldehyde (Jorgensen+12,16; Coutens+15; Taquet+15)
Formamide (Kahane+13; Coutens+16)
Methyl Isocyanate (Ligterink+17, Martin-Domenech+17)
Glycolonitrile (Zeng+18)
Acetamide (Ligterink+18)
Acetic Acid (Jorgensen+16)

See also the GUAPOS survey toward G31.41 (Mininni+20; Colzi+21)

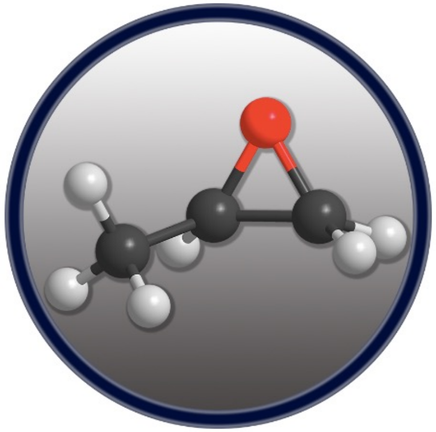
Amino acetonitrile (Belloche+08)
Iso-propyl cyanide (branched molecule)(Belloche+14)
Urea (Belloche+19)
N-methylformamide (Belloche+17)



Urea:
a key
prebiotic
molecule
(Belloche+19)



Urea
(NH_2CONH_2)



Propylene Oxide
(CH_3CHCH_2O)

Propylene
Oxide:
A chiral
molecule
(McGuire+16)

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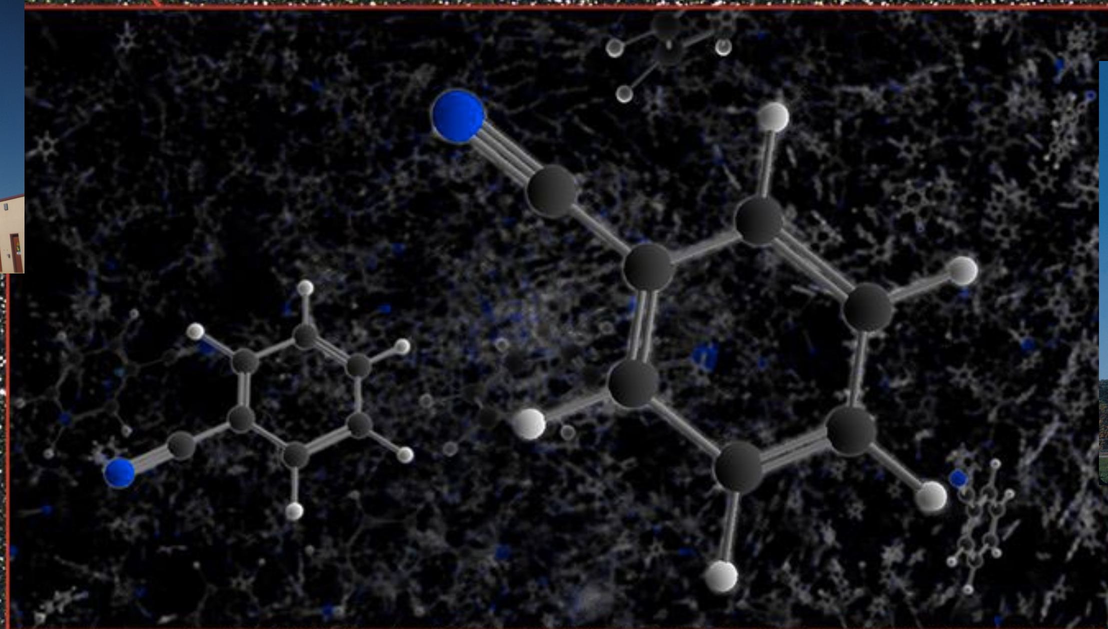
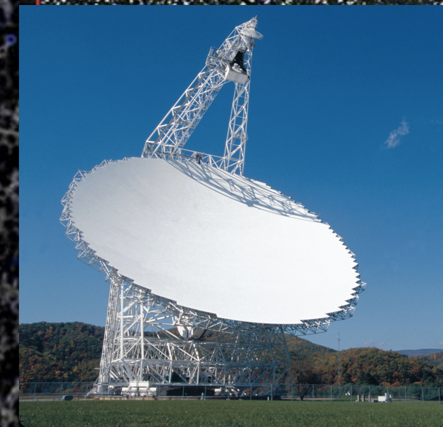
Aromatic Molecules in TMC-1

Yebes 40m
QUIJOTE
(Cernicharo's group)

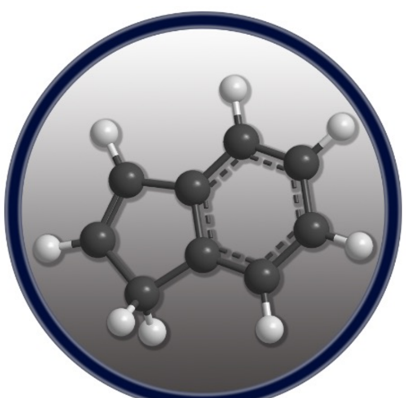


McGuire+18

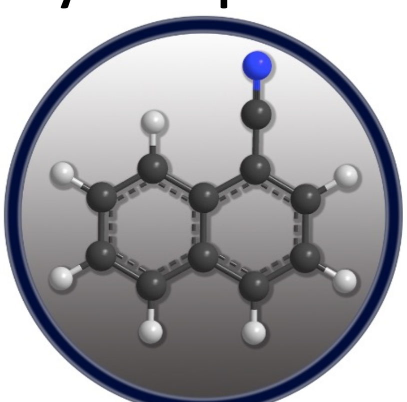


GBT
GOTHAM
(McGuire's group)

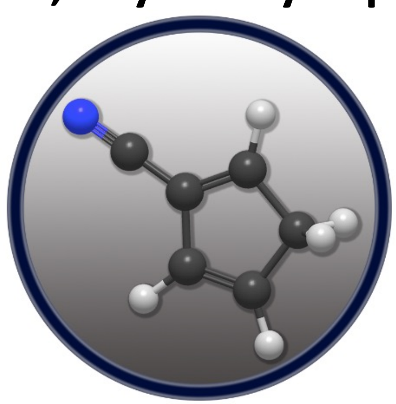
Indene



1,2-cyanonaphtalene



1,2-cyano-cyclopentadiene



Burkhardt+21; Mcguire+21; Cernicharo+21a,b,c,d,e; Lee+21; McCarthy+21; Agundez+21; Marcelino+21; Cabezas+21

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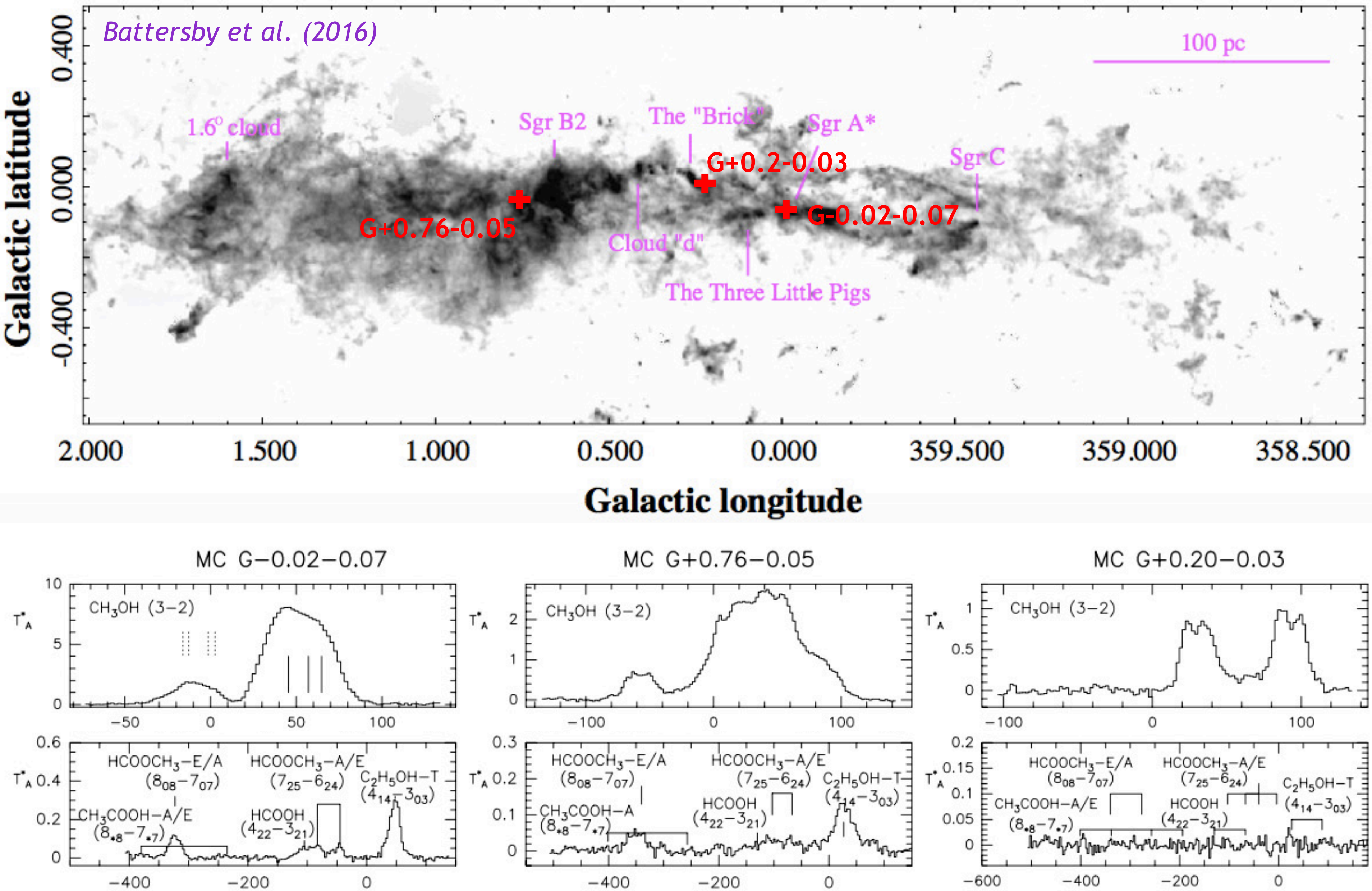
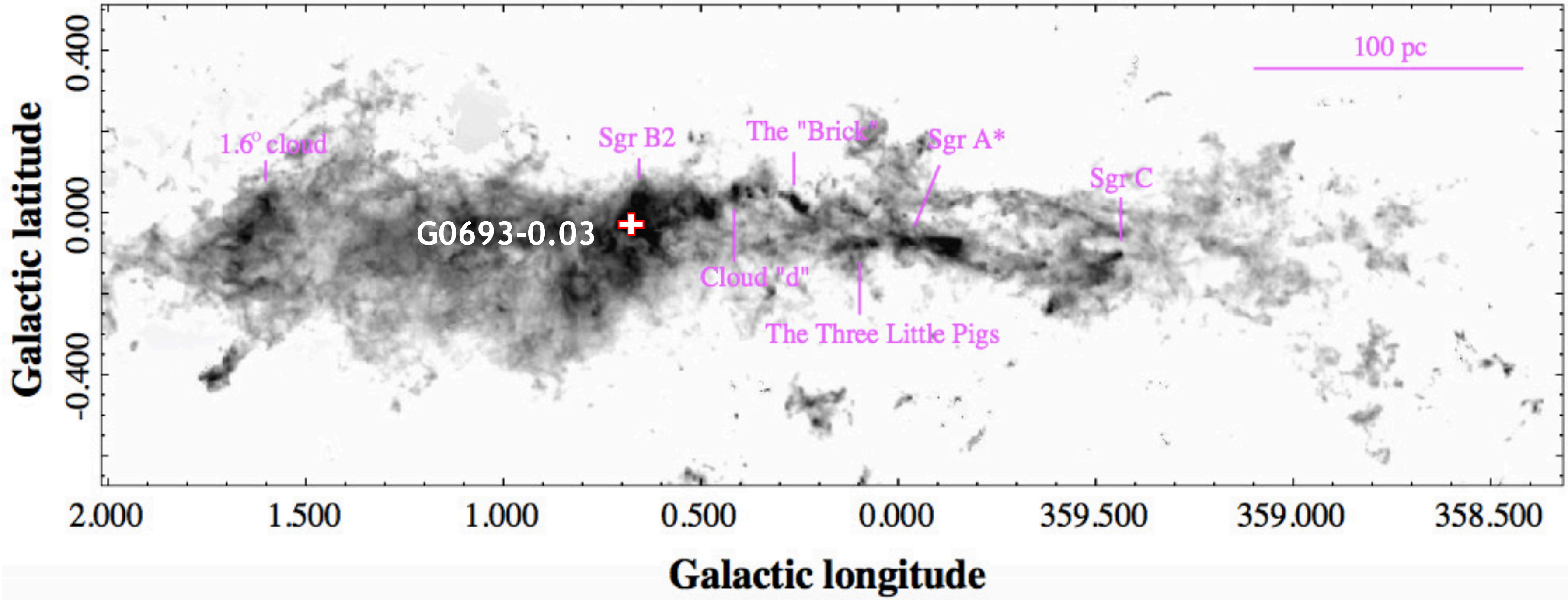
  (Martin-Pintado+2001;Requena-Torres+2006,2008;Widicus-Weaver+2017;Zeng+2018)

