ATMoS

Simulations of molecular spectra for detection of biosignature gases and other volatiles

Clara Sousa-Silva
MIT

8th July 2018, Cumberland

Collaborators

Sara Seager

William Bains

Janusz Petkowski

ATMoS

Simulations of molecular spectra for detection of biosignature gases and other volatiles

Clara Sousa-Silva
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14th June 2018, CfA

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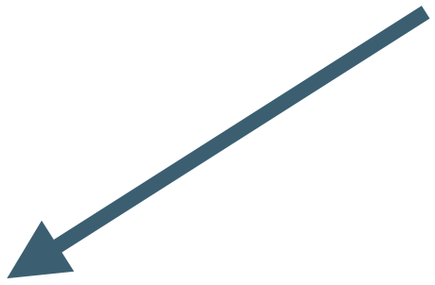
Janusz Petkowski

(**A**pproximate **T**heoretical **Mo**lecular **S**pectra)



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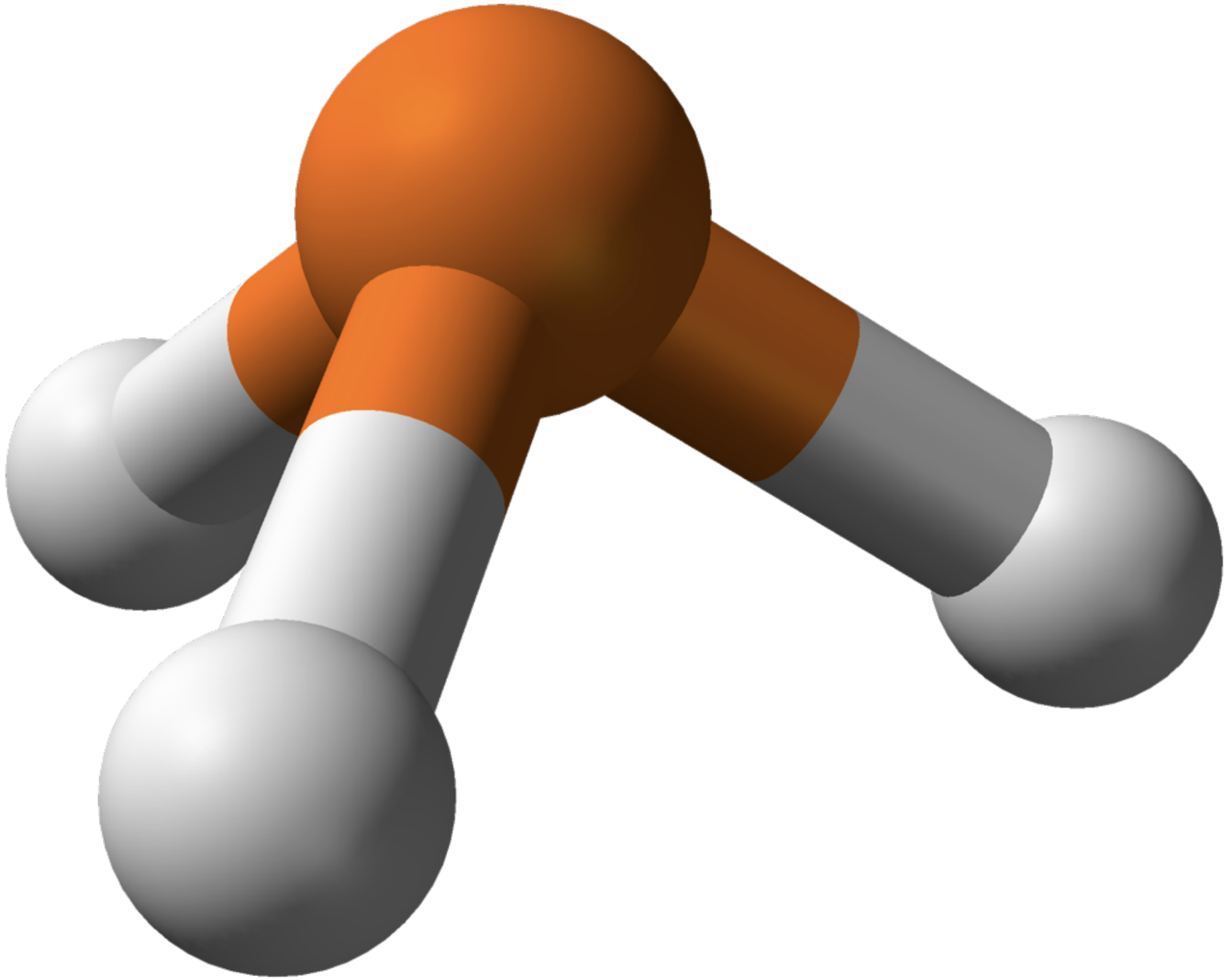
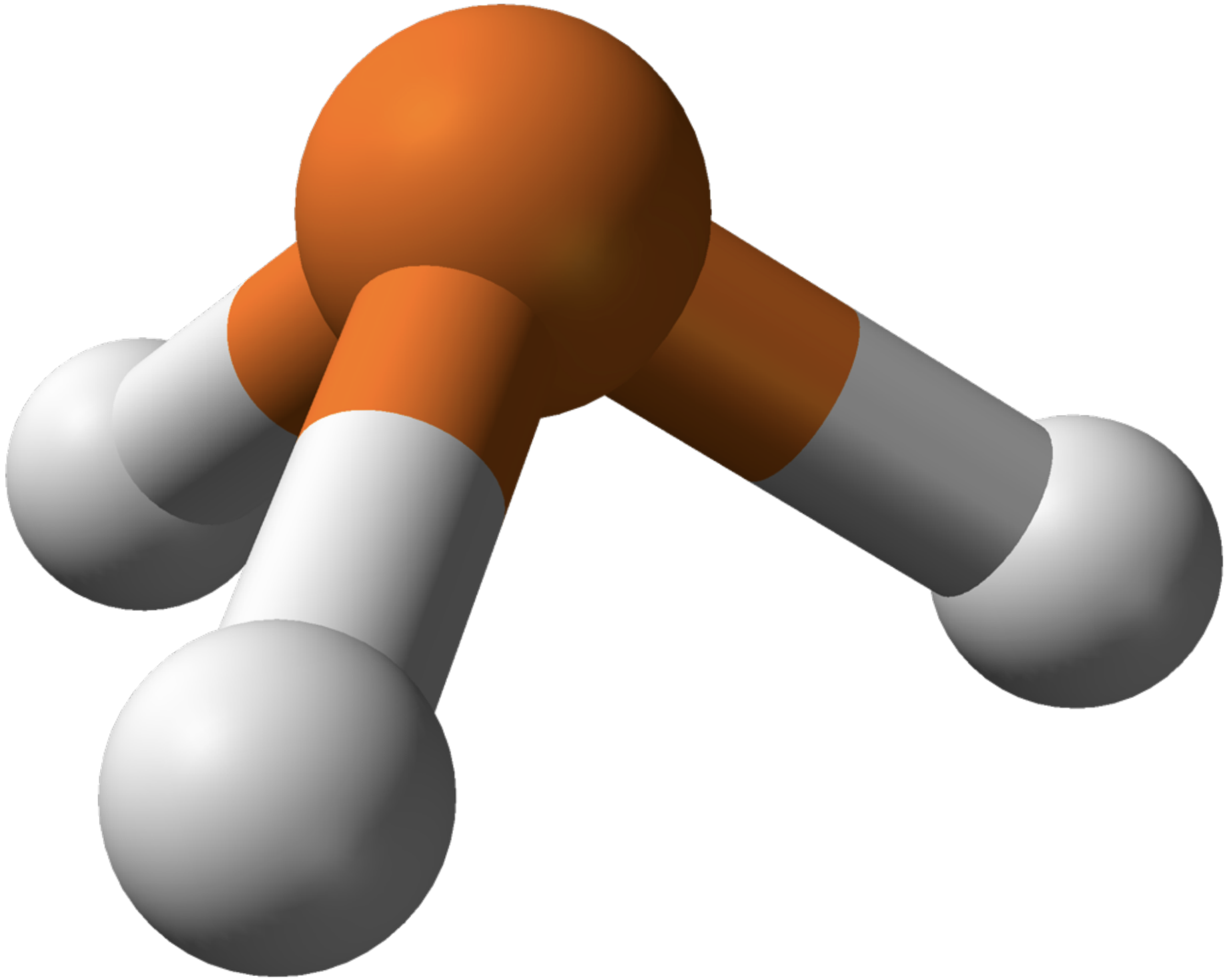
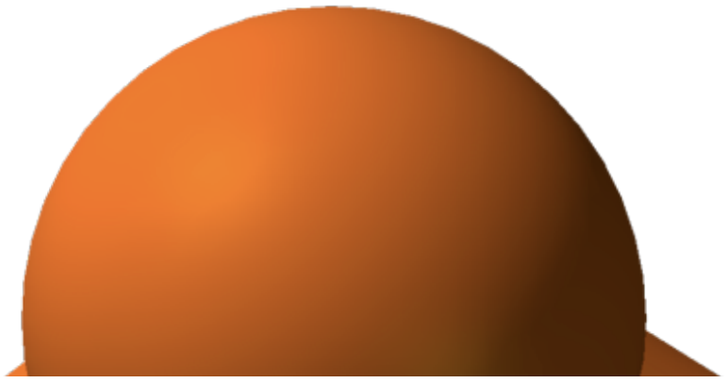






ELSEVIER

Journal of Molecular Spectroscopy

Volume 288, June 2013, Pages 28-37

A computed room temperature line list for phosphine

Clara Sousa-Silva ✉, Sergei N. Yurchenko, Jonathan Tennyson

⊞ Show more

https://doi.org/10.1016/j.jms.2013.04.002

Journal of Quantitative Spectroscopy and Radiative Transfer

Volume 142, July 2014, Pages 66-74

High temperature partition functions and thermodynamic data for ammonia and phosphine

Clara Sousa-Silva, Nicholas Hesketh, Sergei N. Yurchenko, Christian Hill, Jonathan Tennyson

Show more

https://doi.org/10.1016/j.jqsrt.2014.03.012

Journal of Quantitative Spectroscopy and Radiative Transfer

Volume 142, July 2014, Pages 66-74

Communication: Tunnelling splitting in the phosphine molecule

The Journal of Chemical Physics **145**, 091102 (2016); https://doi.org/10.1063/1.4962259

Clara Sousa-Silva, Jonathan Tennyson, *and* Sergey N. Yurchenko

https://doi.org/10.1016/j.jqsrt.2014.03.012

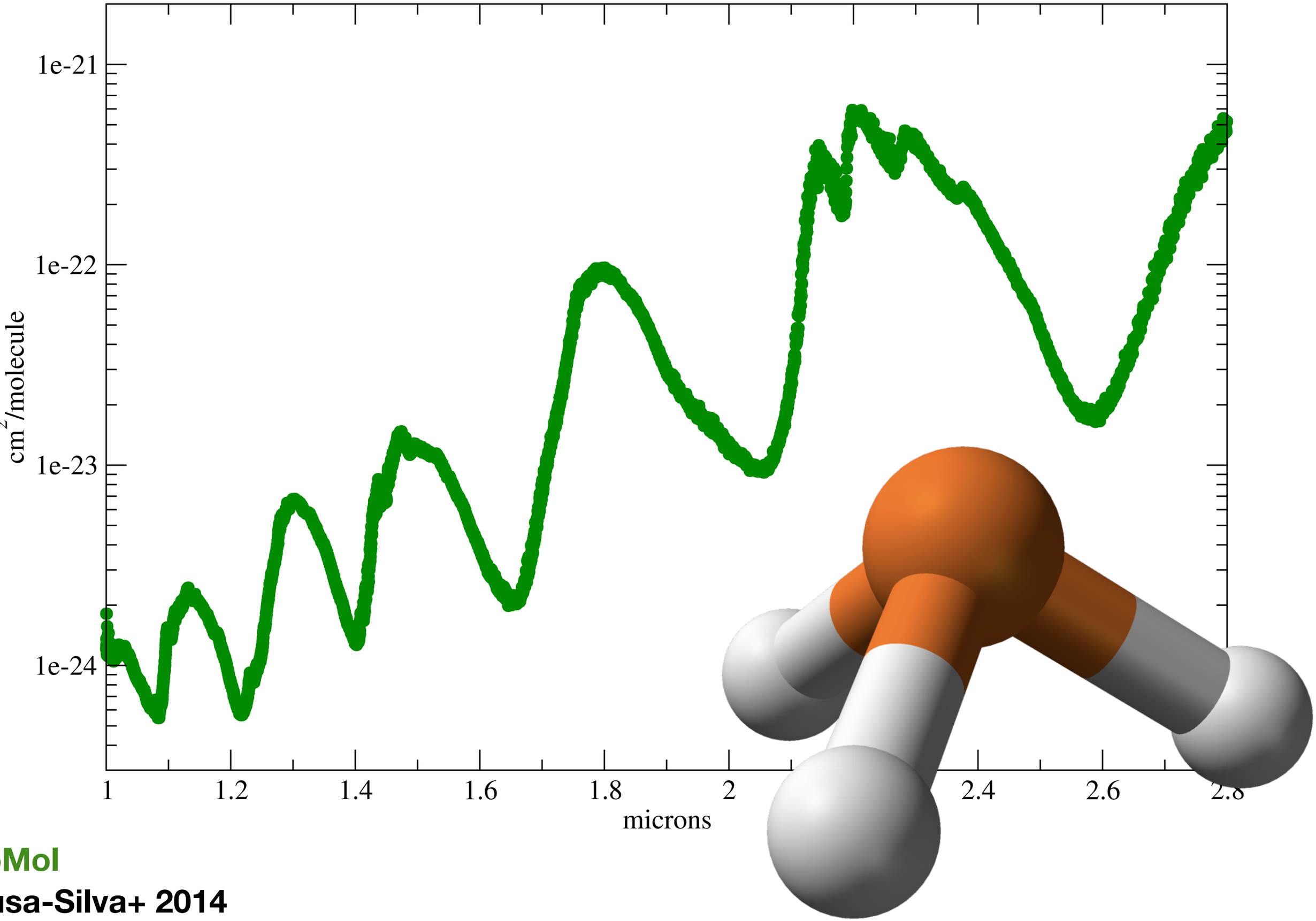
ExoMol line lists – VII. The rotation–vibration spectrum of phosphine up to 1500 K

Clara Sousa-Silva ✉, Ahmed F. Al-Refaie, Jonathan Tennyson, Sergei N. Yurchenko

Monthly Notices of the Royal Astronomical Society, Volume 446, Issue 3, 21 January 2015, Pages 2337–2347, https://doi.org/10.1093/mnras/stu2246