Widespread COM emission in the Galactic Center



Martin-Pintado et al. (2001); Requena-Torres et al. (2006,2008); Zeng et al. (2018)

G+0.693-0.03

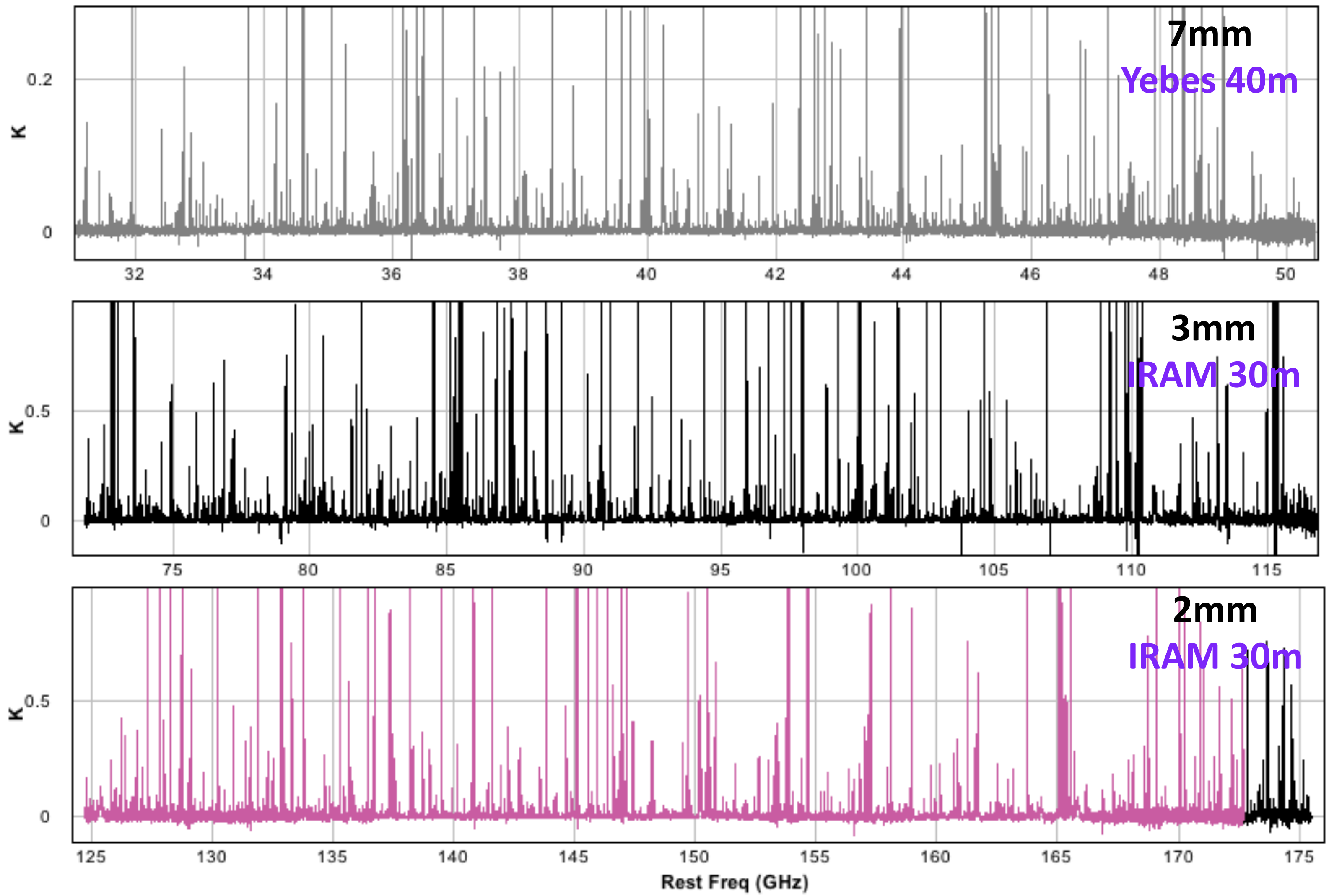


Quiescent (no sign of star-formation) and its chemistry affected by a cloud-cloud collision

(Hasegawa+94;Sato+00; Tsuboi+15; Wu+17; Zeng+20; Armijos-Abendaño+20)

- $n(H_2)$~$4x10^4$ cm^{-3}
- T_{dust}<20 K
- T_{gas}>100 K
- Low T_{ex} of the molecular gas (<15 K).
- *Huge advantage for COM searches in "crowded" spectral surveys*

Surveys with IRAM 30m & Yebes 40m



>170 species detected --- >50% of them are COMs

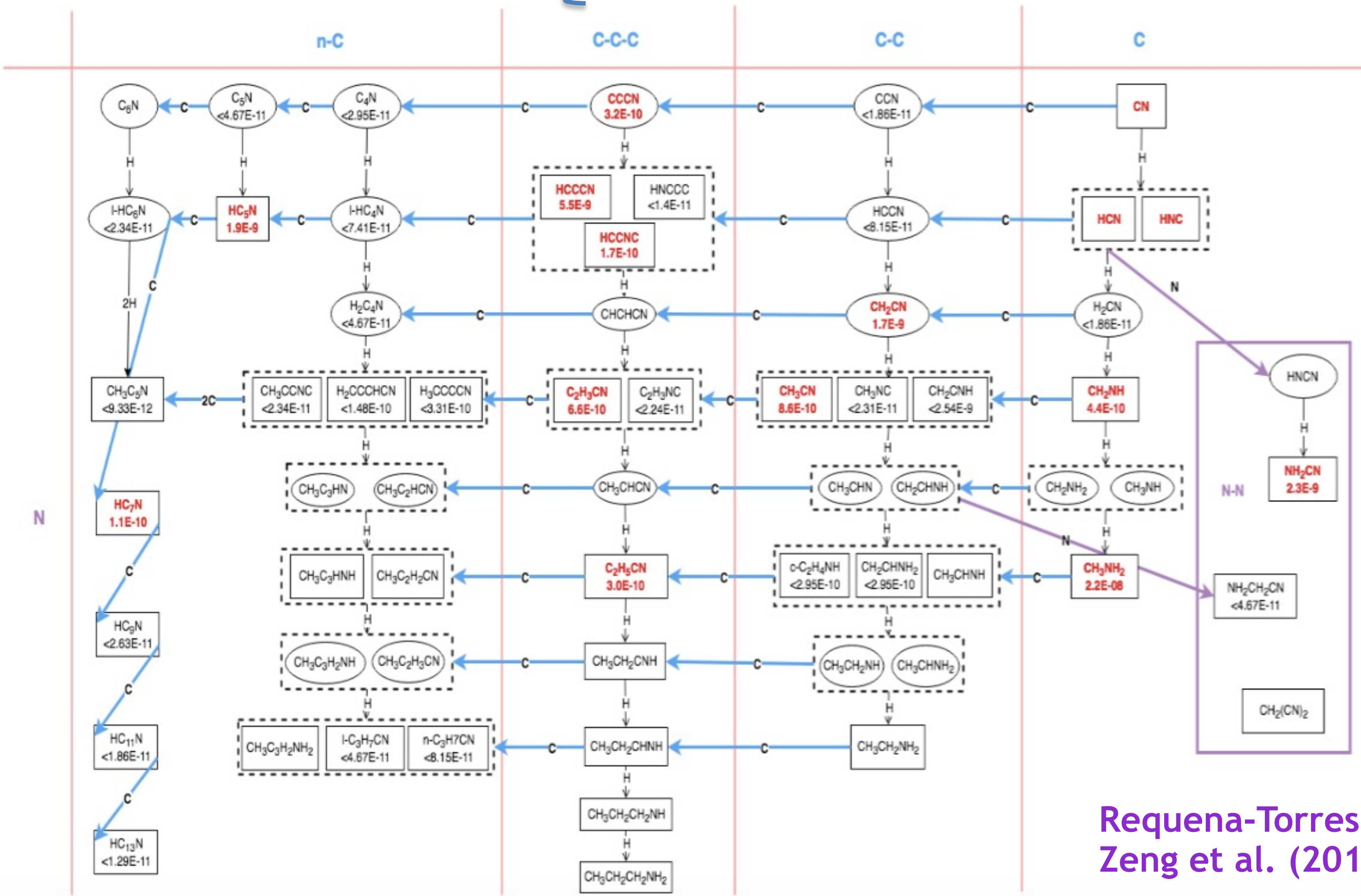
One of the most important reservoirs of COMs in the Galaxy

(Requena-Torres et al. 2008; Widicus-Weaver et al. 2017; Zeng et al. 2018)

Chemical Inventory in G+0.693-0.03

Rich in COMs with:

1) *Oxygen (-OH, -OCHO, -COOH)*
2) *Nitrogen (-CN and -NH/NH_2)*
3) *Sulfur (including -SH)*



Requena-Torres et al. (2008)
Zeng et al. (2018)

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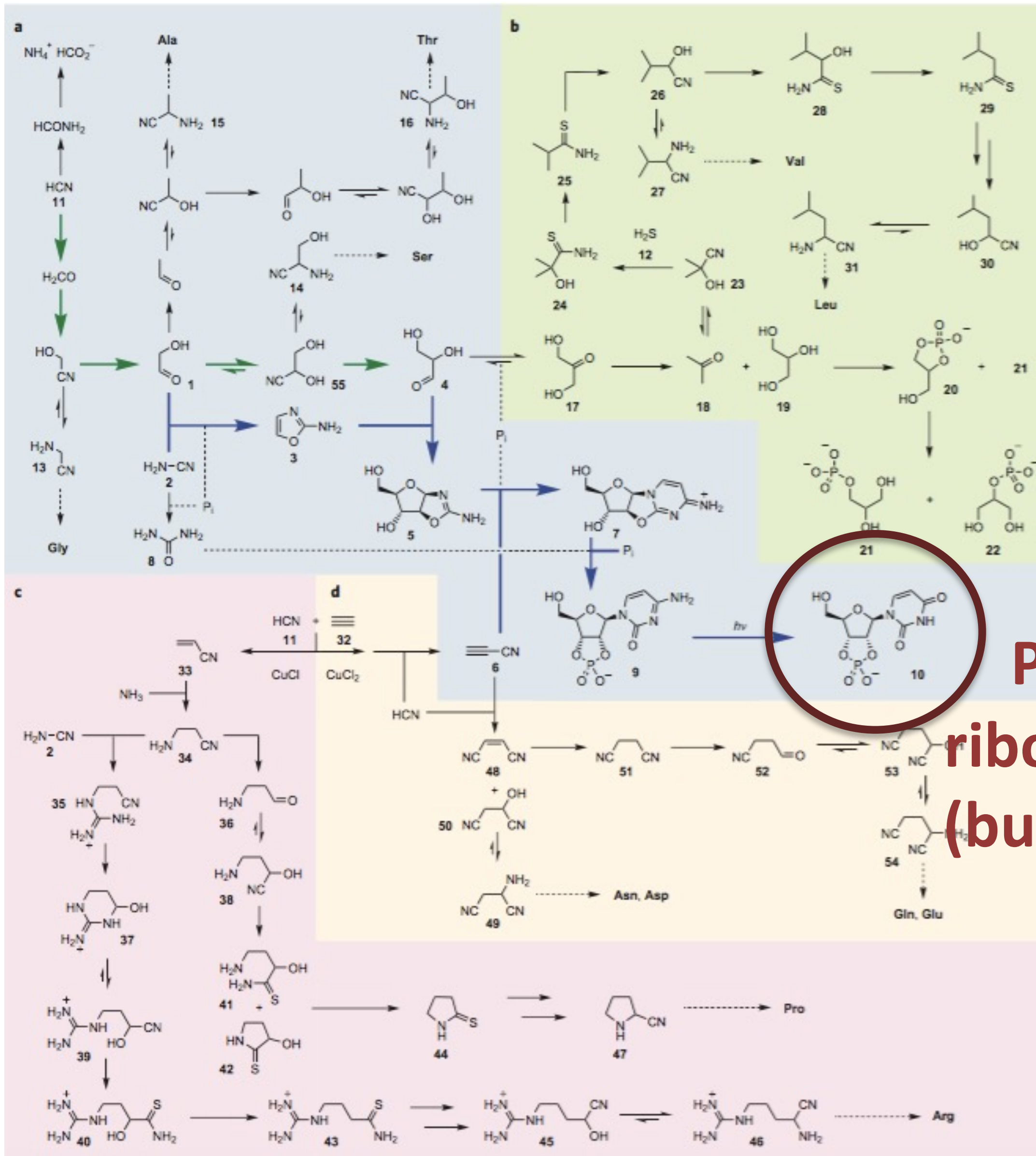
Toward the RNA-world in the ISM

Primordial RNA-world chemical scheme (Powner+2009; Patel+2015)

RNA Precursors

Sugars & Lipid precursors



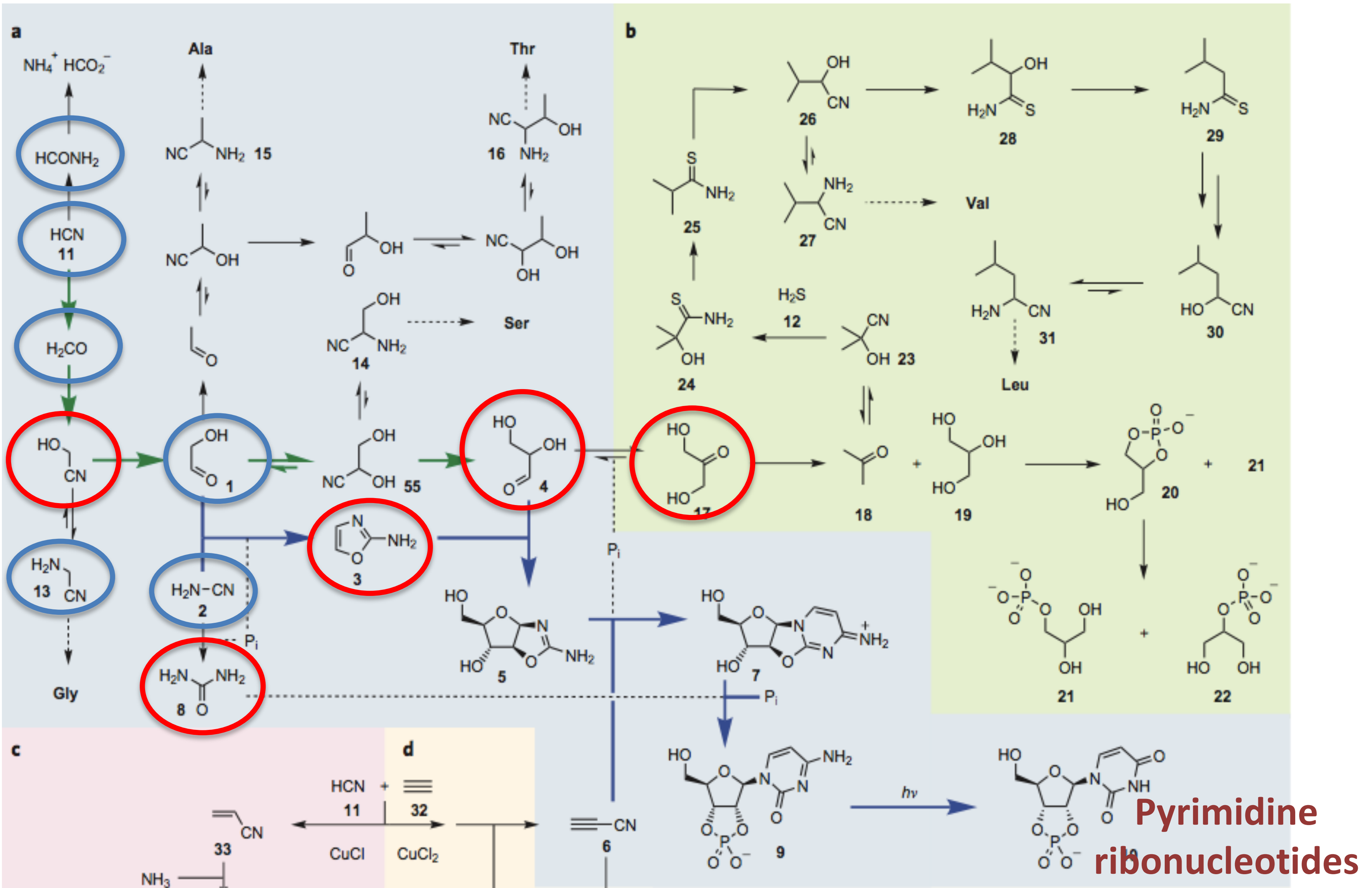
Pyrimidine ribonucleotides (building blocks of RNA)

Amino Acids

Toward the RNA world in the ISM

Urea, 2-amino-oxazole, glyceraldehyde & dihydroxyacetone

Patel et al. (2015)



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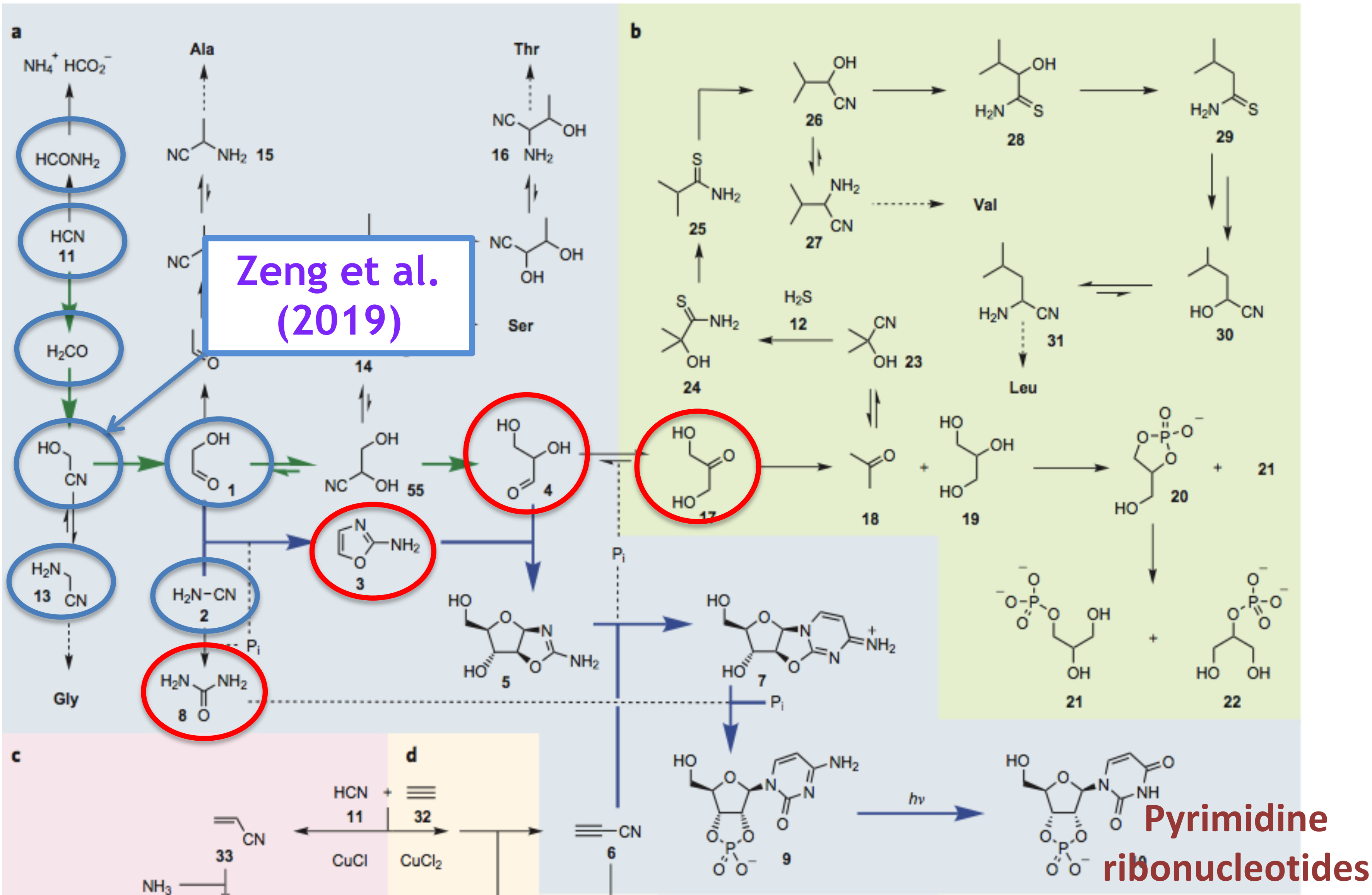
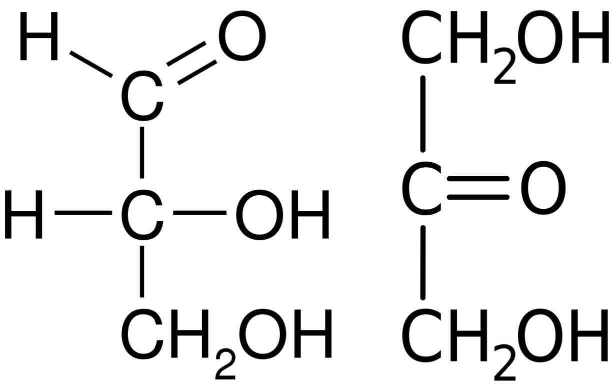


Toward the RNA world in G+0.693

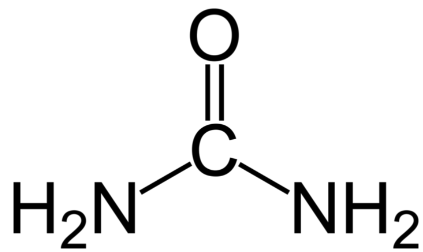
glyceraldehyde
&
dihydroxyacetone



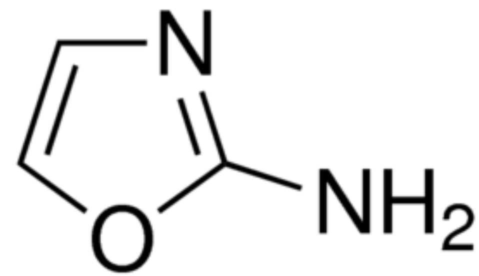
Upper limits
$\chi < (0.5\text{-}1.0)\times10^{-10}$

Consistent with previous searches by Apponi+06

Urea



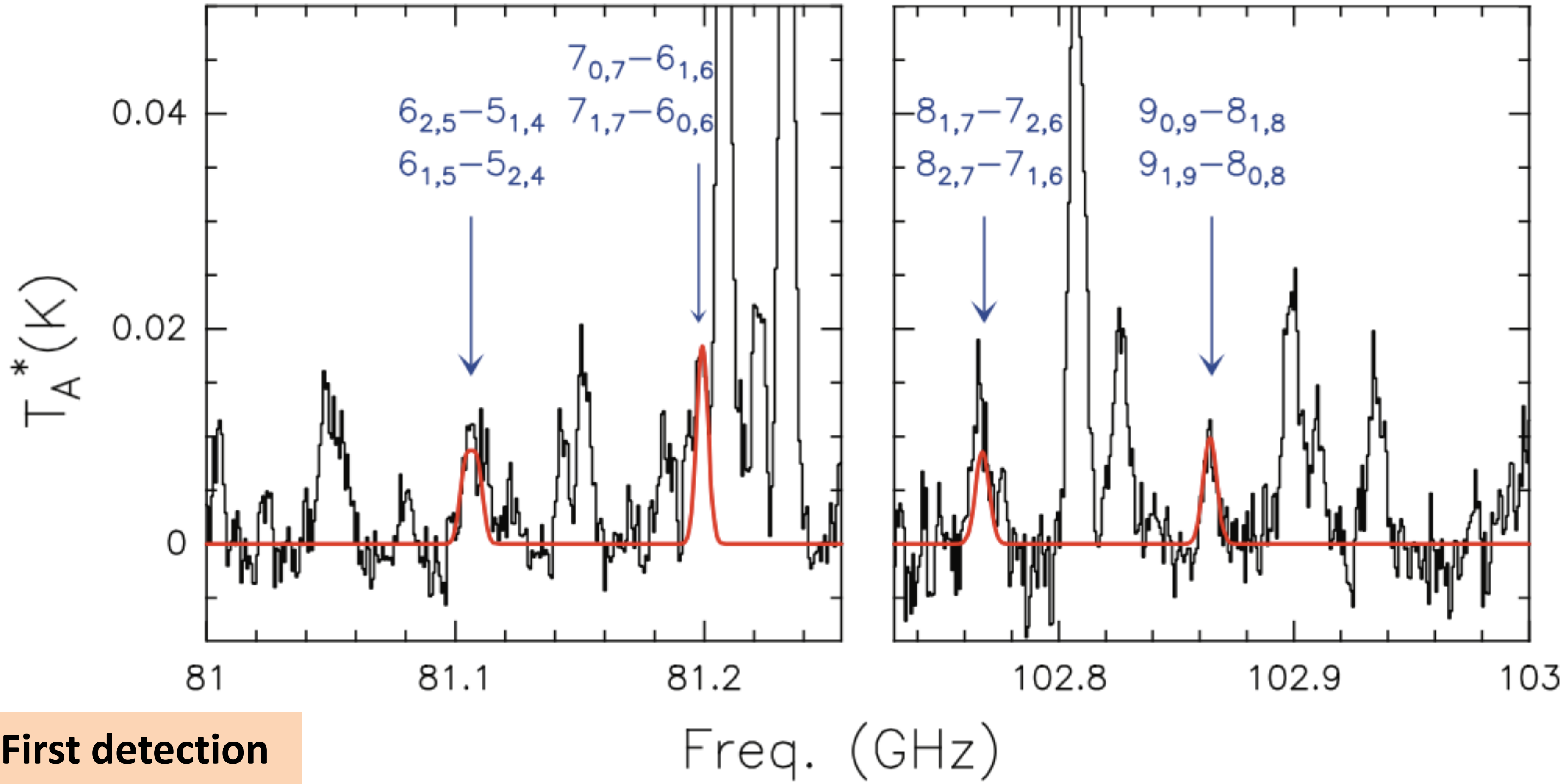
2-amino-oxazole



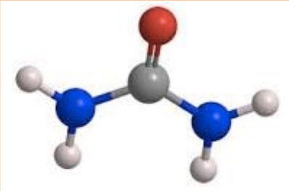
Jimenez-Serra+(2020), Astrobiology, 20, 7

Urea (NH_2CONH_2) in G+0.693-0.027

Jimenez-Serra+(2020)