Published: 26 November 2014 **Article history** ▾

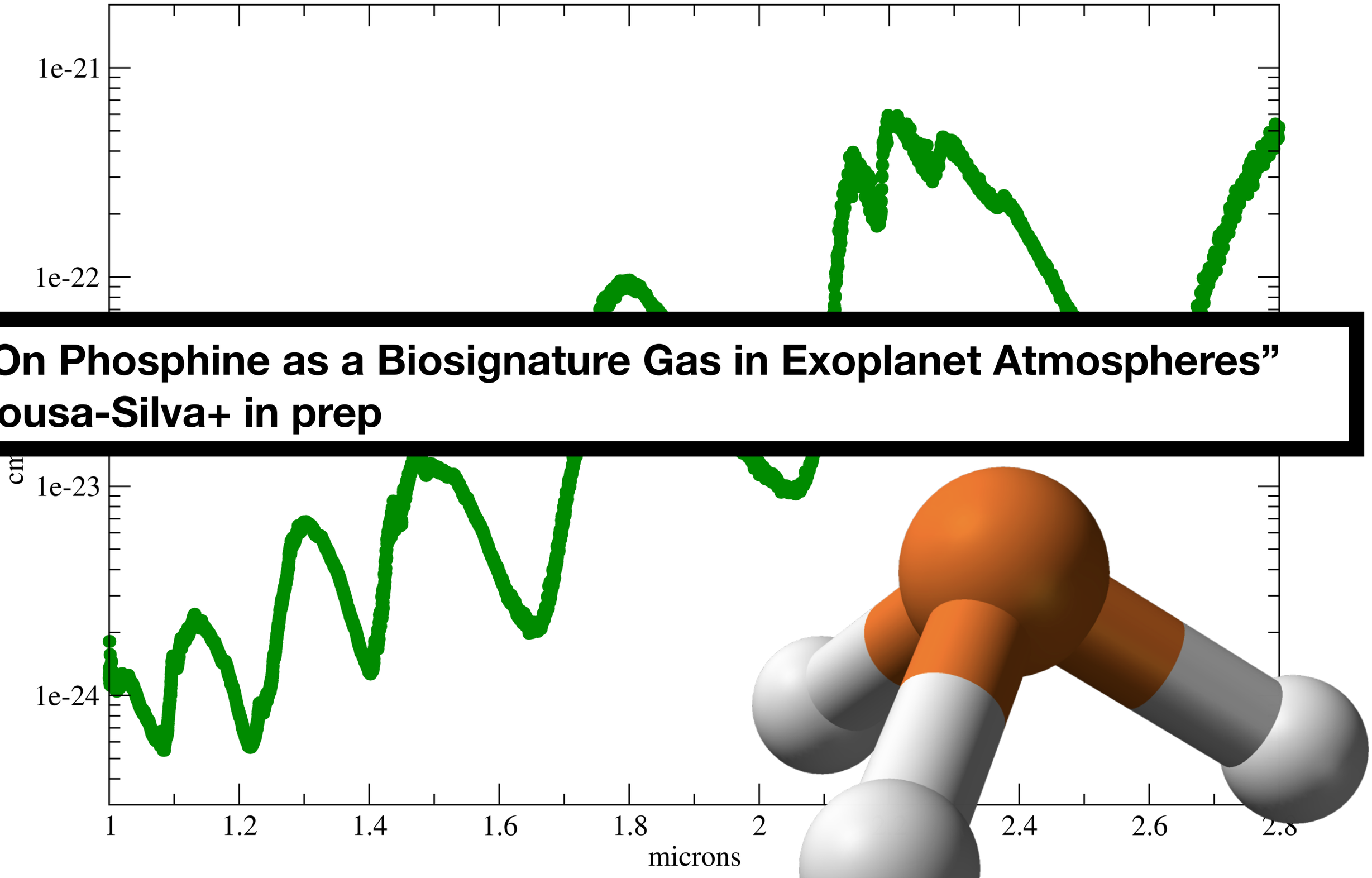
phosphine at 300 K



ExoMol

Sousa-Silva+ 2014

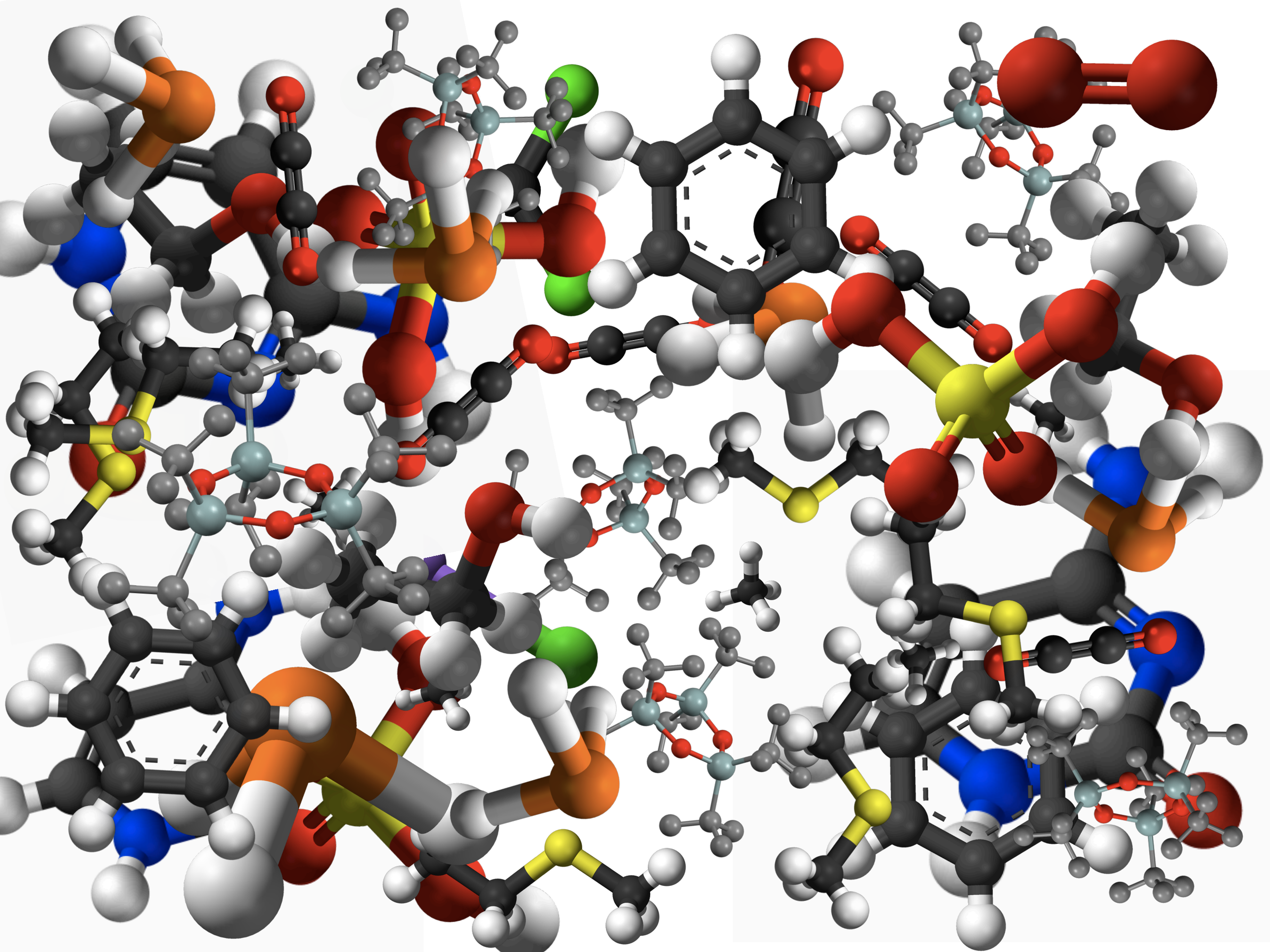
phosphine at 300 K

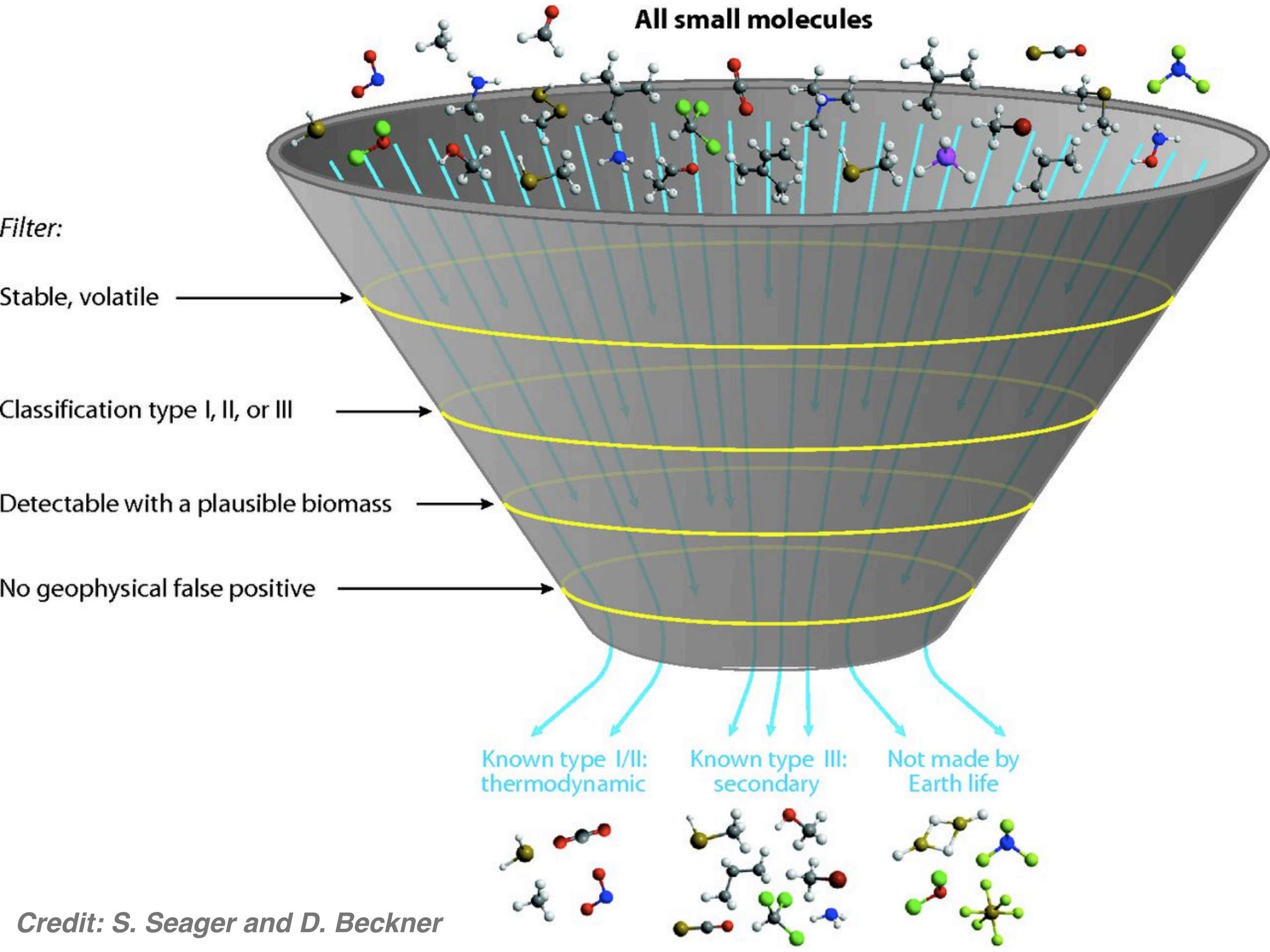


“On Phosphine as a Biosignature Gas in Exoplanet Atmospheres”
Sousa-Silva+ in prep

ExoMol

Sousa-Silva+ 2014





Credit: S. Seager and D. Beckner

All small molecules

Filter:

Stable, volatile →

Classification type I, II, or III →

Detectable with a plausible biomass →

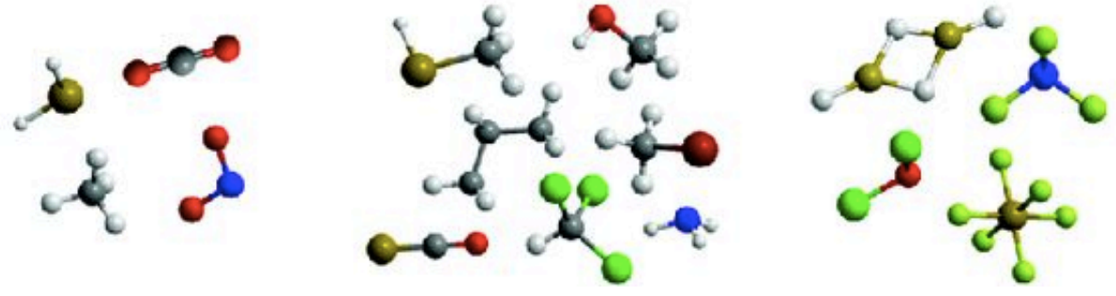
No geophysical false positive →

16,367

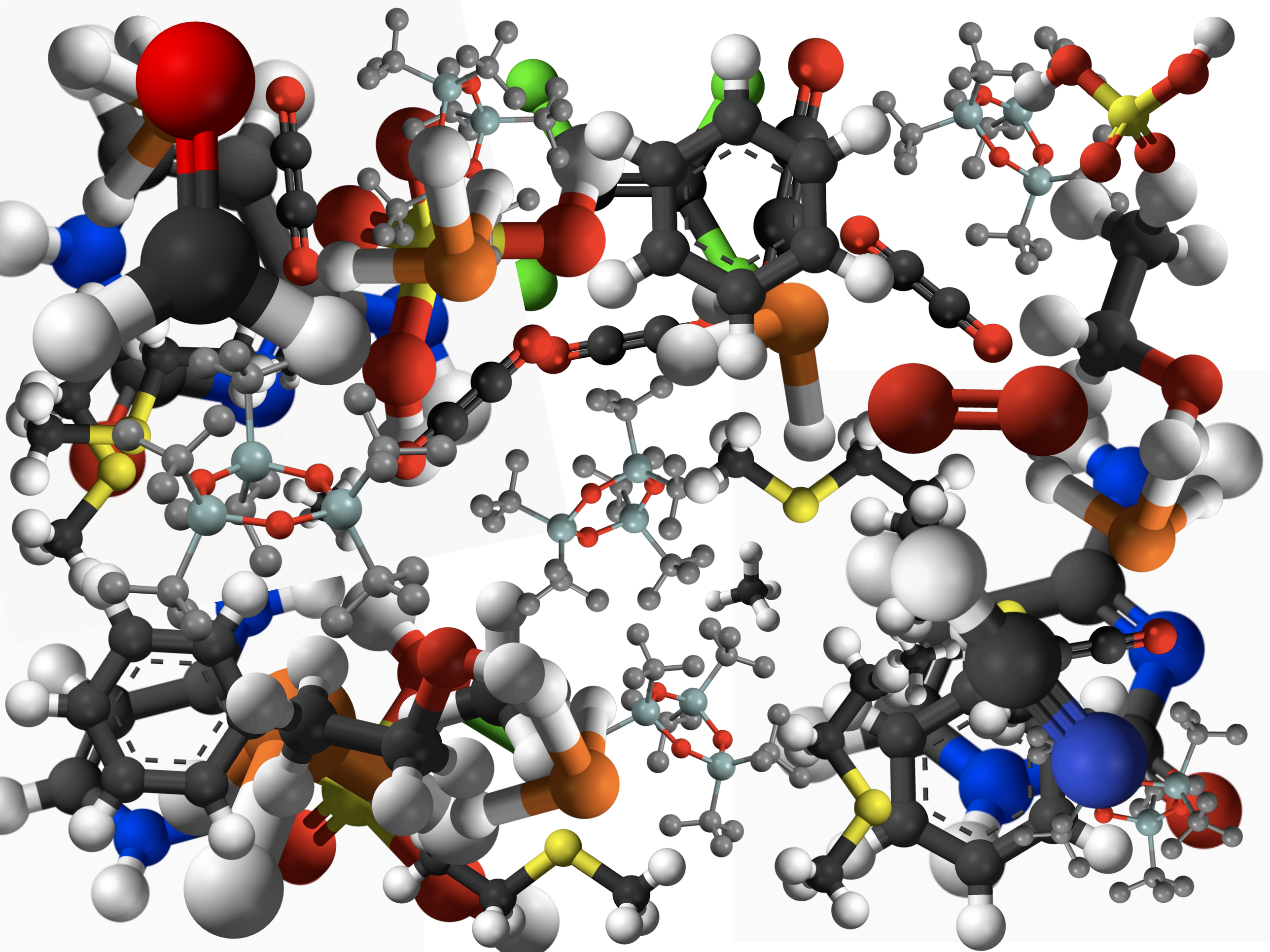
Known type I/II: thermodynamic

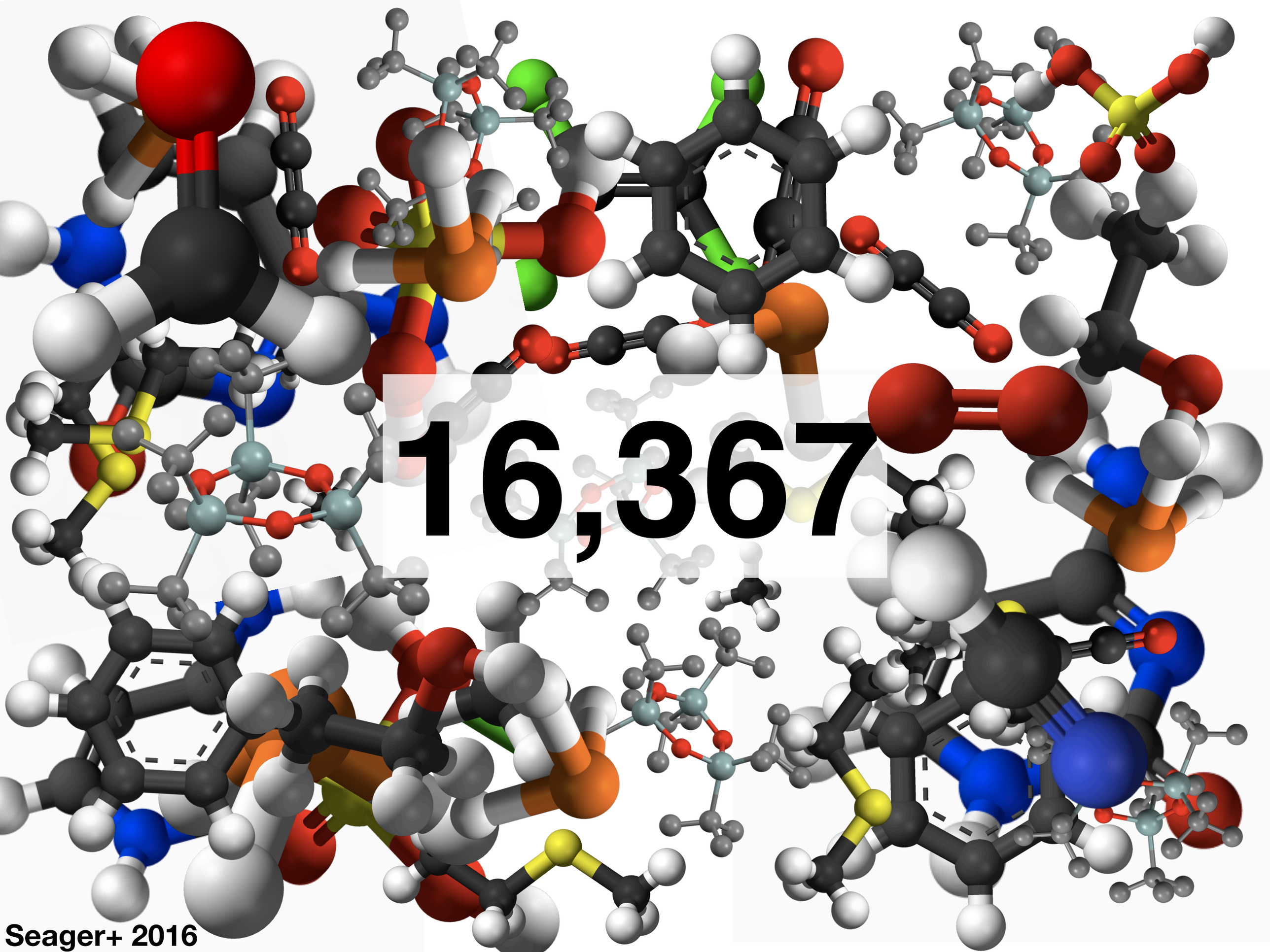
Known type III: secondary

Not made by Earth life



Credit: S. Seager and D. Beckner




16,367
Seager+ 2016

~600

Seager+ 2016

~50

Seager+ 2016

- 1 person
- 1 molecule
- 100s CPUhrs
- 100s GPUs
- 4 years

- 1 person
- 1 molecule
- 100s CPUhrs **X** 15,747 molecules **=** 62,988 years
- 100s GPUs
- 4 years

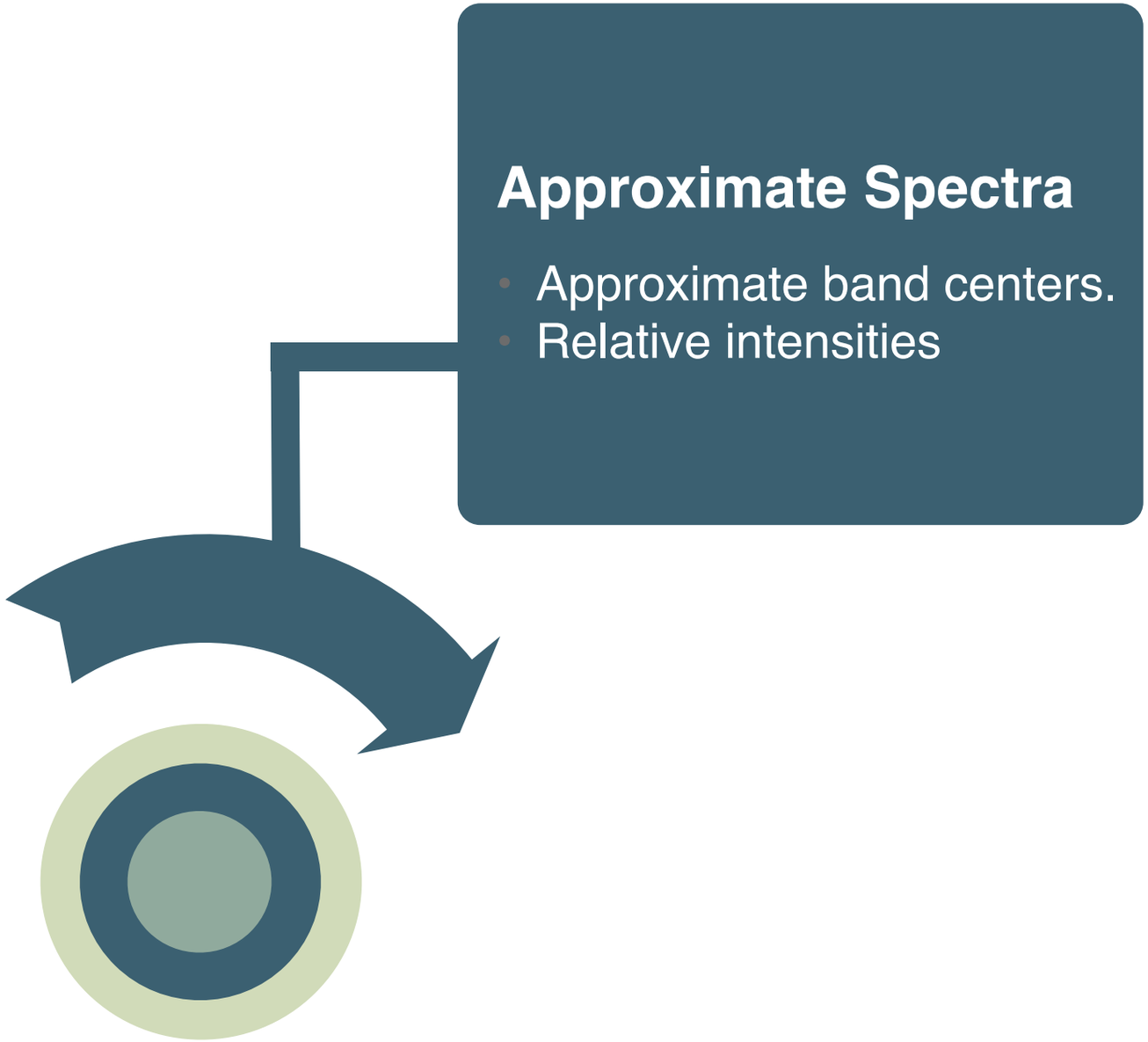
ATMoS:

Approximate

Theoretical

Molecular

Spectra



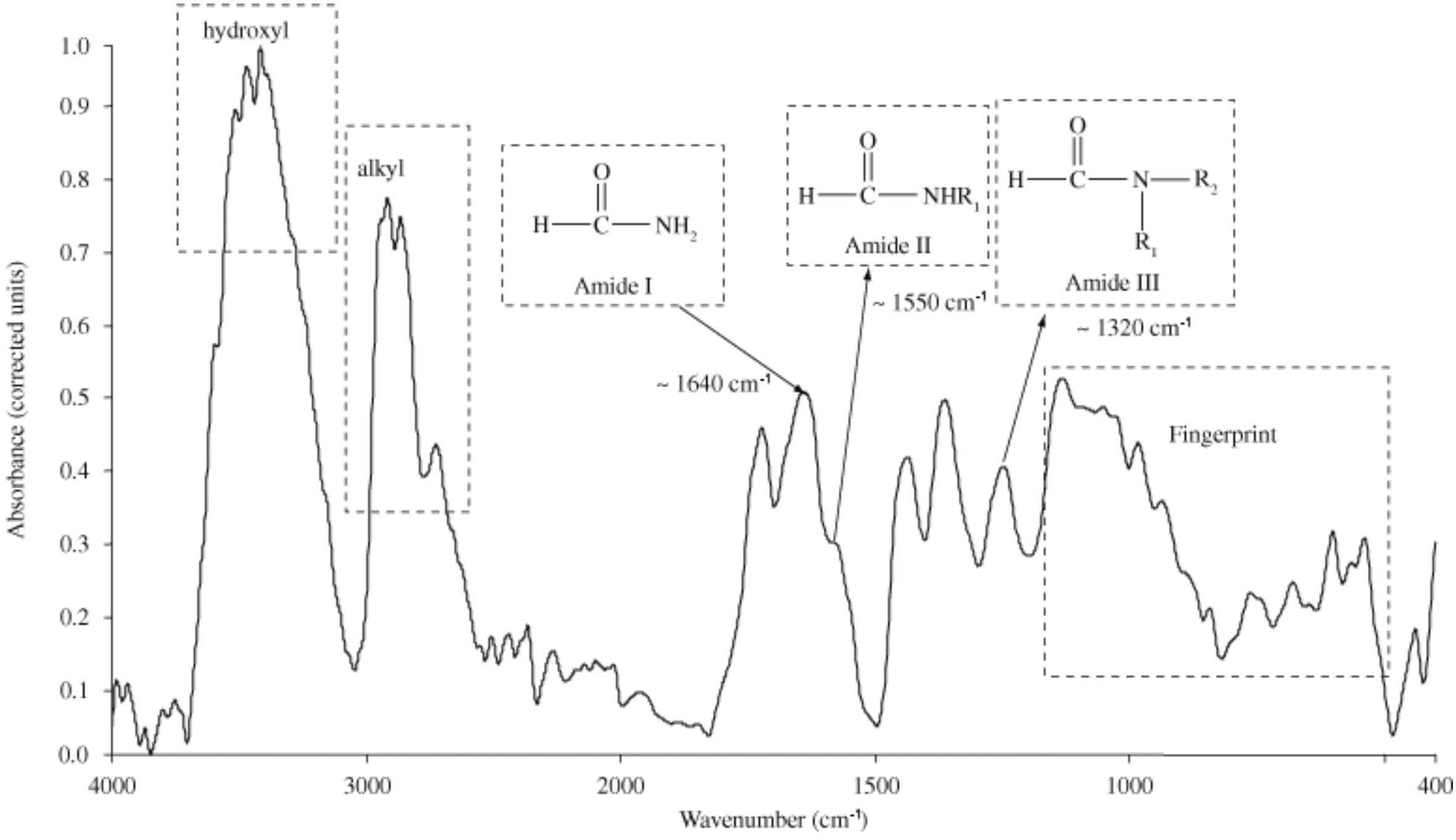


Figure 5. FTIR spectrum of pure MPB70 recombinant protein produced, purified and characterized.