First detection of urea in ISM by Belloche+19

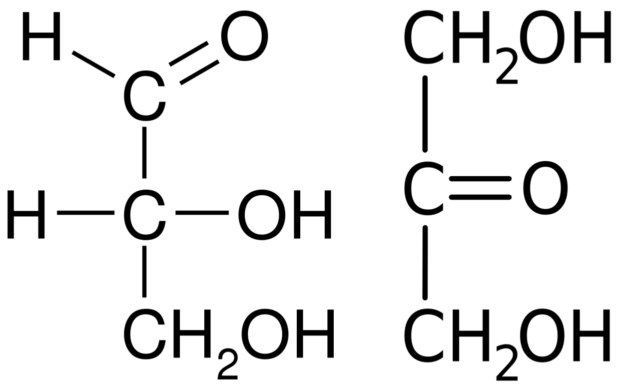


N (NH_2CONH_2) = $(6.3\pm0.1)\times10^{12}$ cm^{-2}

X (NH_2CONH_2) = 4.7×10^{-11} wrt molecular H_2

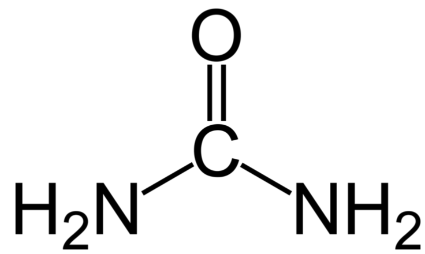
Toward the RNA world in G+0.693

glyceraldehyde
&
dihydroxyacetone



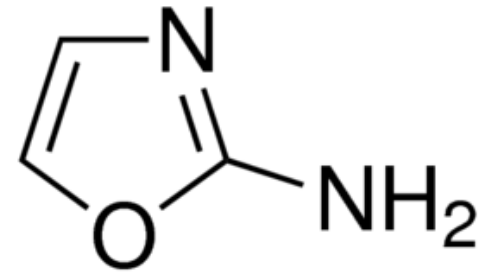
Upper limits
$\chi < (0.5\text{-}1.0)\times10^{-10}$

Urea



Detected
$X \sim 5\times10^{-11}$

2-amino-oxazole

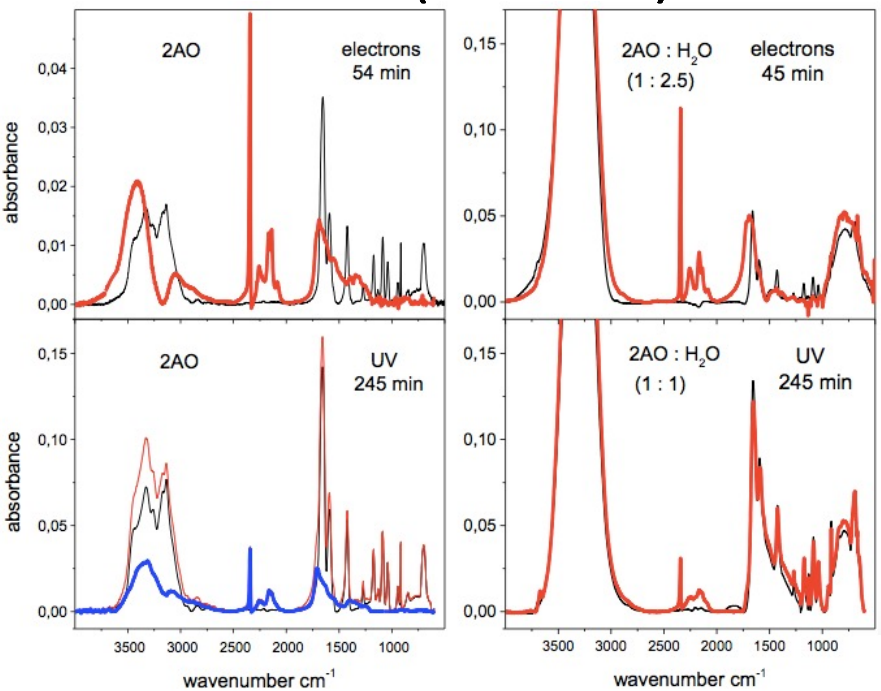


Upper limits
$\chi < 8.0\times10^{-11}$

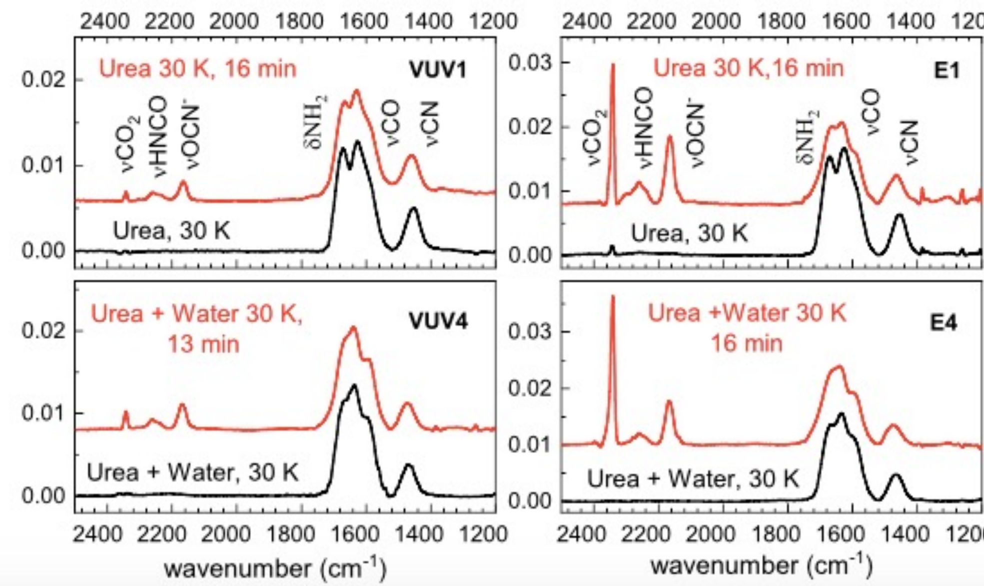
Jimenez-Serra+(2020), Astrobiology, 20, 7

Energetic processing of urea and 2-aminooxazole

2-amino-oxazole (Mate+2021)



Urea (Herrero+2022)

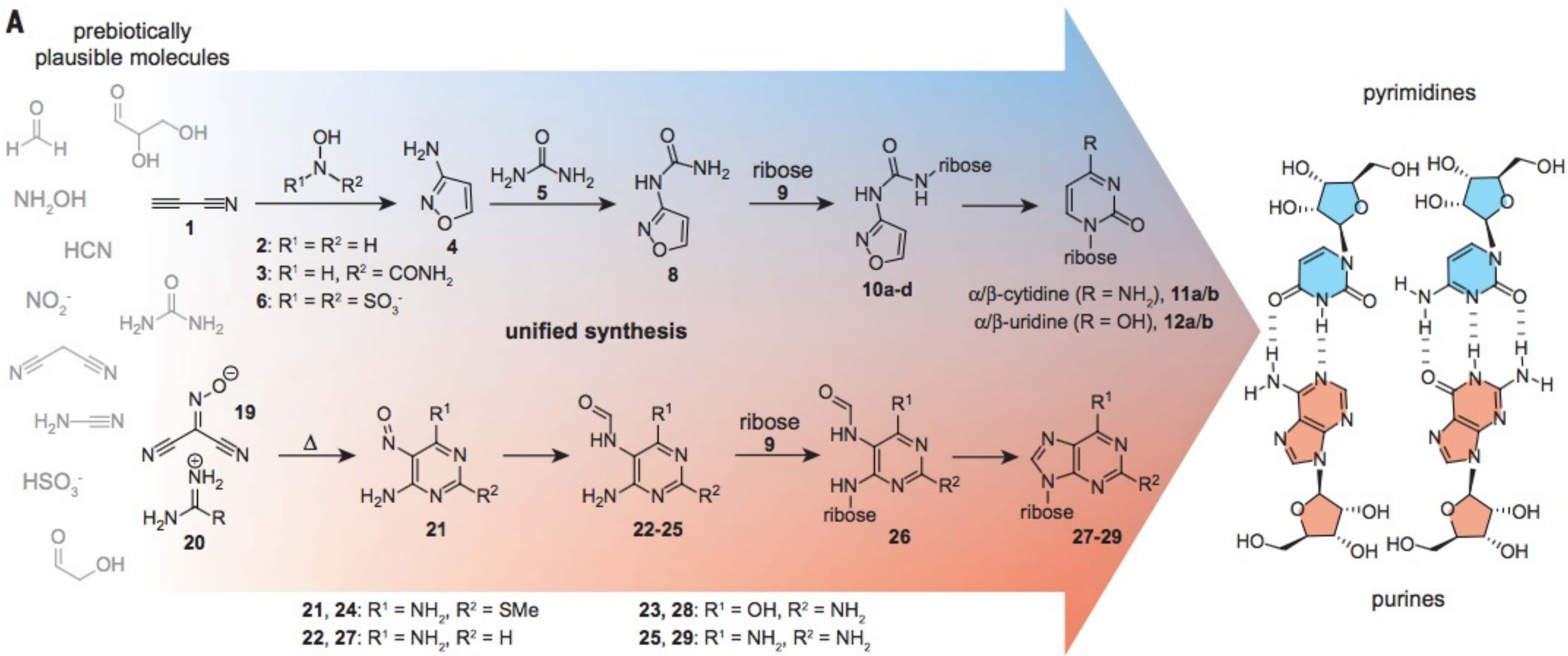


Ices of pure 2AO/urea and of 2AO/urea:H_2O mixes irradiated with UV photons and e-'s simulating CRs

-> *photo-destruction rates*

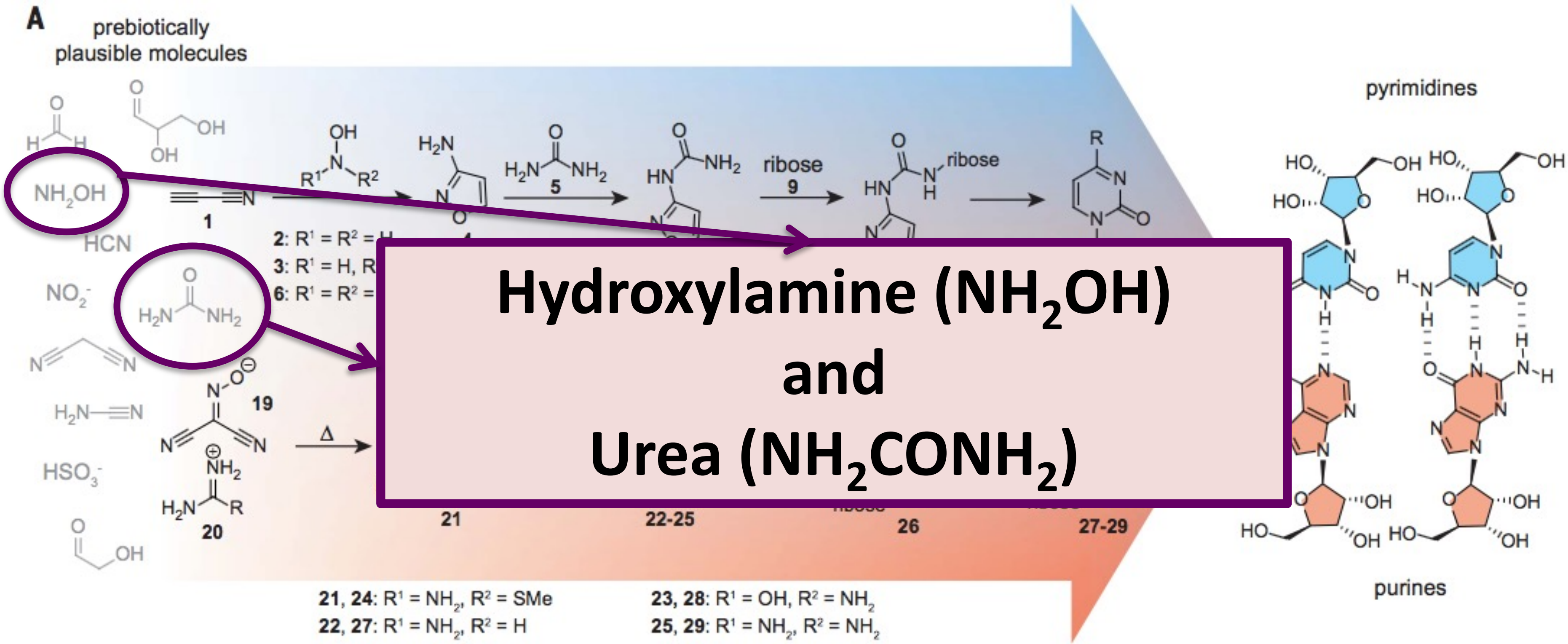
Urea is more resilient to irradiation than 2-amino-oxazole

The primordial RNA-world hypothesis



Concurrent formation of all four RNA ribonucleotides (pyrimidine AND purine)
Becker et al. (2019, Science, 366, 6461)

The primordial RNA-world hypothesis

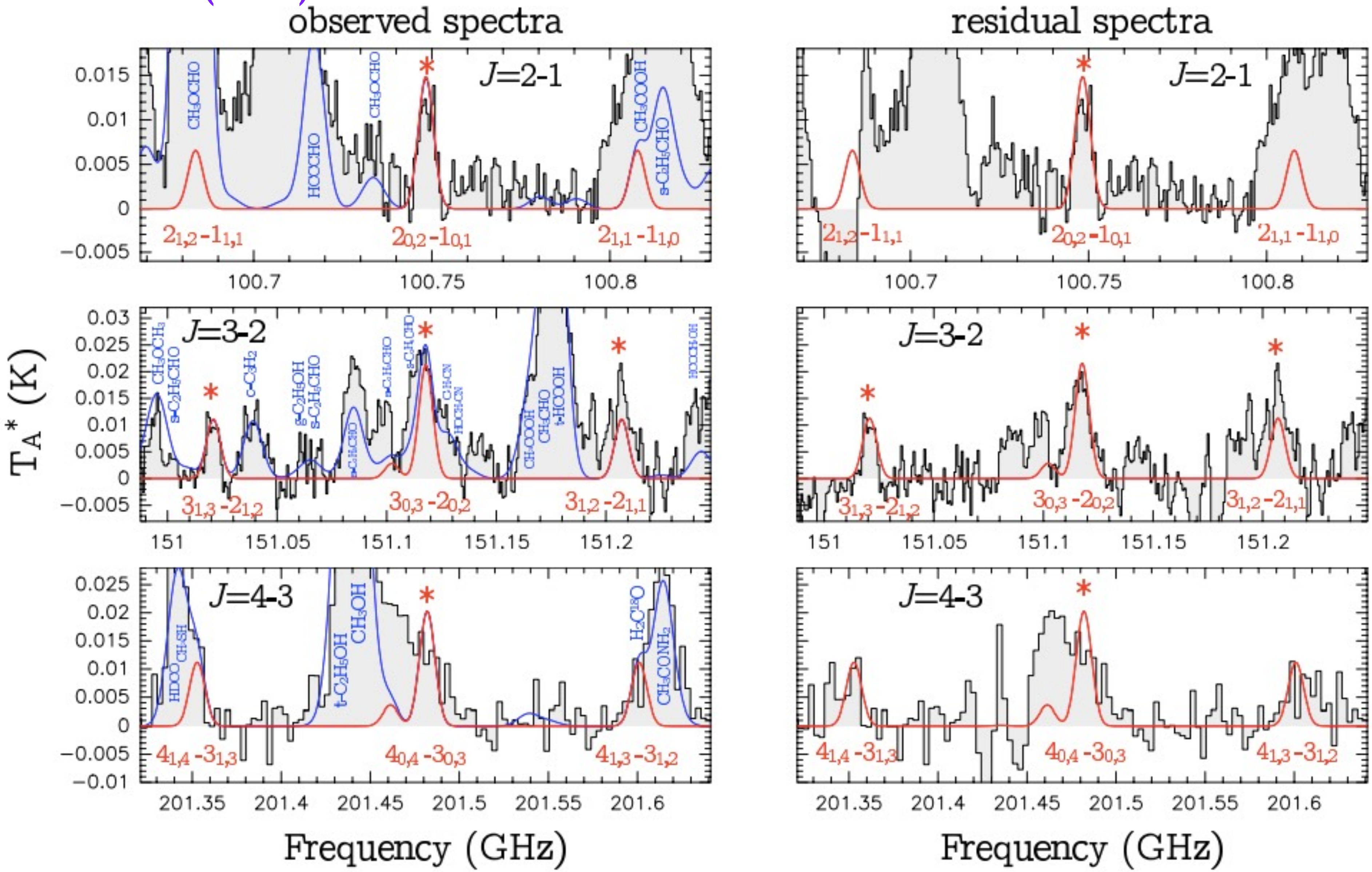


Hydroxylamine (NH_2OH)
and
Urea (NH_2CONH_2)

Concurrent formation of all four RNA ribonucleotides (pyrimidine AND purine)
Becker et al. (2019, Science, 366, 6461)

Discovery of NH_2OH in the ISM

Rivilla et al. (2020)

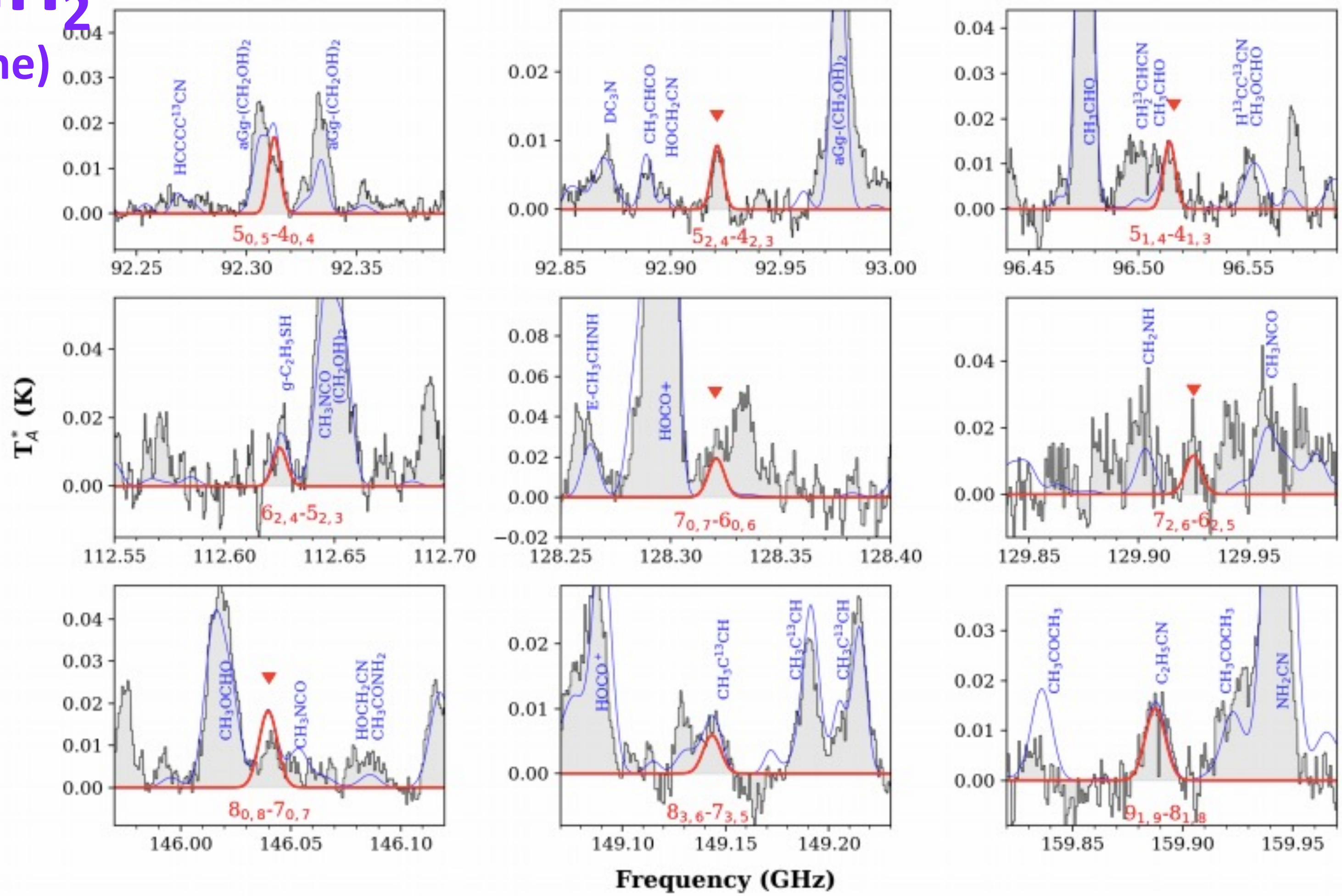


Probing the chemical complexity of amines in the ISM: detection of vinylamine ($C_2H_3NH_2$) and tentative detection of ethylamine ($C_2H_5NH_2$)

Shaoshan Zeng,[1] Izaskun Jiménez-Serra,[2] Víctor M. Rivilla,[2,3] Jesús Martín-Pintado,[2] Lucas F. Rodríguez-Almeida,[2] Belén Tercero,[4] Pablo de Vicente,[4] Fernando Rico-Villas,[2] Laura Colzi,[2,3] Sergio Martín,[5,6] and Miguel A. Requena-Torres[7,8]

$C_2H_3NH_2$ (vinyl amine)

Zeng et al. (2021)

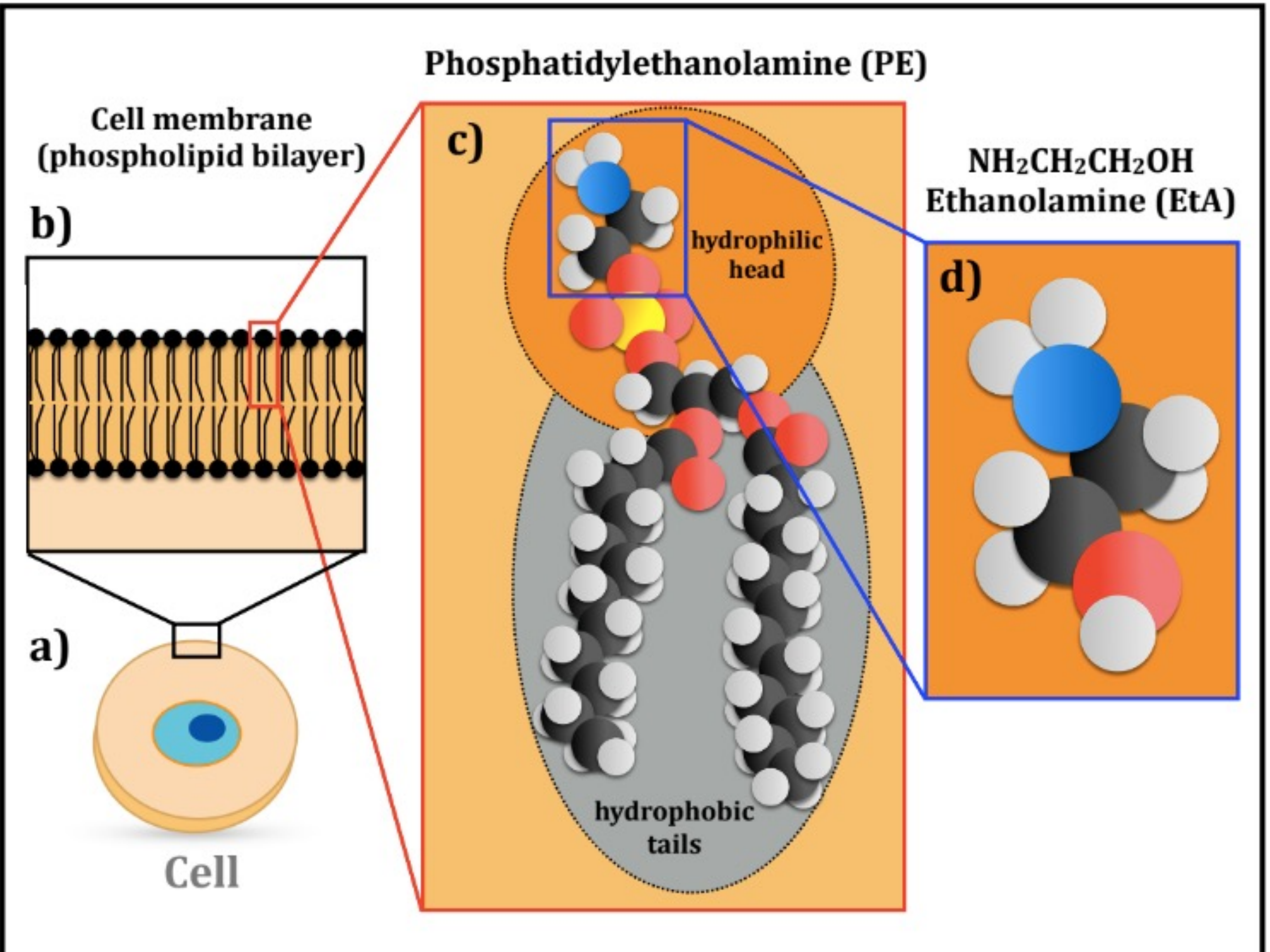


While $C_2H_5NH_2$ likely forms on grains, $C_2H_3NH_2$ is a product of the recombination dissociation of $C_2H_5NH_2$ + H^+/H_3^+