Fonseca dos Reis + 2006

organic chemistry

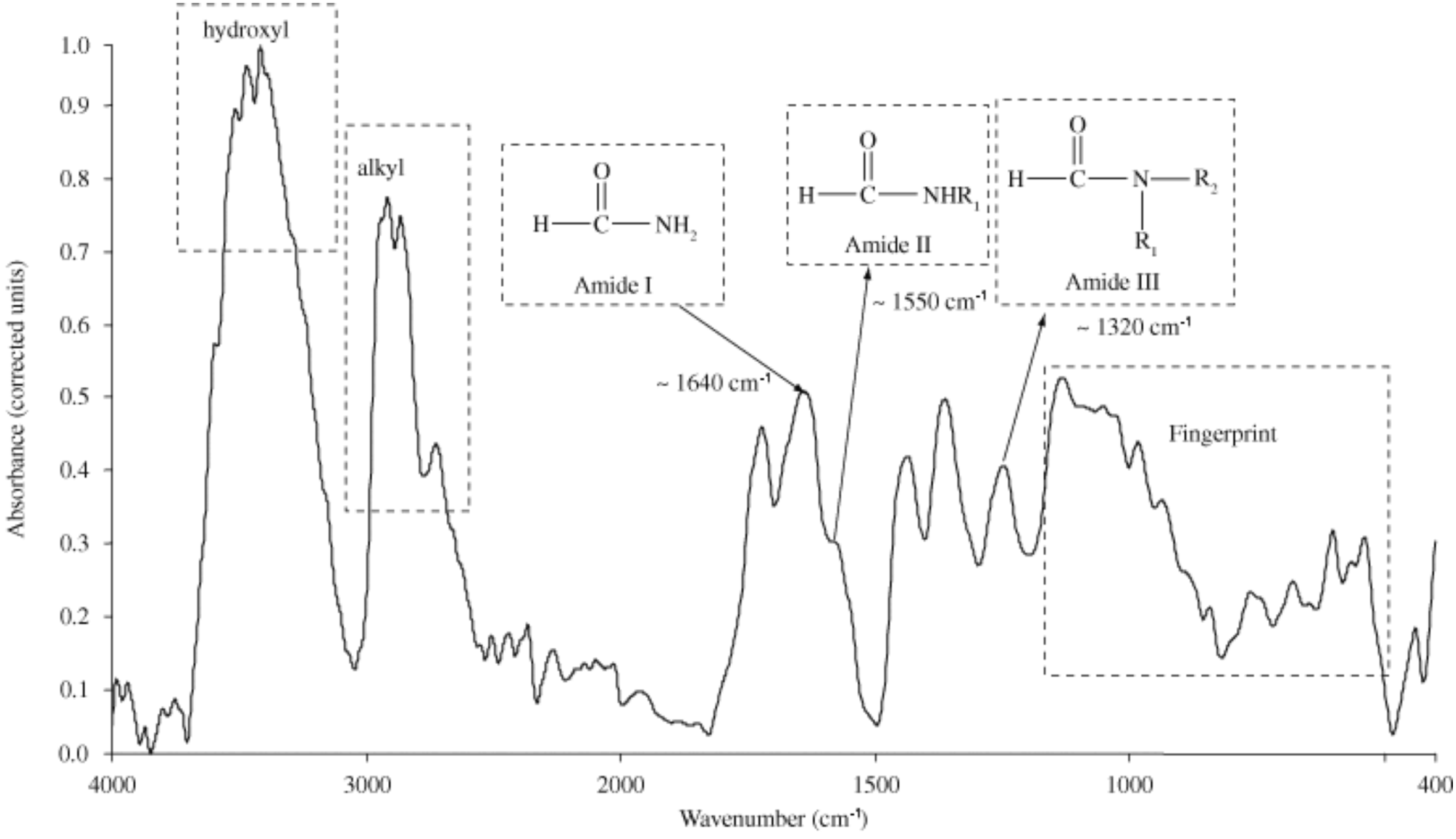


Figure 5. FTIR spectrum of pure MPB70 recombinant protein produced, purified and characterized.

Fonseca dos Reis + 2006

organic chemistry

Alkane C - H	2850 - 2975 cm^{-1}
Alkyne (C≡C)	2100 - 2250 cm^{-1}
Amines (N-H)	3300 - 3350 cm^{-1}
Ketone (RCOR)	~1540 cm^{-1}
...	? cm^{-1}

etc

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- ... — ? cm^{-1}

etc

Type	MSMILE	Vib type	Low freq	High Freq	Inten	Shape	Source	Class	Sub-Type	Notes
=C-H	[H]C([H])=C([H])[!#1]	stretch	3010	3040	m	-1	ir.pdf	Alkenes	mono-alkyl(vinyl group)	R-CH=CH2
=C-H	[H]C([H])=C([H])[!#1]	stretch	3075	3095	m	-1	ir.pdf	Alkenes	mono-alkyl(vinyl group)	R-CH=CH2
=C-H	[H]\C([!#1])=C(/[H])[!#1]	stretch	3010	3040	m	-1	ir.pdf	Alkenes	di-alkyl(cis)	RCH=CHR
=C-H	[H]\C([!#1])=C(\[H])[!#1]	stretch	3010	3040	m	-1	ir.pdf	Alkenes	di-alkyl(trans)	RCH=CHR
=C-H	[H]C([H])=C([!#1])[!#1]	stretch	3075	3095	m	-1	ir.pdf	Alkenes	di-alkyl(geminal)	R2C=CH2
=C-H	[H]C([!#1])=C([!#1])[!#1]	stretch	3010	3040	m	-1	ir.pdf	Alkenes	tri-alkyl	R2C=CHR
=C-H	[H]C([H])=C([H])[!#1]	bend	905	920	s	-1	ir.pdf	Alkenes	mono-alkyl(vinyl group)	R-CH=CH2
=C-H	[H]C([H])=C([H])[!#1]	bend	985	1000	s	-1	ir.pdf	Alkenes	mono-alkyl(vinyl group)	R-CH=CH2
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=C-H	[H]C([H])=C([H])[!#1]	bend	1410	1420	m	-1	ir.pdf	Alkenes	mono-alkyl(vinyl group)	R-CH=CH2
=C-H	[H]\C([!#1])=C(/[H])[!#1]	bend	680	730	s	-1	ir.pdf	Alkenes	di-alkyl(cis)	RCH=CHR
=C-H	[H]\C([!#1])=C(\[H])[!#1]	bend	960	970	s	-1	ir.pdf	Alkenes	di-alkyl(trans)	RCH=CHR
=C-H	[H]\C([!#1])=C(\[H])[!#1]	bend	1295	1310	m	-1	ir.pdf	Alkenes	di-alkyl(trans)	RCH=CHR
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=C-H	[H]C([H])=C([!#1])[!#1]	bend	1410	1420	s	-1	ir.pdf	Alkenes	di-alkyl(geminal)	R2C=CH2
=C-H	[H]C([!#1])=C([!#1])[!#1]	bend	790	840	s	-1	ir.pdf	Alkenes	tri-alkyl	R2C=CHR
=C-H	[H]C1=C([H])C([H])=C([!#1])C([H])=C1[H]	bend	730	770	s	-1	ir.pdf	Arenes	mono-alkyl	R-C6H5
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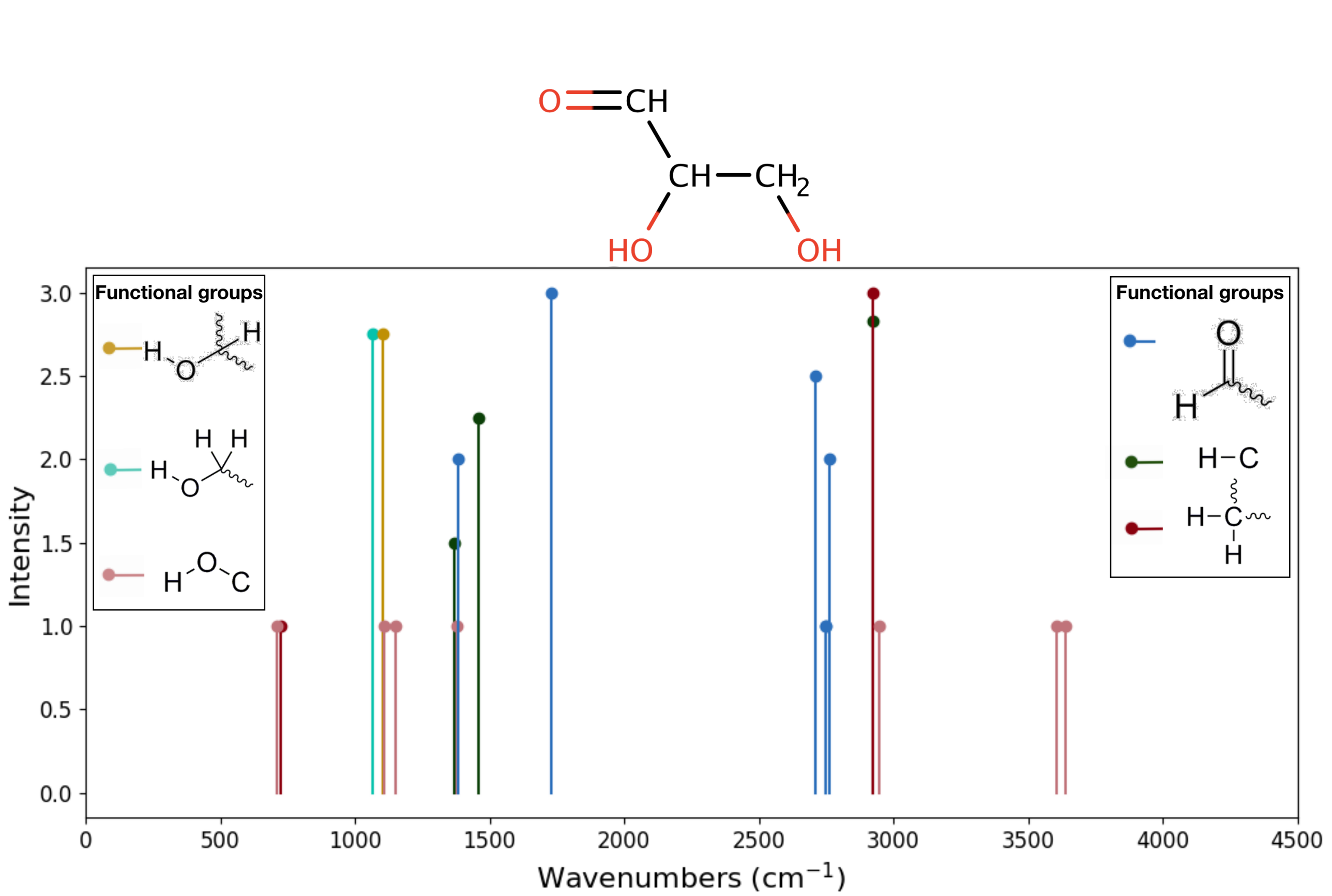
O
CH
CH
CH2
HO
OH
Functional groups
Functional groups
H
O
H
H
H
O
H
O
C
H
O
H
H−C
H−C
H
3.0
2.5
2.0
1.5
1.0
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Intensity
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1000
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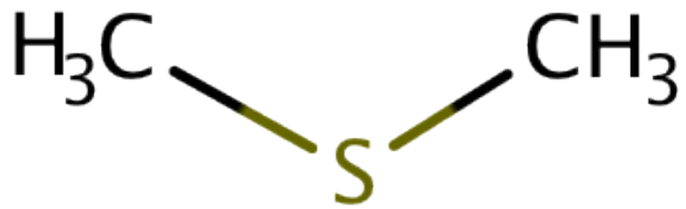
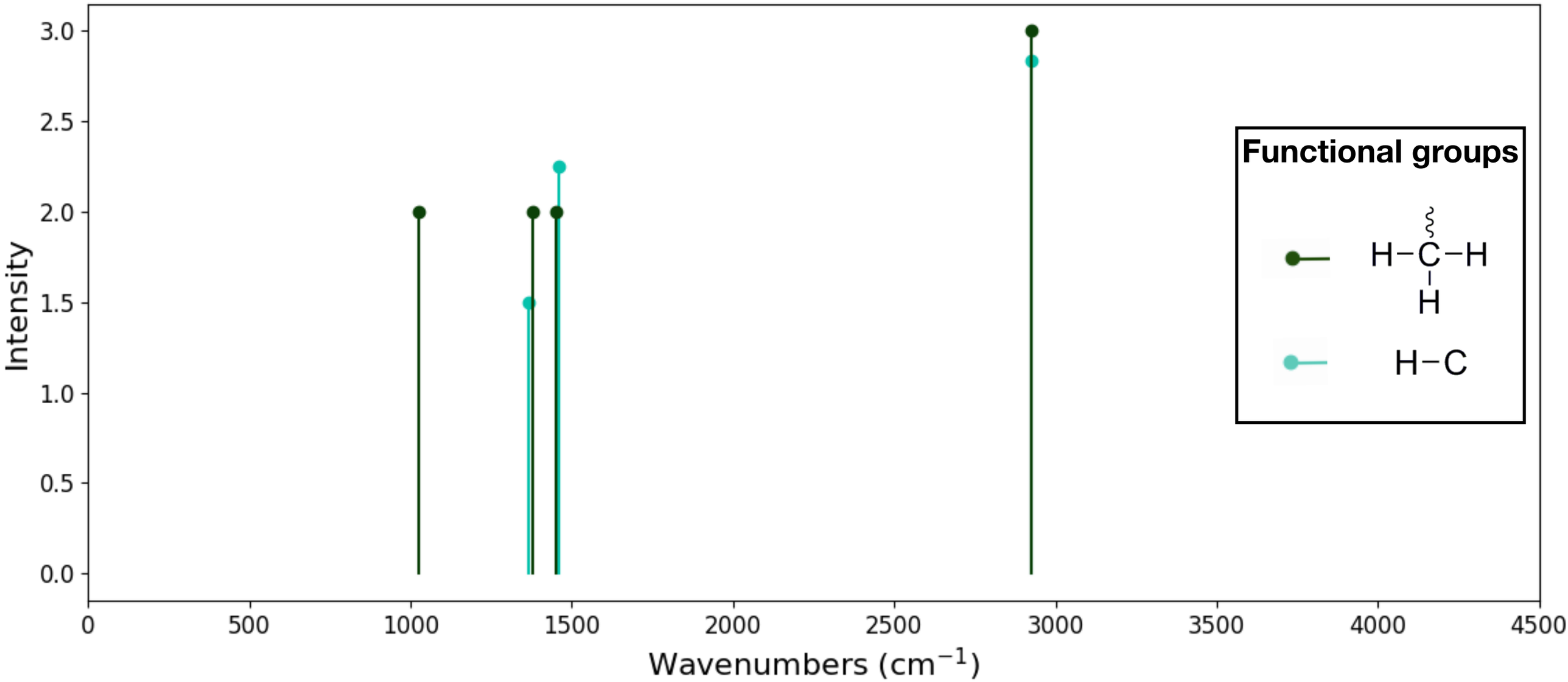
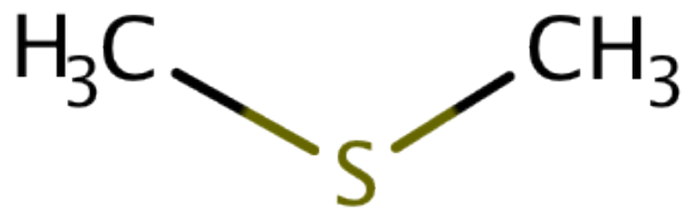
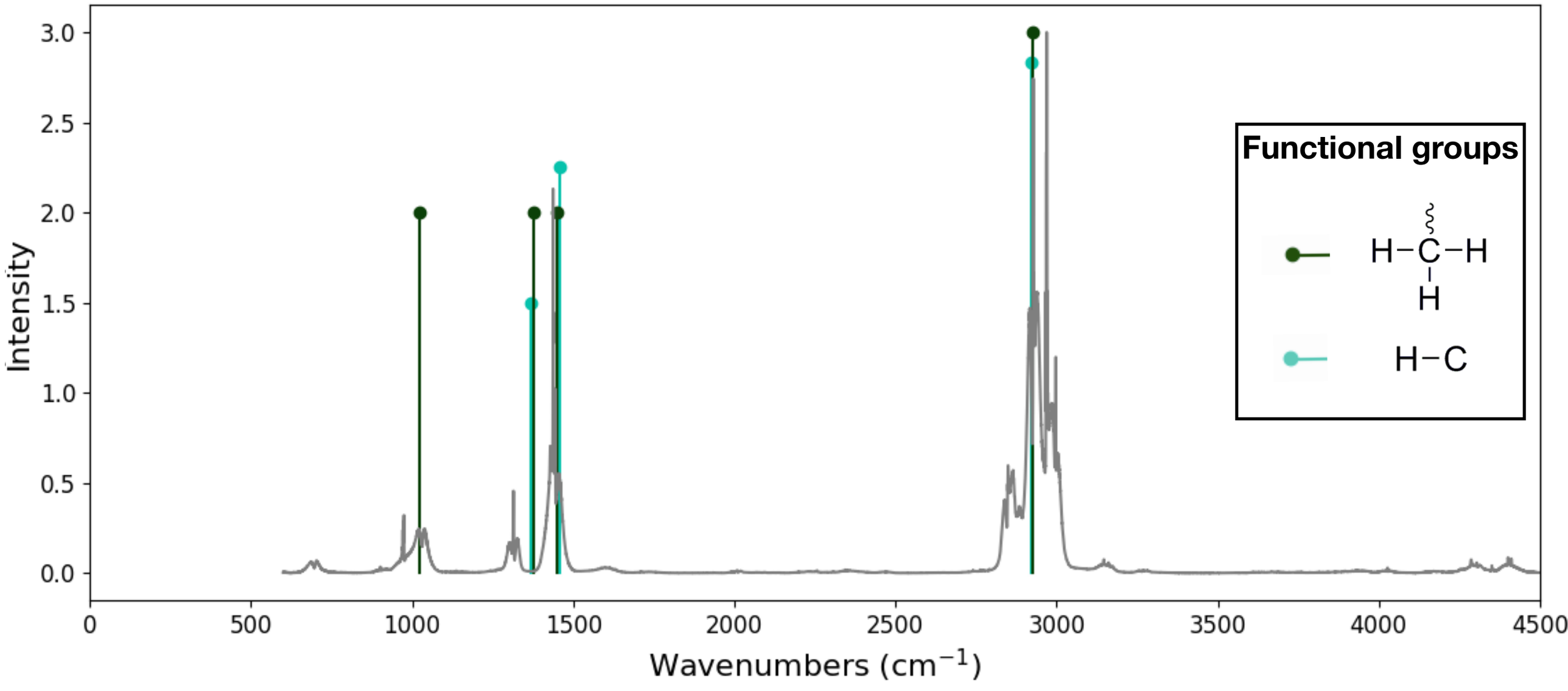
2500
3000
3500
4000
4500
Wavenumbers (cm−1)