Discovery of the simplest phospholipid head group

Rivilla, Jimenez-Serra et al. (2021), PNAS, 118, 22

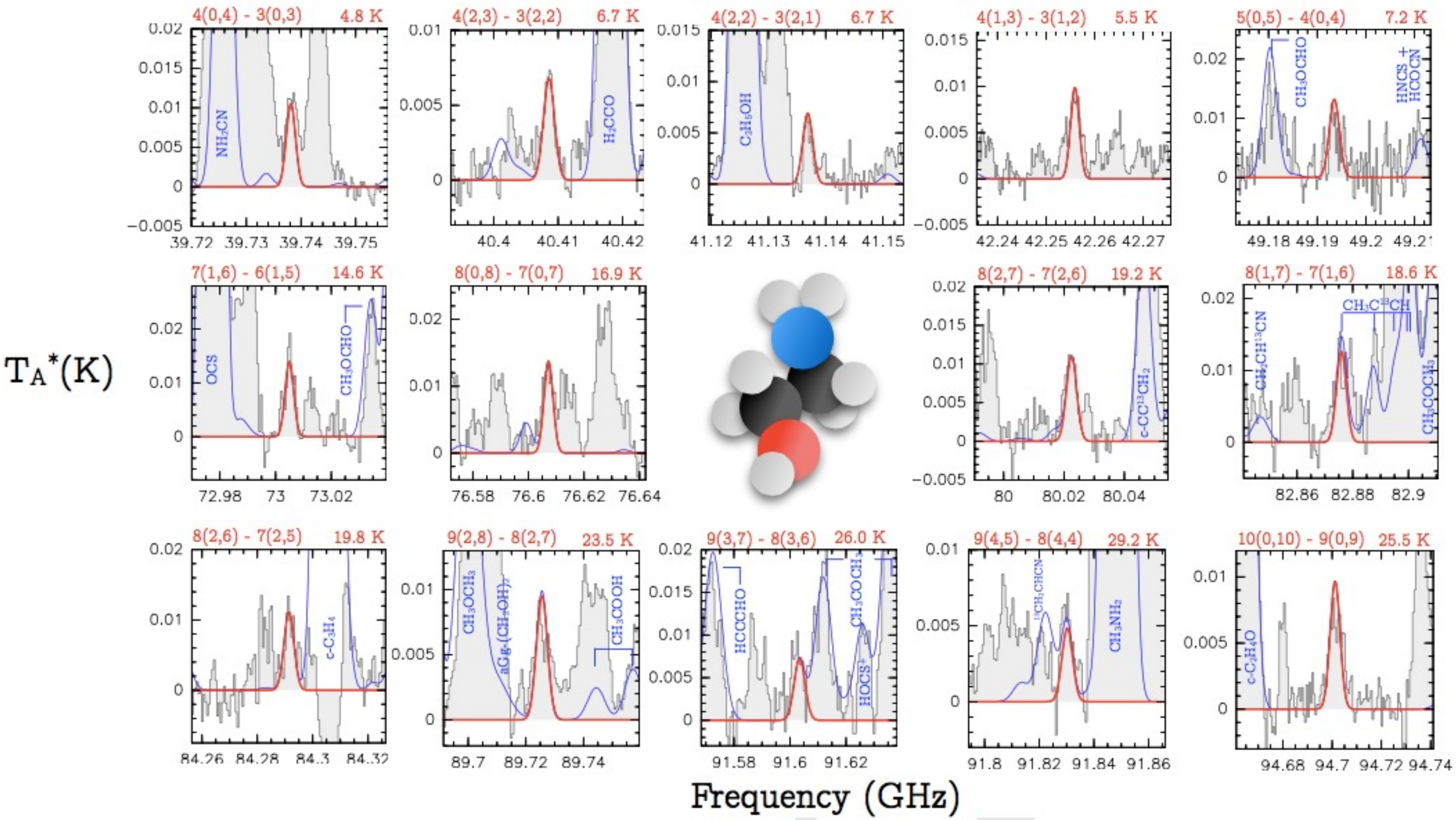
$NH_2CH_2CH_2OH$ (Ethanolamine)



χ(EtA) ~ 10^{-10}

EtA/H_2O ratio consistent with the one measured in the Almahata Sitta meteorite

Discovery of the simplest phospholipid head group

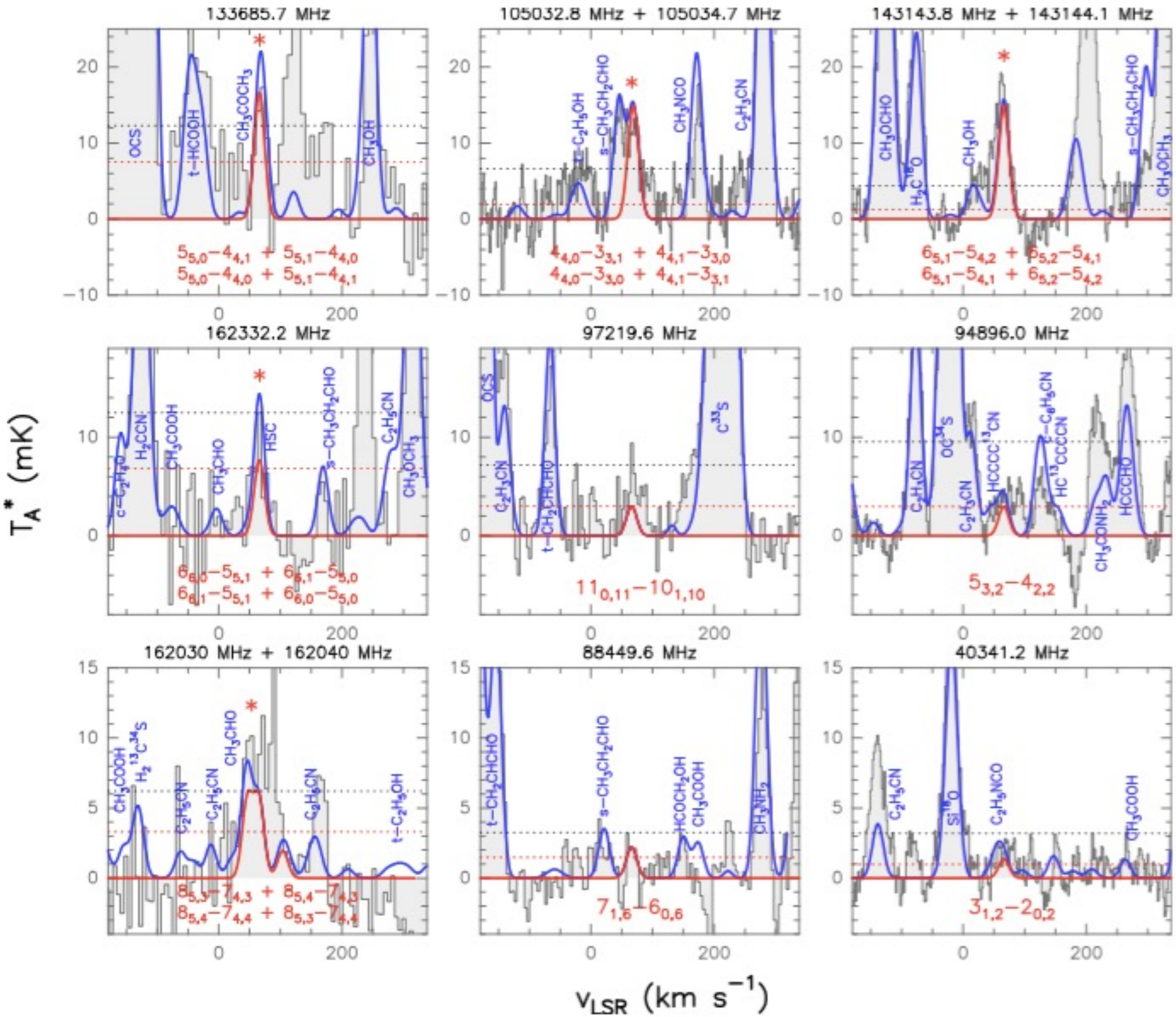


~10^{15} liters of EtA (i.e. Victoria Lake's capacity) could have arrived to Earth

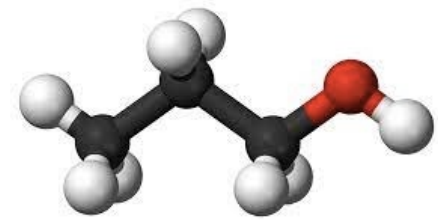
Possibility of EtA being available in early Earth for cell membrane formation

Precursors of fatty alcohols: n-propanol

Jimenez-Serra et al. (2022), A&A, 663, A181



n-C_3H_7OH



Ga and Aa conformers detected

X(n-propanol) ~ 3-4x10^{-10}

Vinyl alcohol (s and a forms) also detected

Ultrasensitive unbiased spectral survey towards G+0.693-0.027

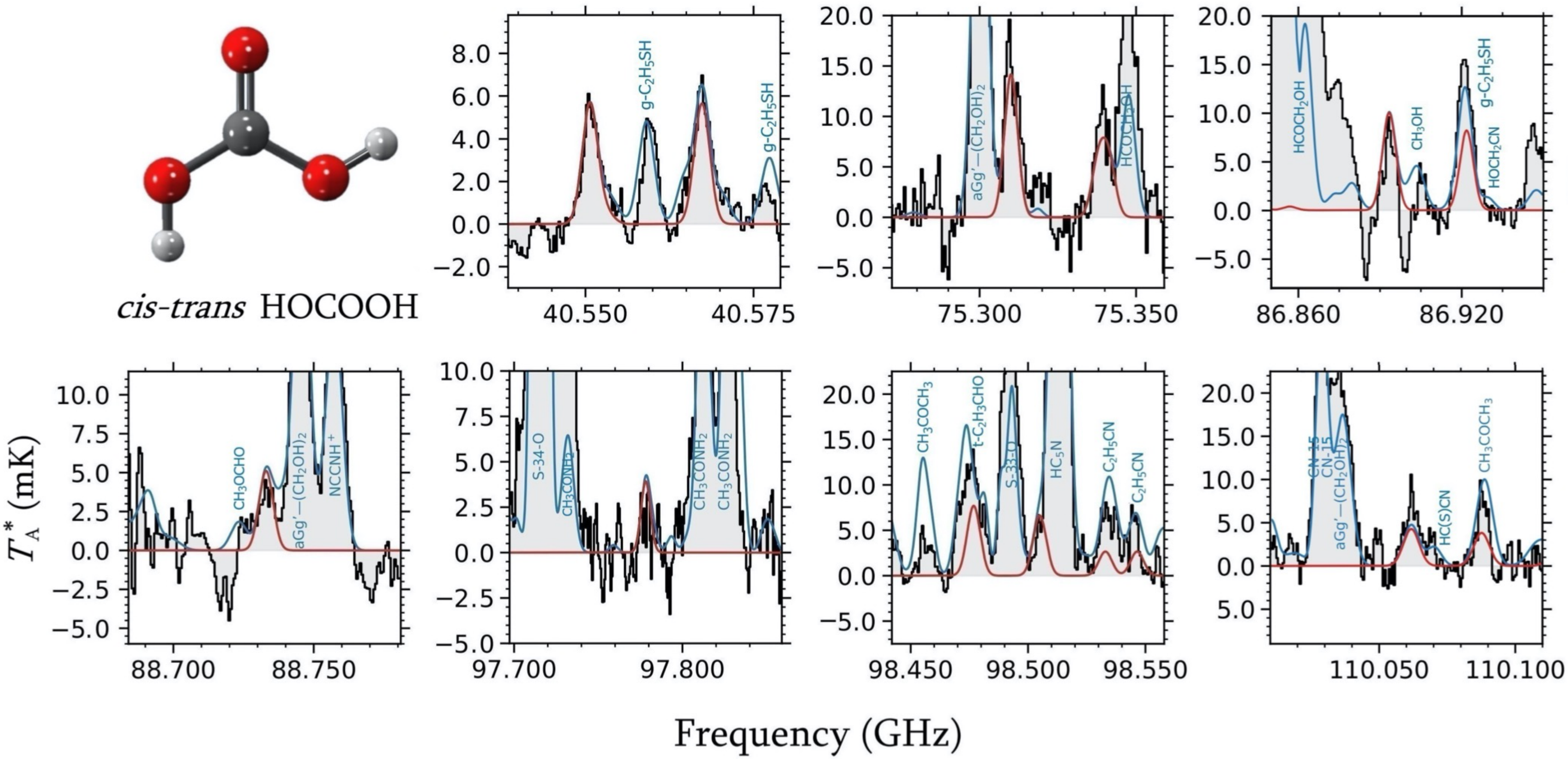
Yebes 40m
(Spain)

IRAM 30m
(Spain)

achieved RMS at sub-mk level

Carbonic acid (HOCOOH)

(Sanz-Novo et al. 2023)

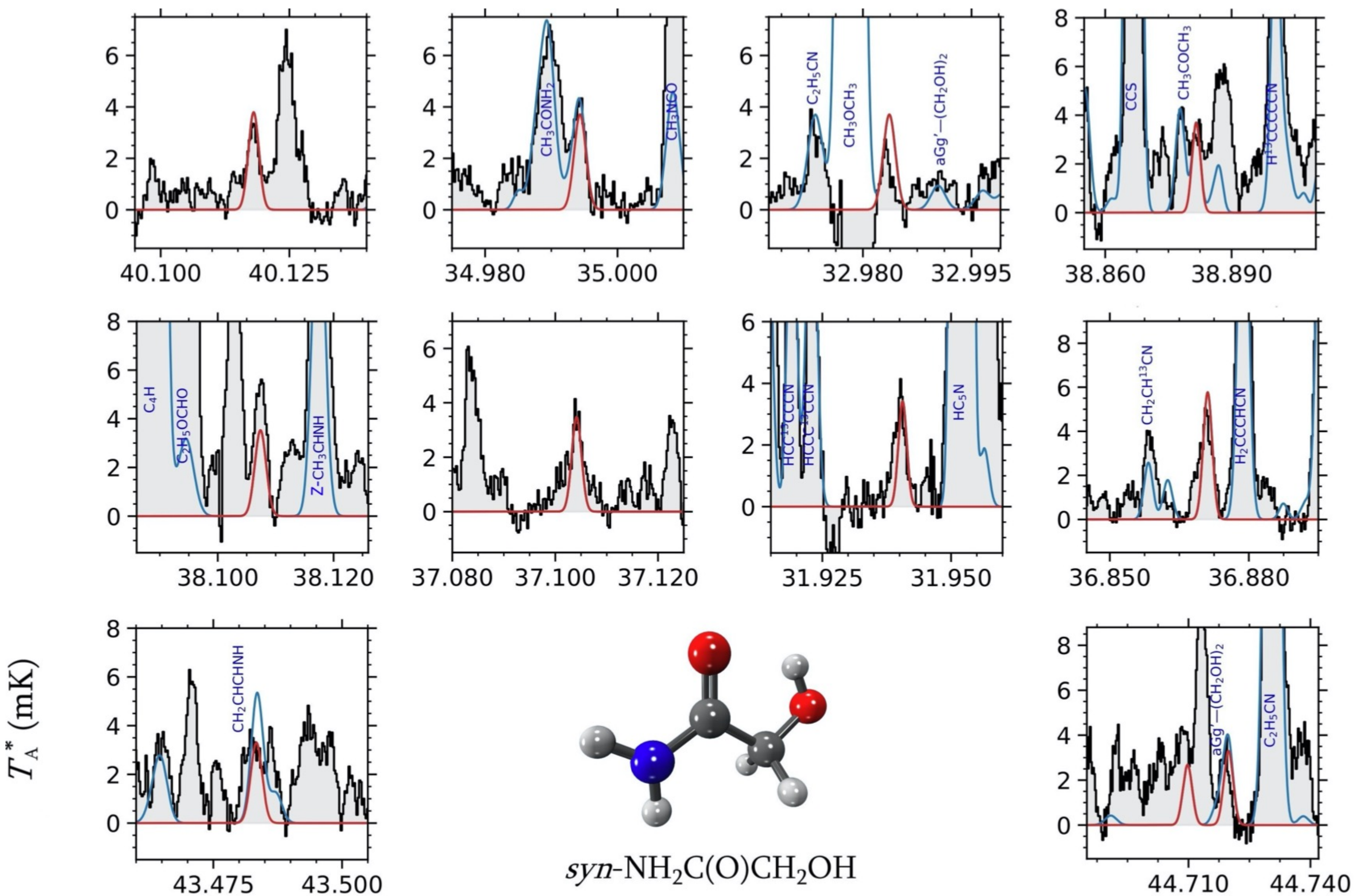


Despite being higher in energy, *only the cis-trans conformer detected* *(χ(HOCOOH) ~ 4.7x10^{-11} with respect to H_2)*

Cis-cis conf. (the lowest in energy) has a dipole moment 10 x smaller

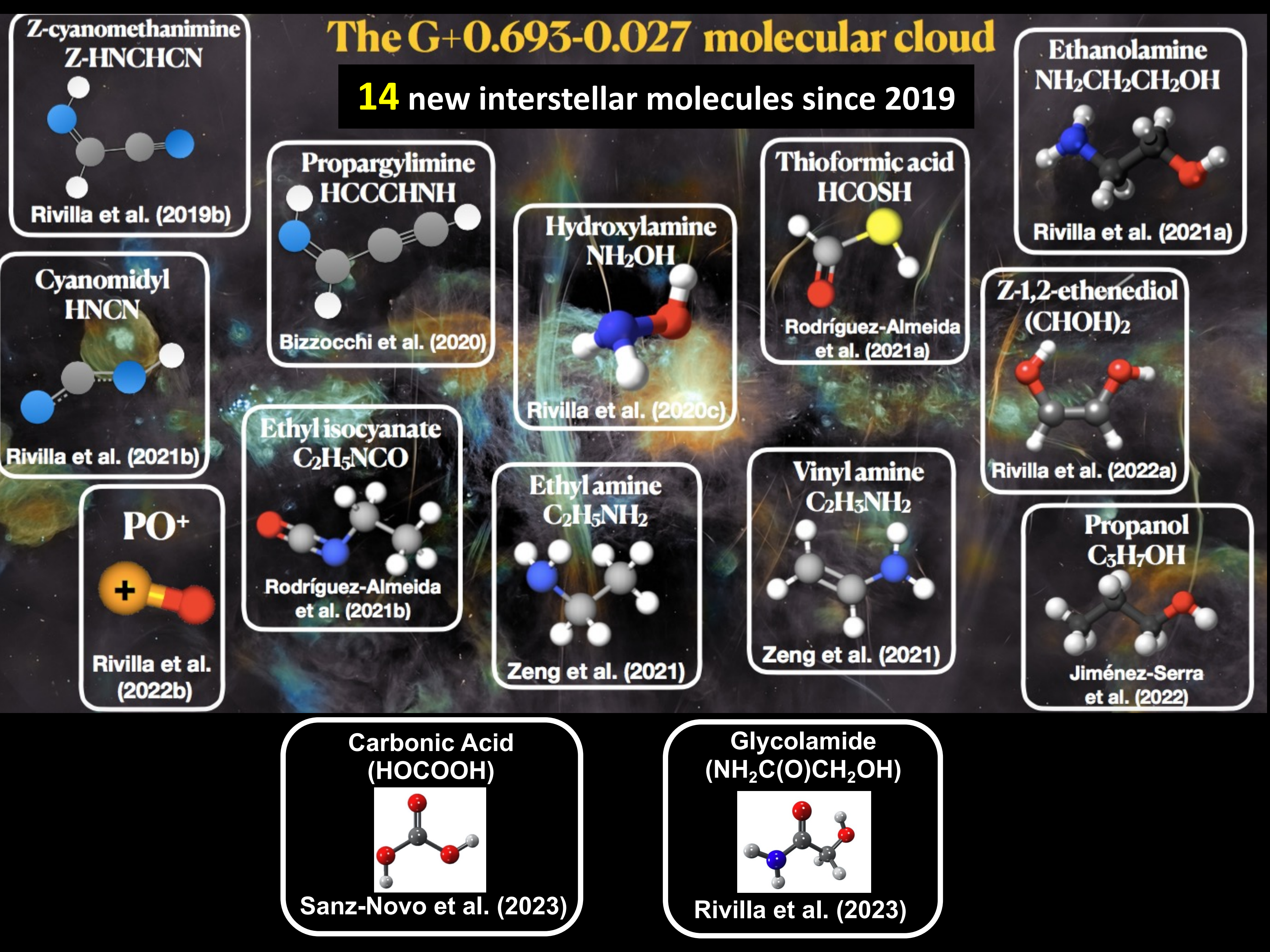
Glycolamide ($NH_2C(O)CH_2OH$): an isomer of glycine detected in the ISM

(Rivilla et al. 2023)



χ(Glycolamide) ~ 5.5×10^{-11} with respect to H_2

(G+0.693 rich in amides; see Zeng et al. 2023)



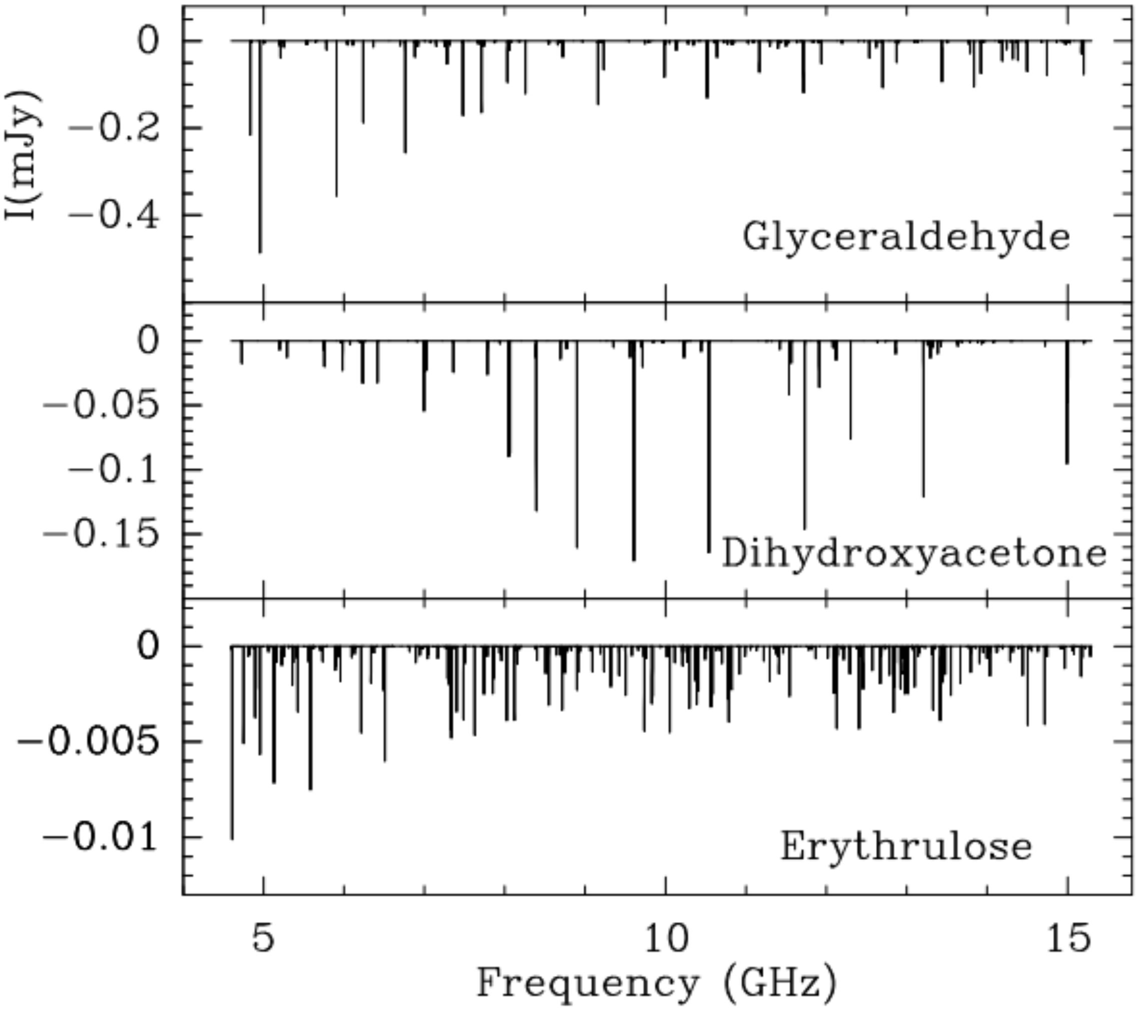
The G+0.693-0.027 molecular cloud
14 new interstellar molecules since 2019
Z-cyanomethanimine
Z-HNCHCN
Rivilla et al. (2019b)
Propargylimine
HCCCHNH
Bizzocchi et al. (2020)
Hydroxylamine
NH_2OH
Rivilla et al. (2020c)
Thioformic acid
HCOSH
Rodríguez-Almeida et al. (2021a)
Ethanolamine
$NH_2CH_2CH_2OH$
Rivilla et al. (2021a)
Cyanomidyl
HNCN
Rivilla et al. (2021b)
Z-1,2-ethenediol
$(CHOH)_2$
Rivilla et al. (2022a)
Ethyl isocyanate
C_2H_5NCO
Rodríguez-Almeida et al. (2021b)
Ethyl amine
$C_2H_5NH_2$
Zeng et al. (2021)
Vinyl amine
$C_2H_3NH_2$
Zeng et al. (2021)
PO^+
+
Rivilla et al. (2022b)
Propanol
C_3H_7OH
Jiménez-Serra et al. (2022)
Carbonic Acid
(HOCOOH)
Sanz-Novo et al. (2023)
Glycolamide
$(NH_2C(O)CH_2OH)$
Rivilla et al. (2023)

What is next?

- Perform even deeper spectroscopic surveys in the Q band (30-50 GHz)
- Spectroscopic surveys at low frequencies against a bright background continuum source

Prebiotic COM searches in absorption

Feasibility study for C3 and C4 sugars with SKA



Extended COM-rich GMC

(G+0.693)

Bright HII region (L source)

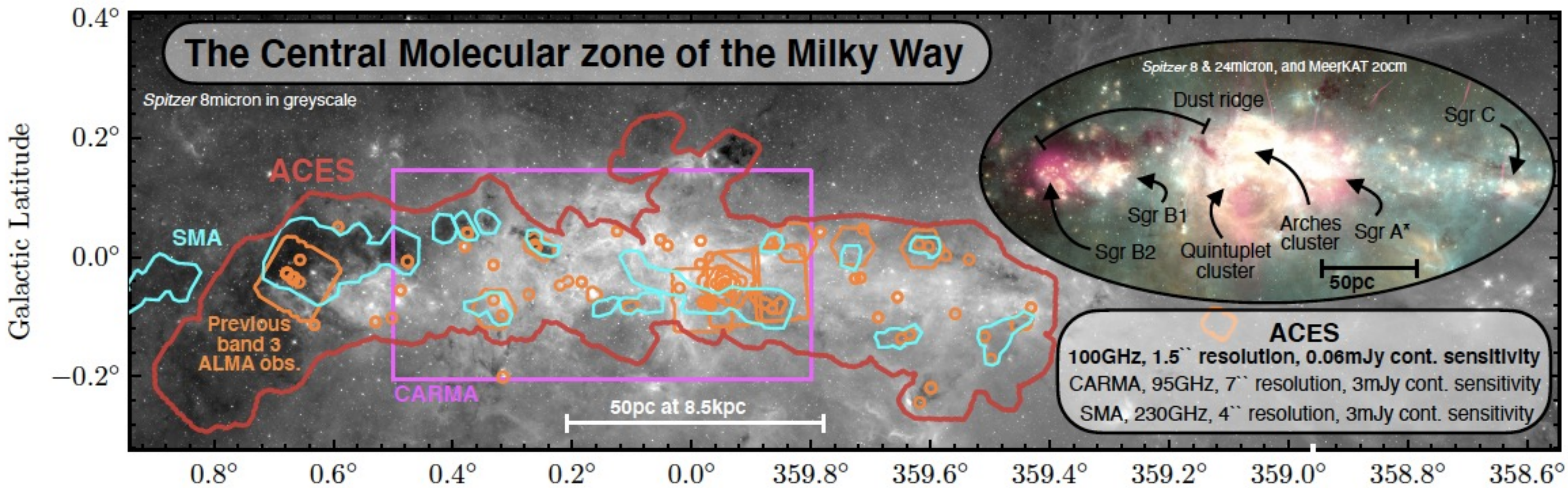
$$T_L = (T_{ex} - T_c - T_{bg}) \times [1 - exp(-\tau_\nu)]$$