Sousa-Silva+ submitted

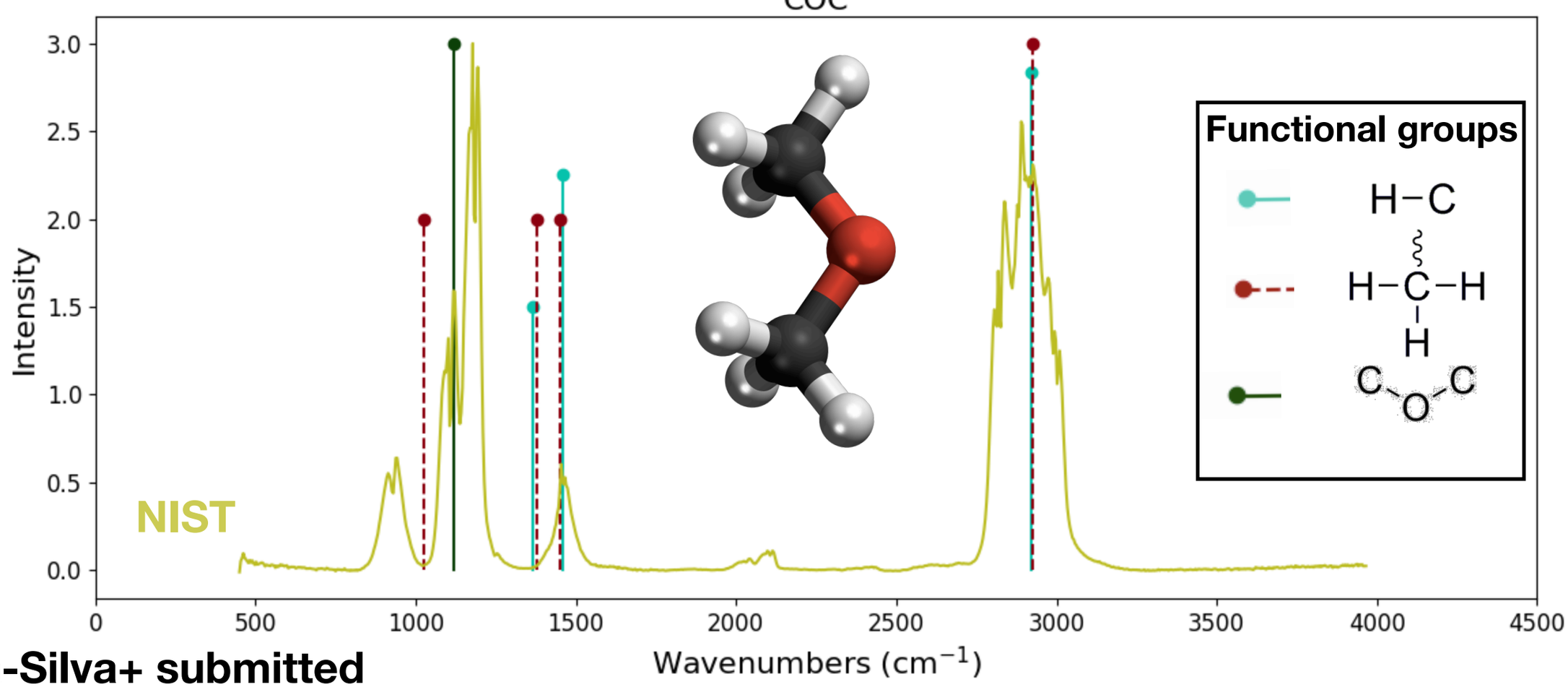




PNNL

Sousa-Silva+ submitted

COC



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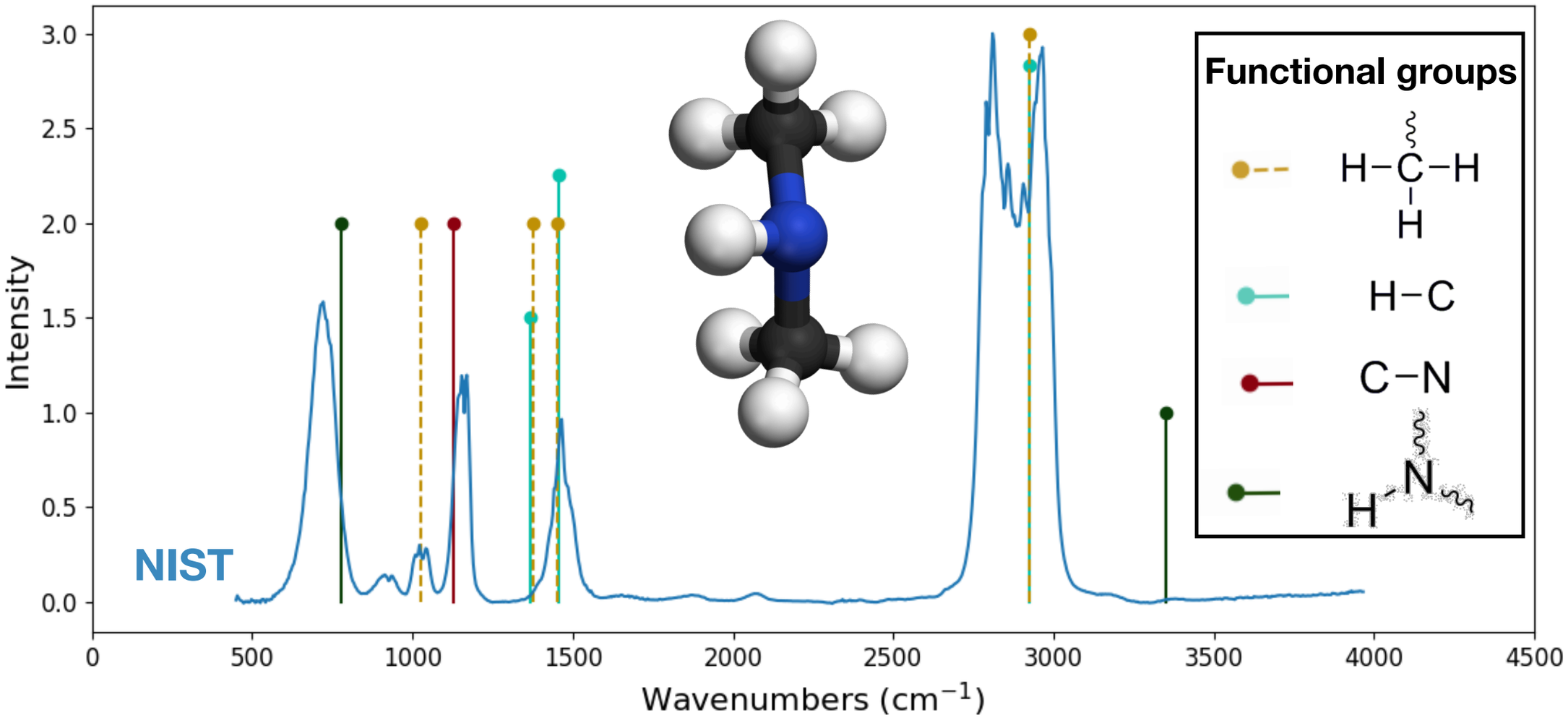

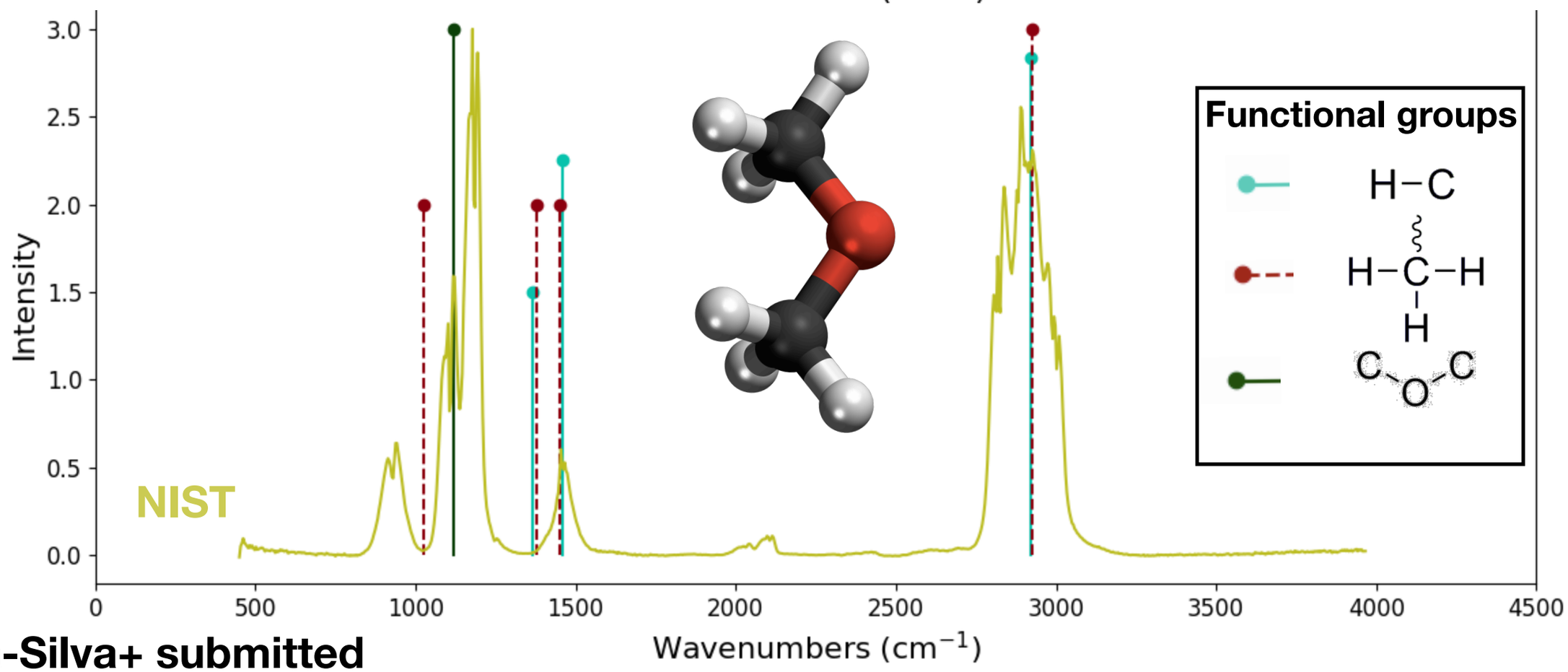

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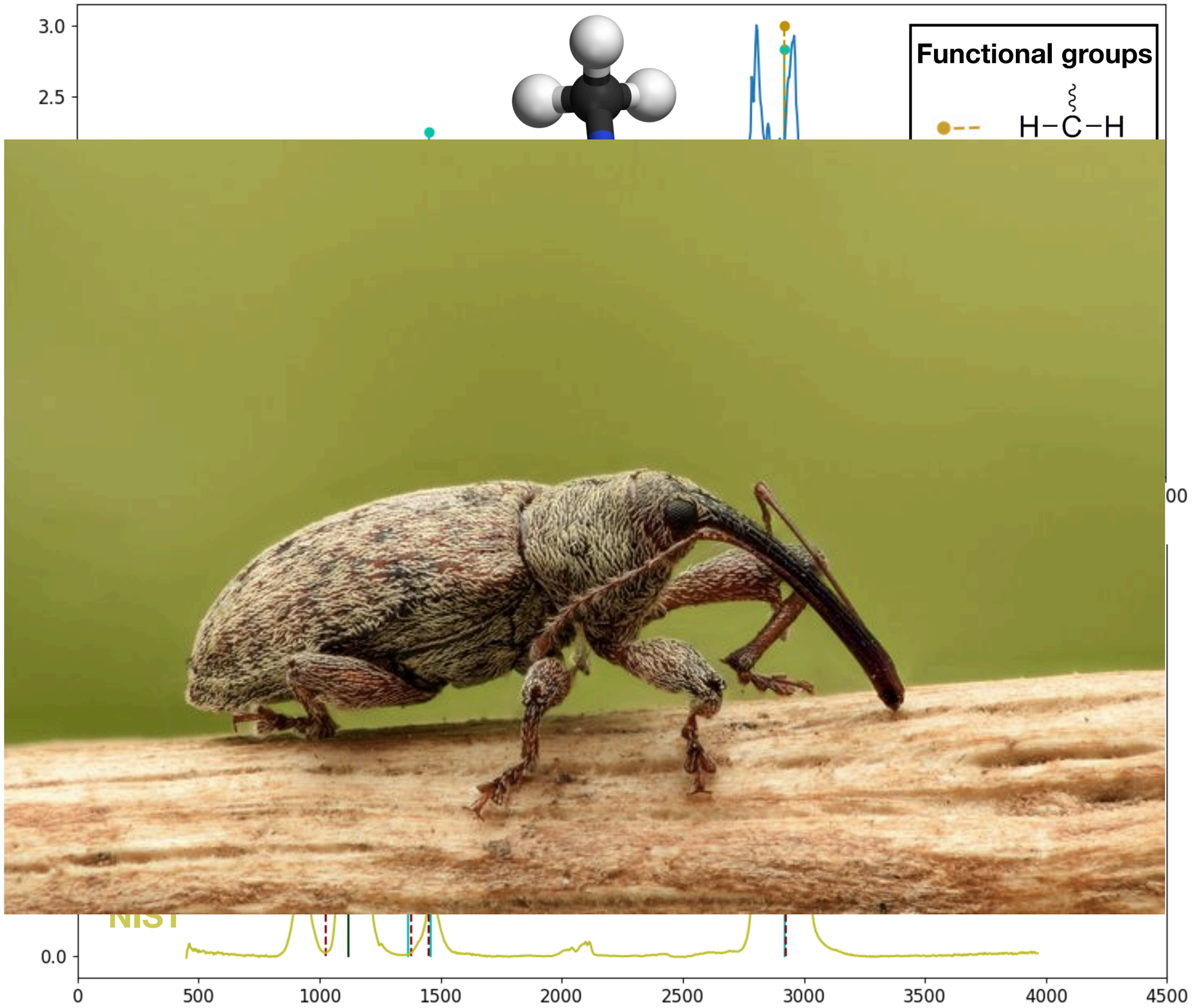

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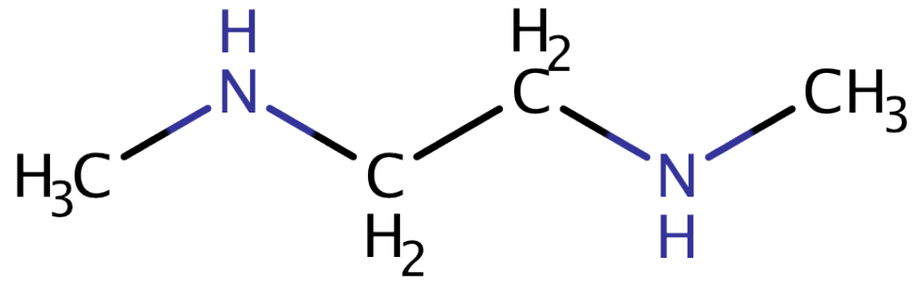

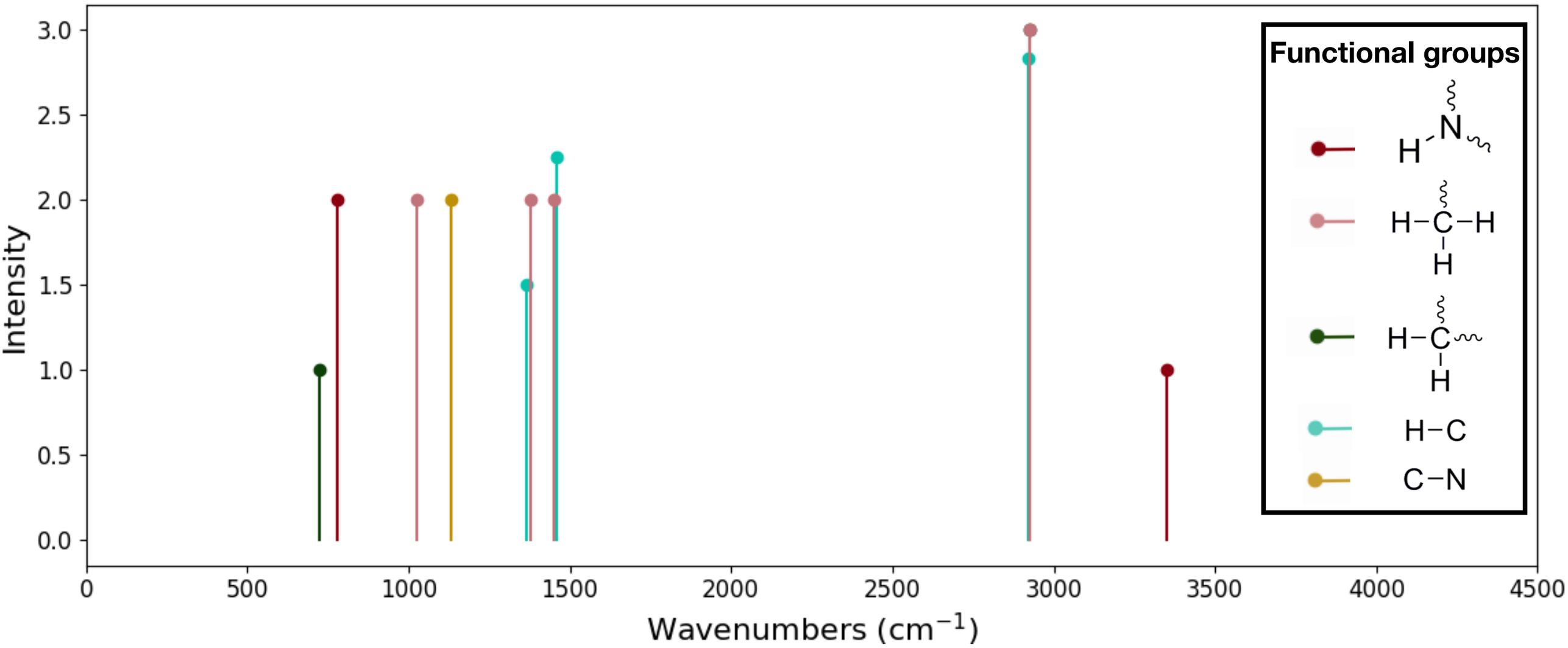

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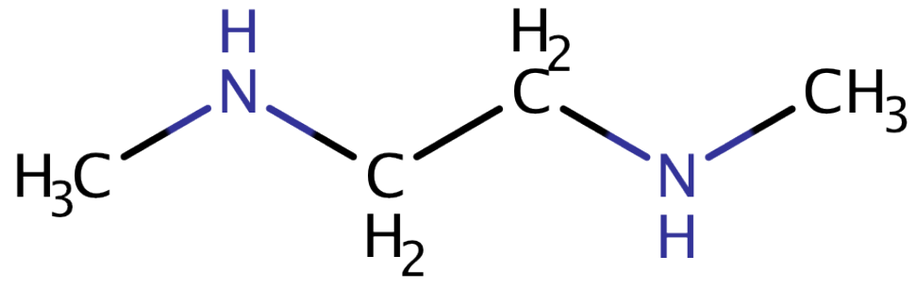
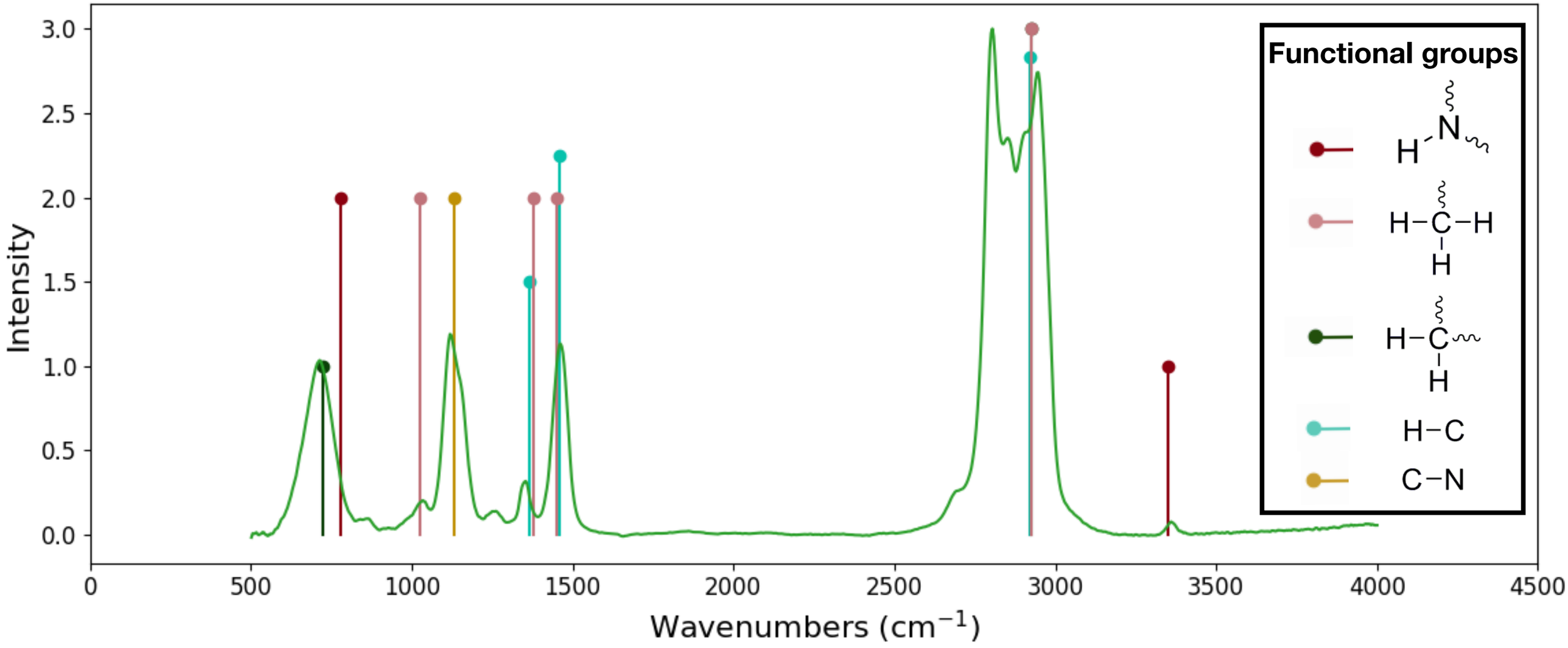
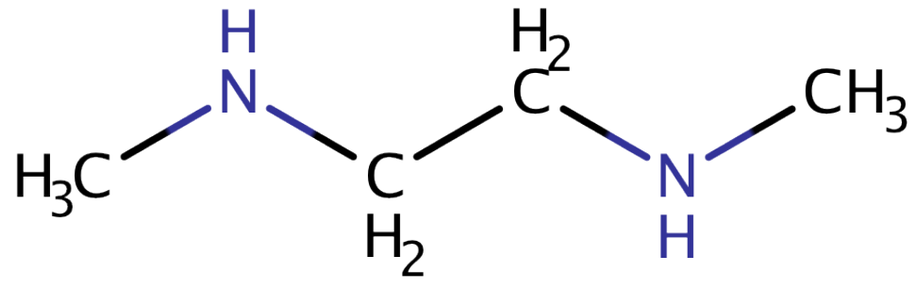
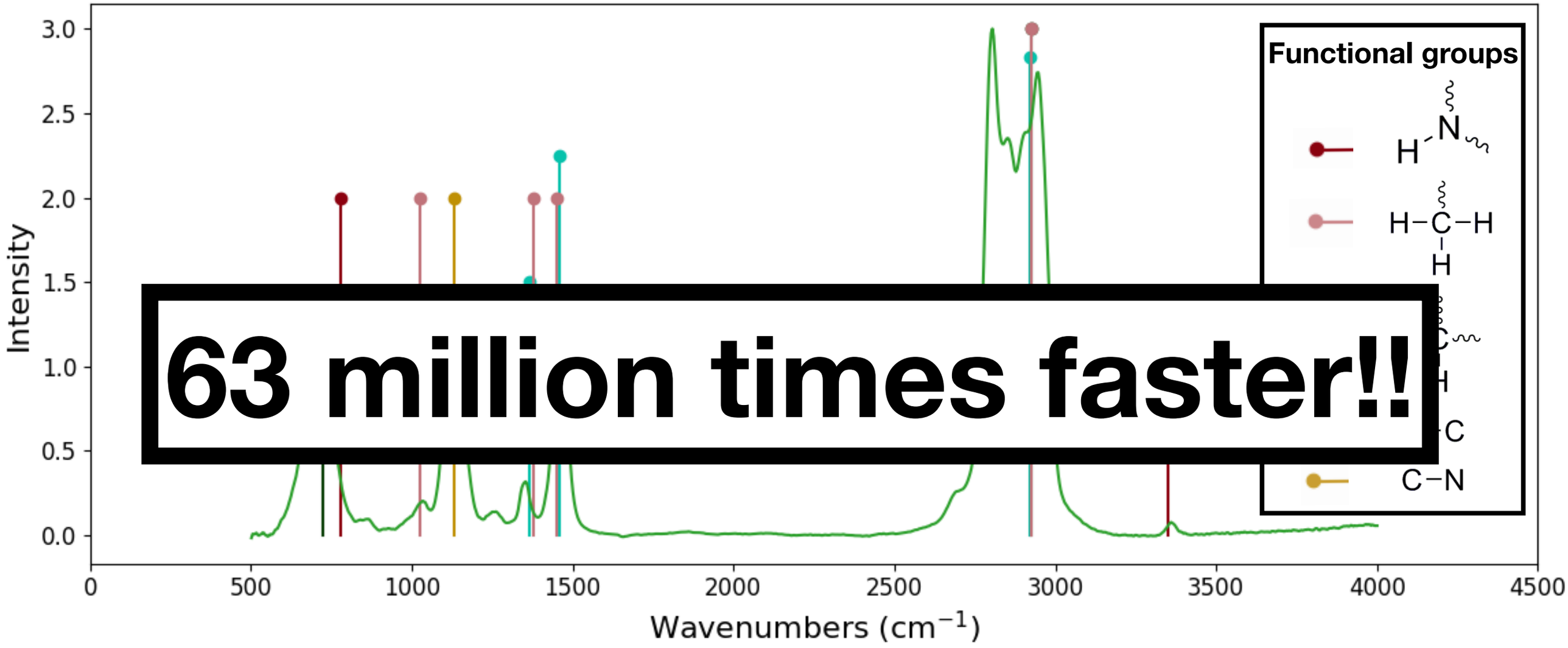




NIST

Sousa-Silva+ submitted





63 million times faster!!