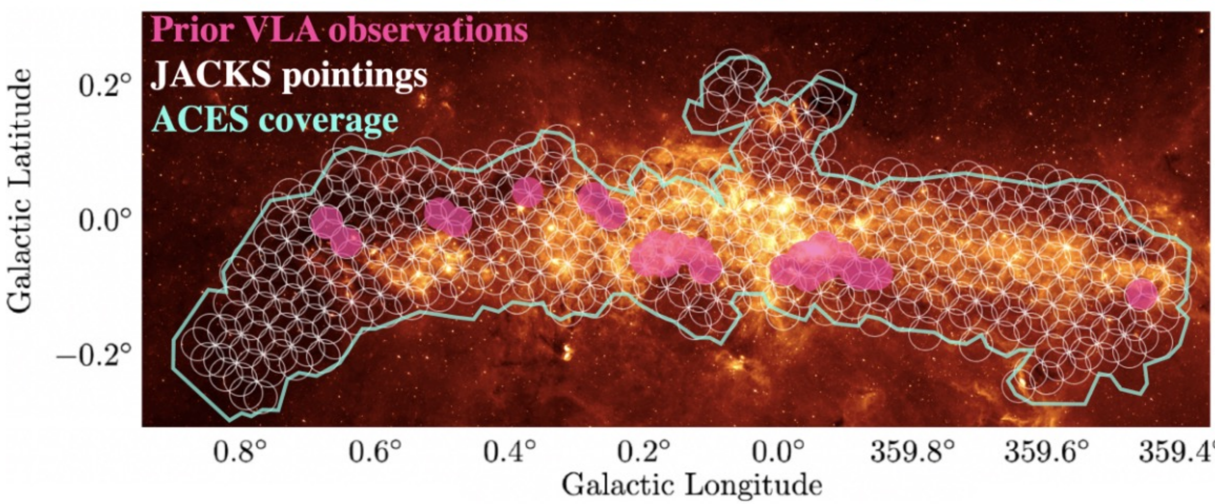
Predictions obtained for SKA Band 5, but transitions in the Q band expected to be >10x brighter

Jimenez-Serra et al. (2022)

Prebiotic COM searches in absorption

ACES: ALMA Central Molecular Zone Exploration Survey (PI: S. Longmore)





ACES ALMA (>1000 hrs):

dense gas rich in COMs

JACKS JVLA (~100 hrs):

radio continuum sources

JACKS: A JVLA Ammonia CMZ K-band Survey (PI: E. Mills)

Outline:

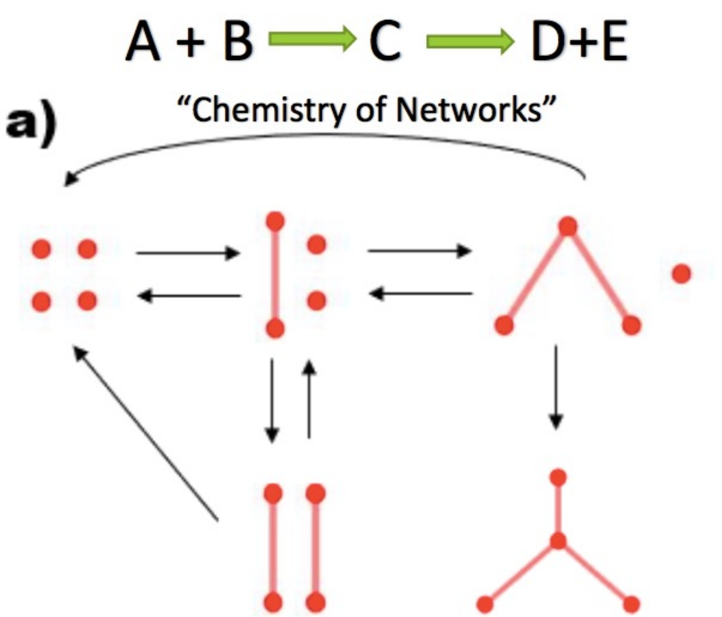
- Complex Organic Molecules (COMs): How do they form and where are they found?
- Search of COMs of prebiotic interest in the ISM
- **Emergence of interstellar chemical complexity explained by Complex Network Theory**

PNAS RESEARCH ARTICLE | PHYSICS
BIOPHYSICS AND COMPUTATIONAL BIOLOGY
2022

The emergence of interstellar molecular complexity explained by interacting networks

Miguel García-Sánchez[a,b,c], Izaskun Jiménez-Serra[a], Fernando Puente-Sánchez[d], and Jacobo Aguirre[a,c,1]

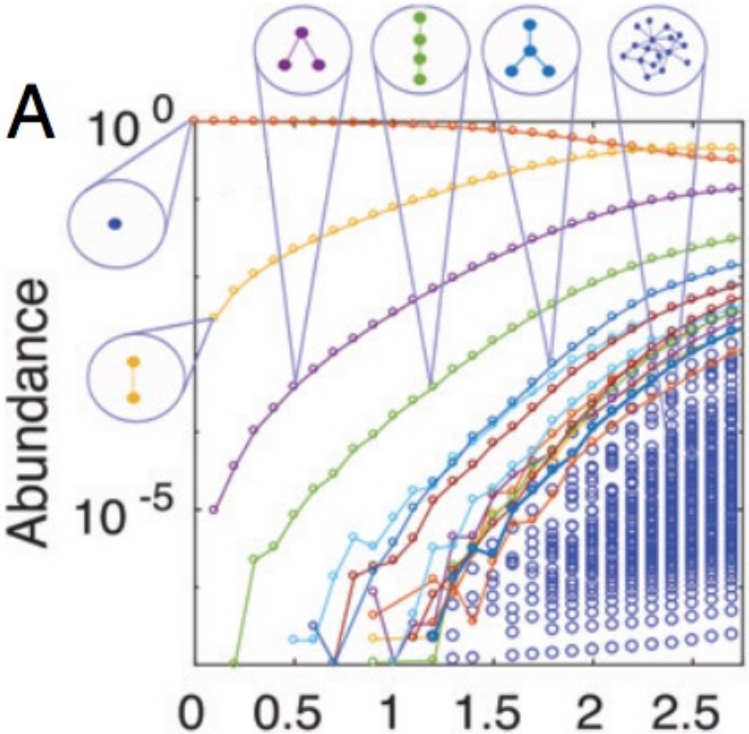
Networld: Computational framework based on Complex Network Theory to create an "artificial chemistry of networks"



(a) Sketch description of the potential evolution of a simple system formed by 4 nodes.

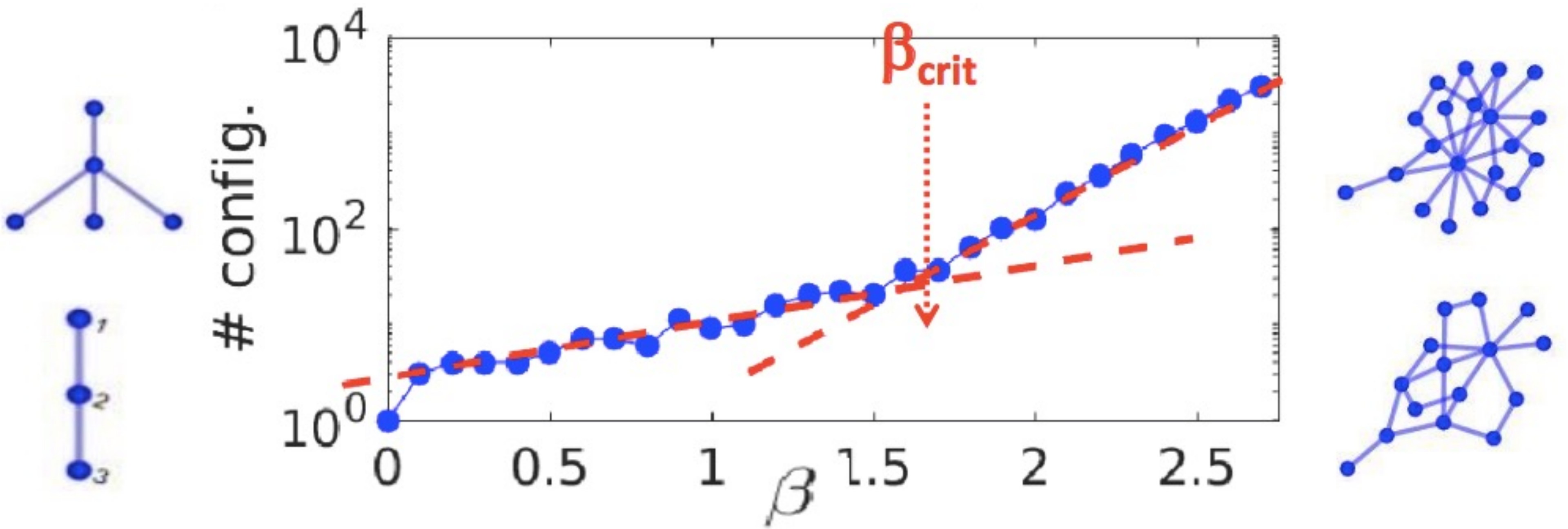
- Simulations start with N nodes
- Nodes interact to form more complex structures that can either connect to other structures or divide into smaller configurations
- Each complex network represents a chemical compound

Transition to complexity when the environment (β) changes

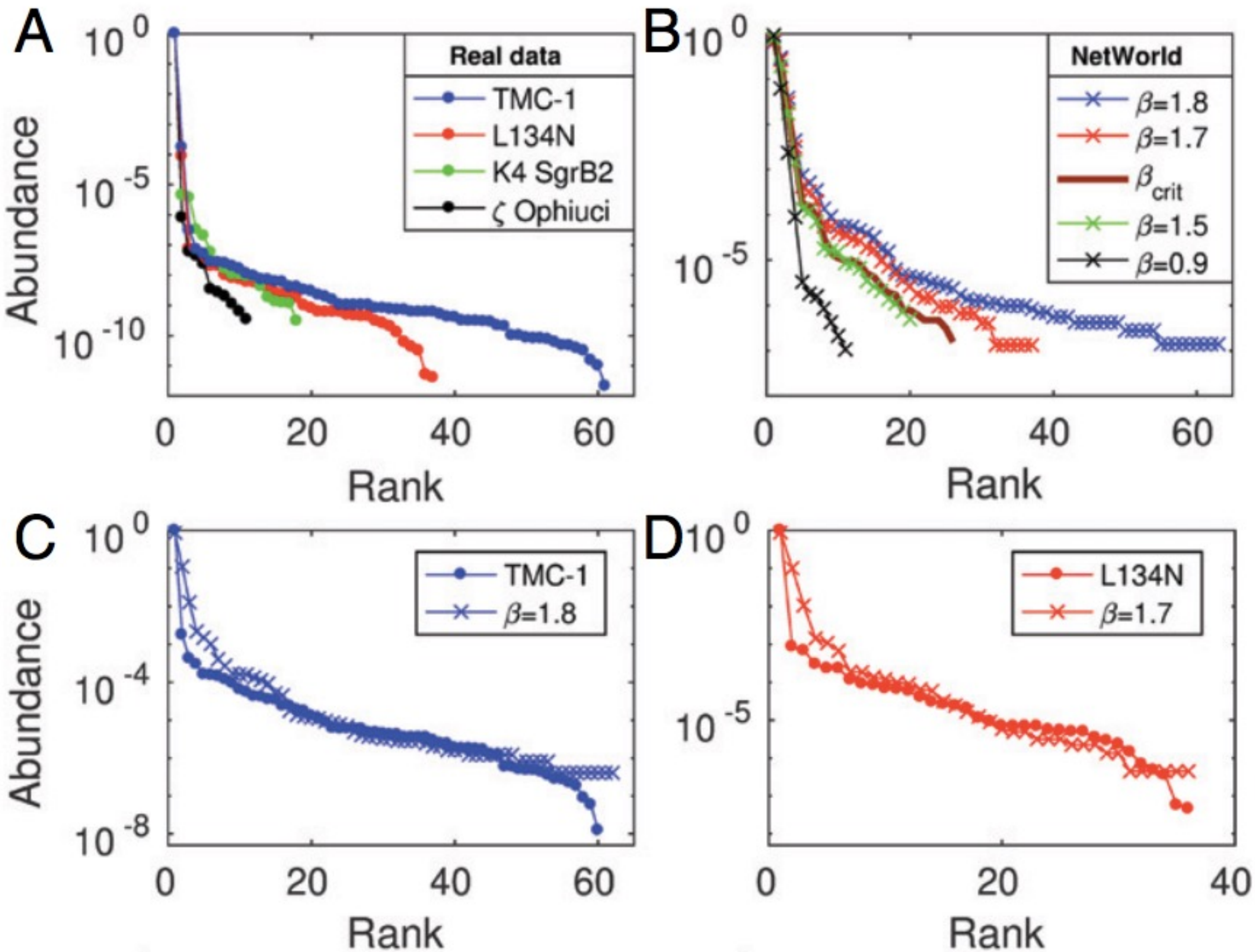


Low β = efficient division of compounds

High β = large compounds become stable



Comparison with astronomical observations



Networld mimics chemical evolution towards complexity in the ISM

- **Precursors of prebiotic systems chemistry form in the ISM**

- **Galactic Center Clouds present multiple advantages for the search of new prebiotic species in the ISM**

- **The rules leading to the emergence of interstellar chemical complexity may be universal**

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