NIST

Sousa-Silva+ submitted

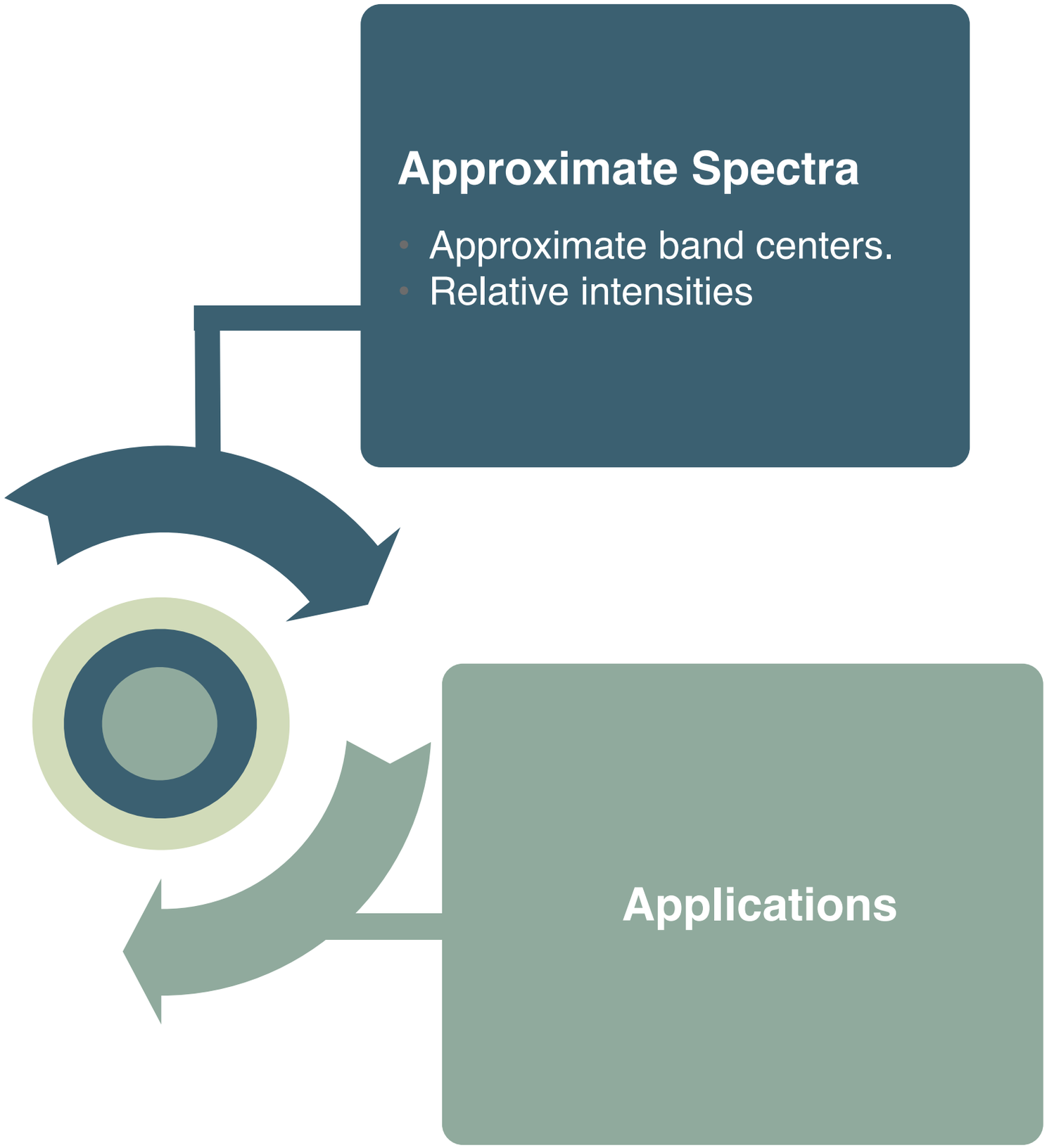
ATMoS:

Approximate

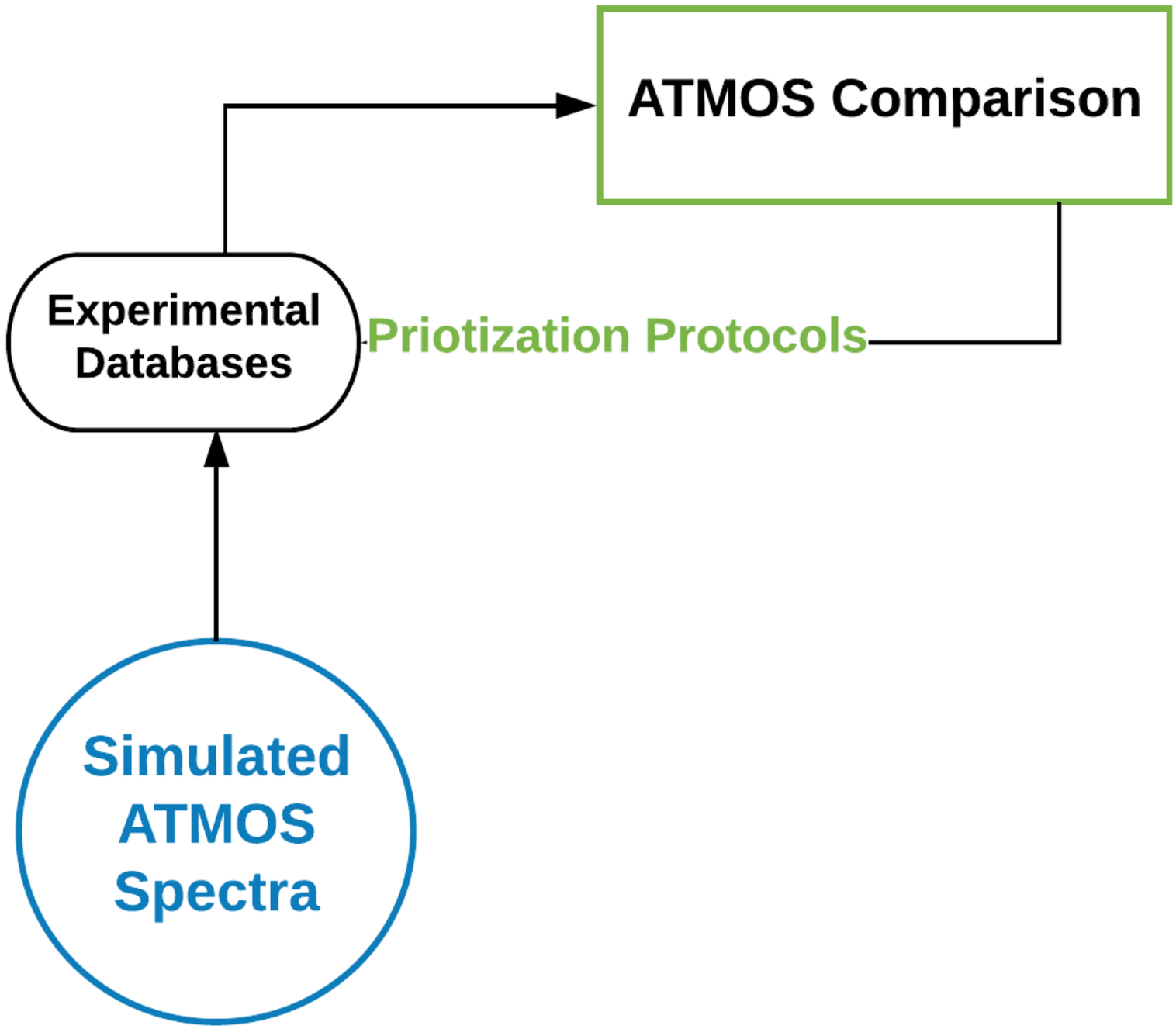
Theoretical

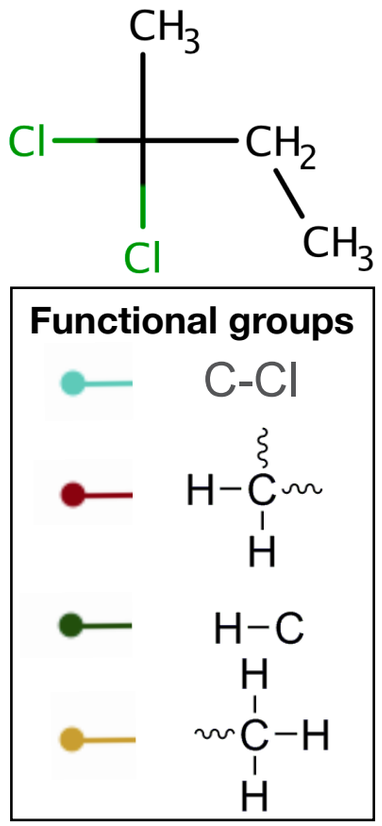
Molecular

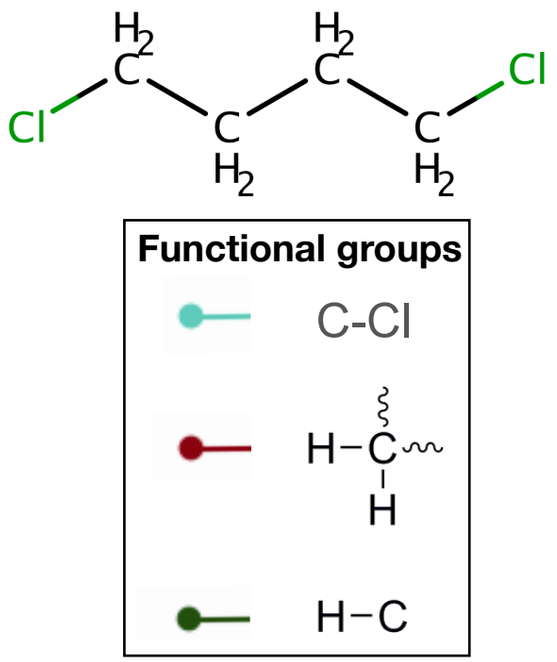
Spectra



ATMoS: Approximate Theoretical Molecular Spectra







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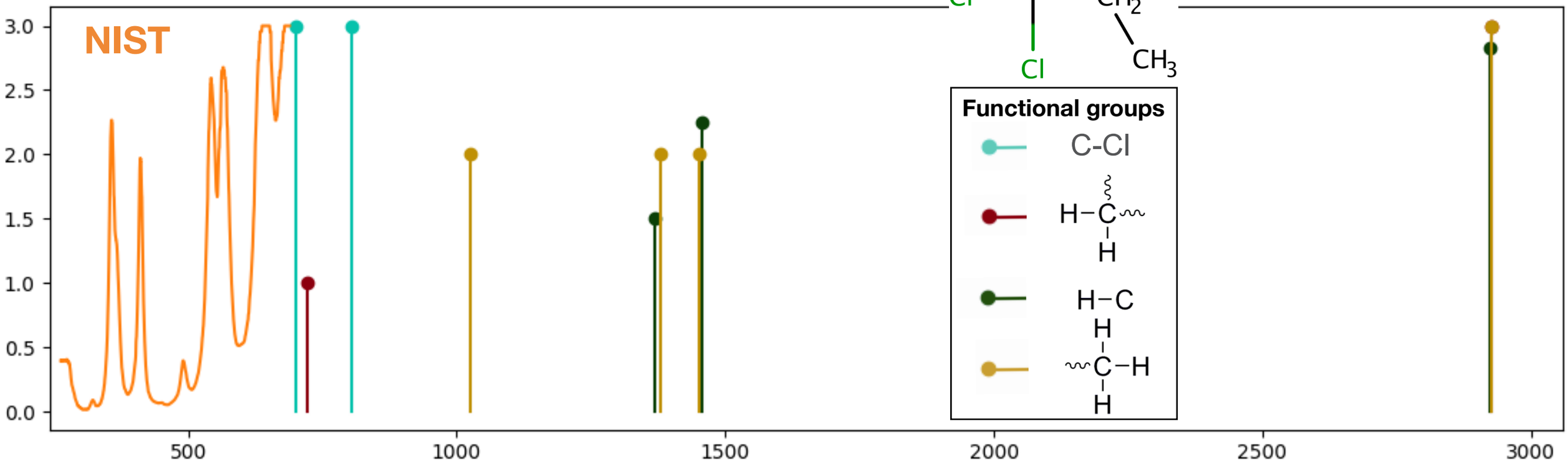

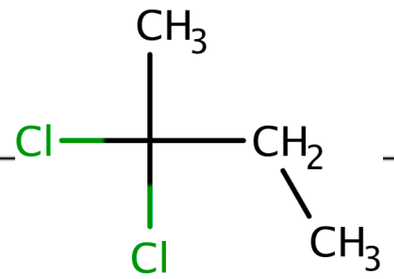

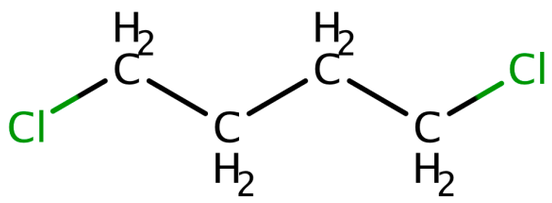

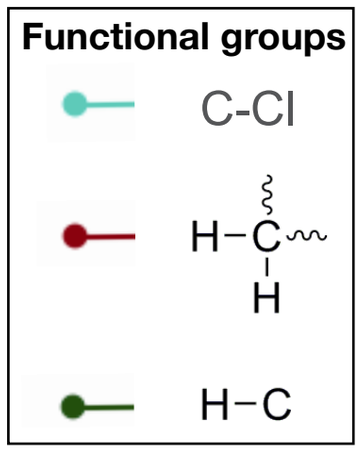

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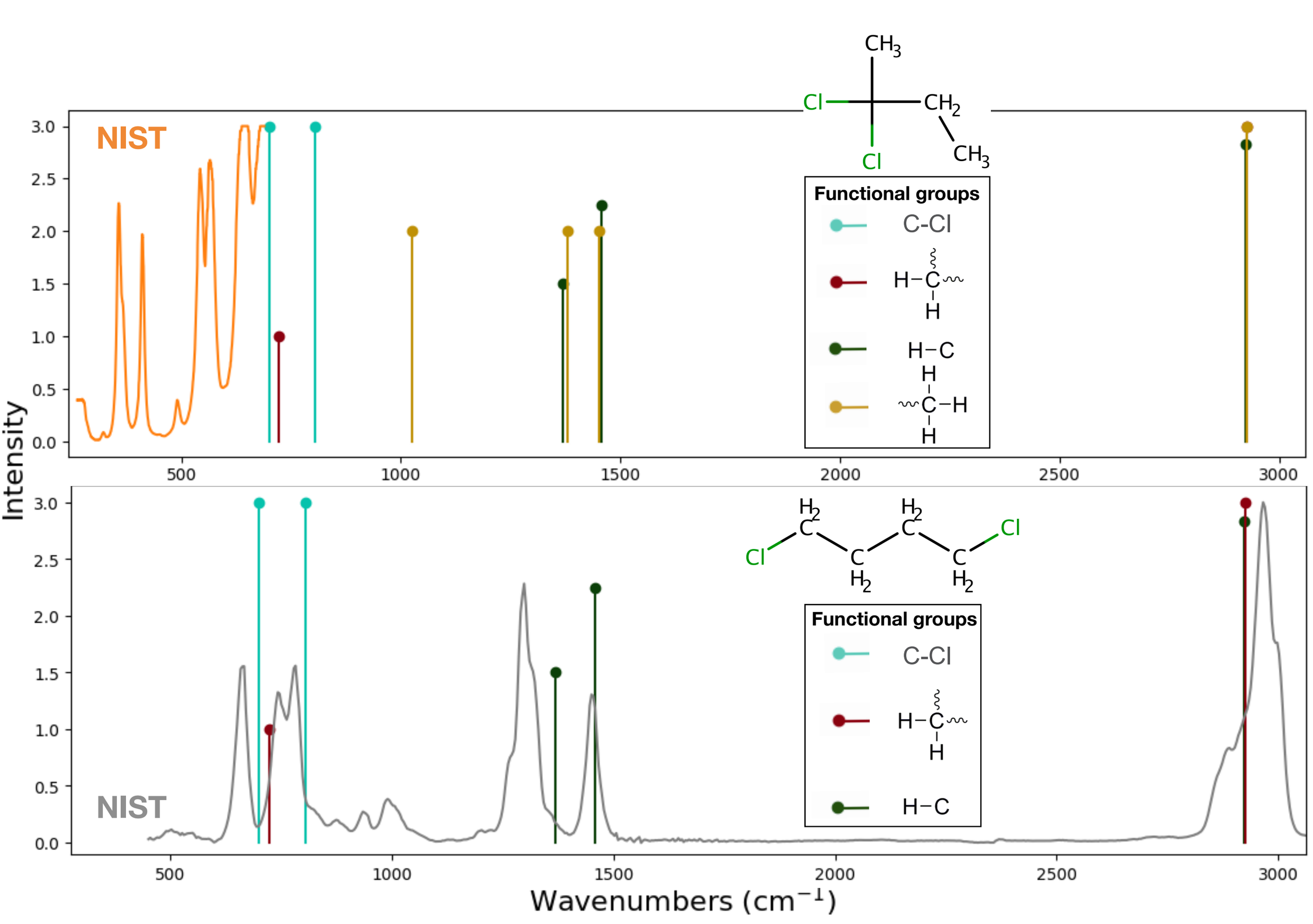
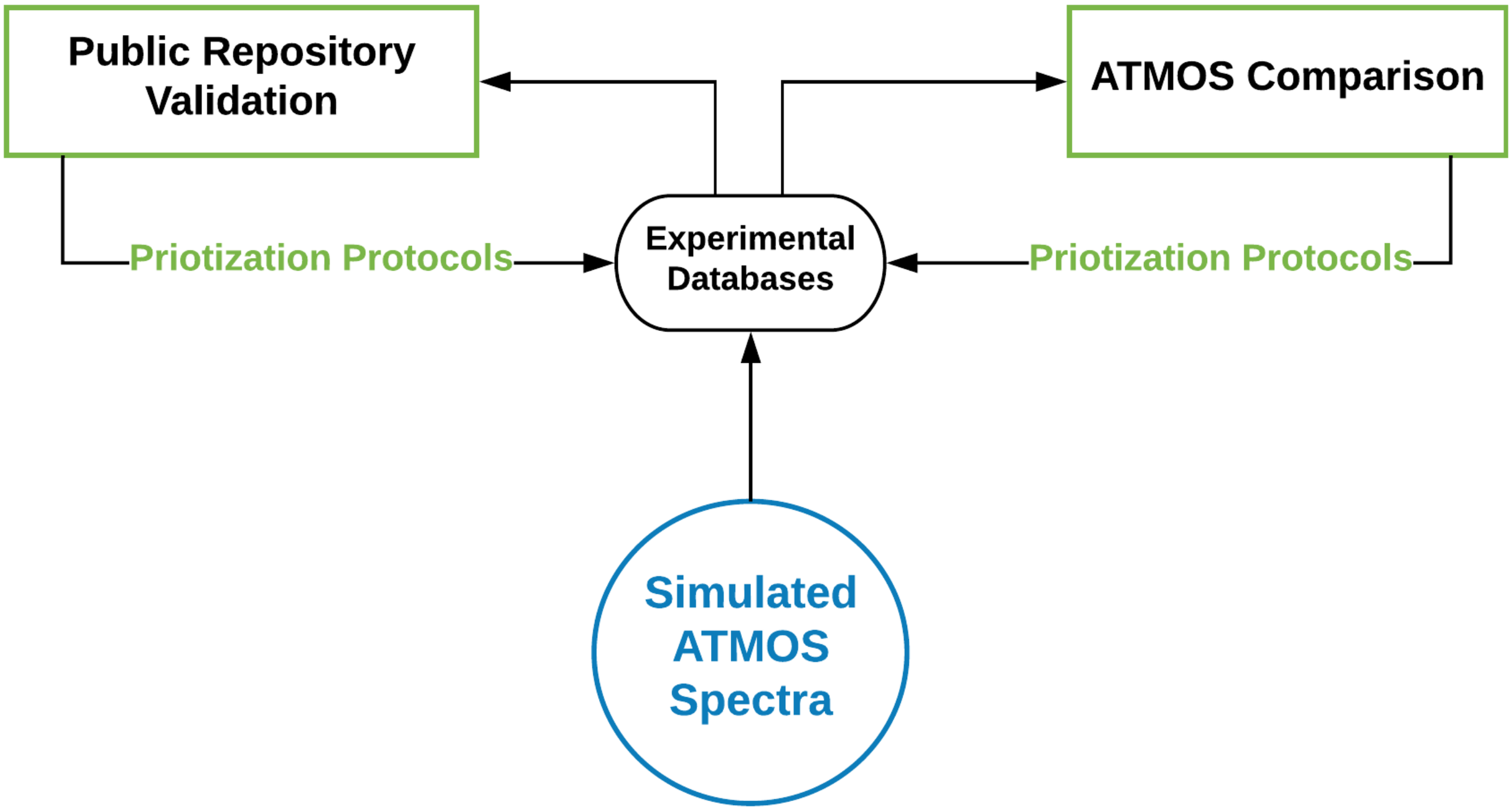
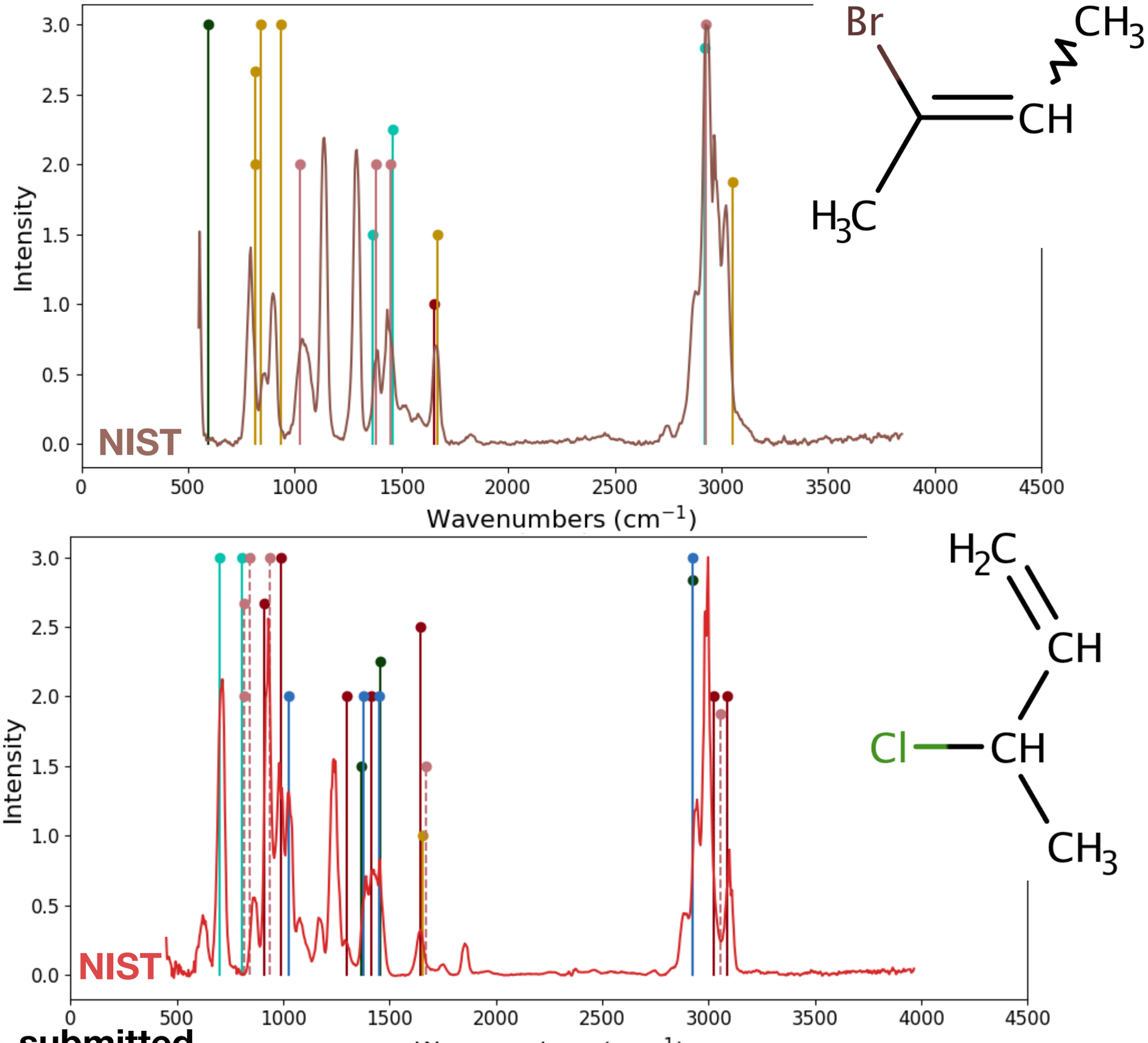


Sousa-Silva+ submitted

ATMoS: Approximate Theoretical Molecular Spectra

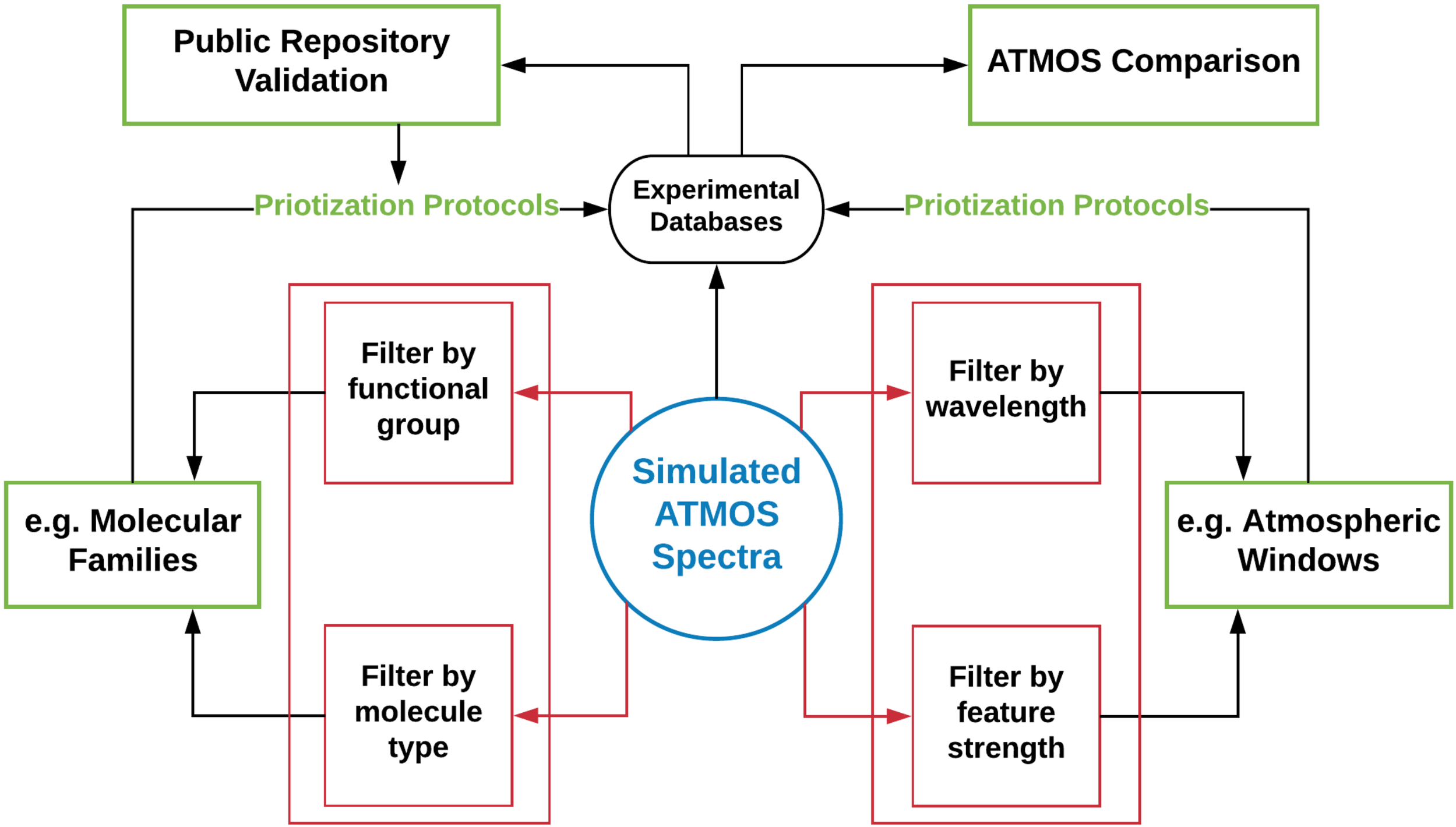


ATMoS: Approximate Theoretical Molecular Spectra

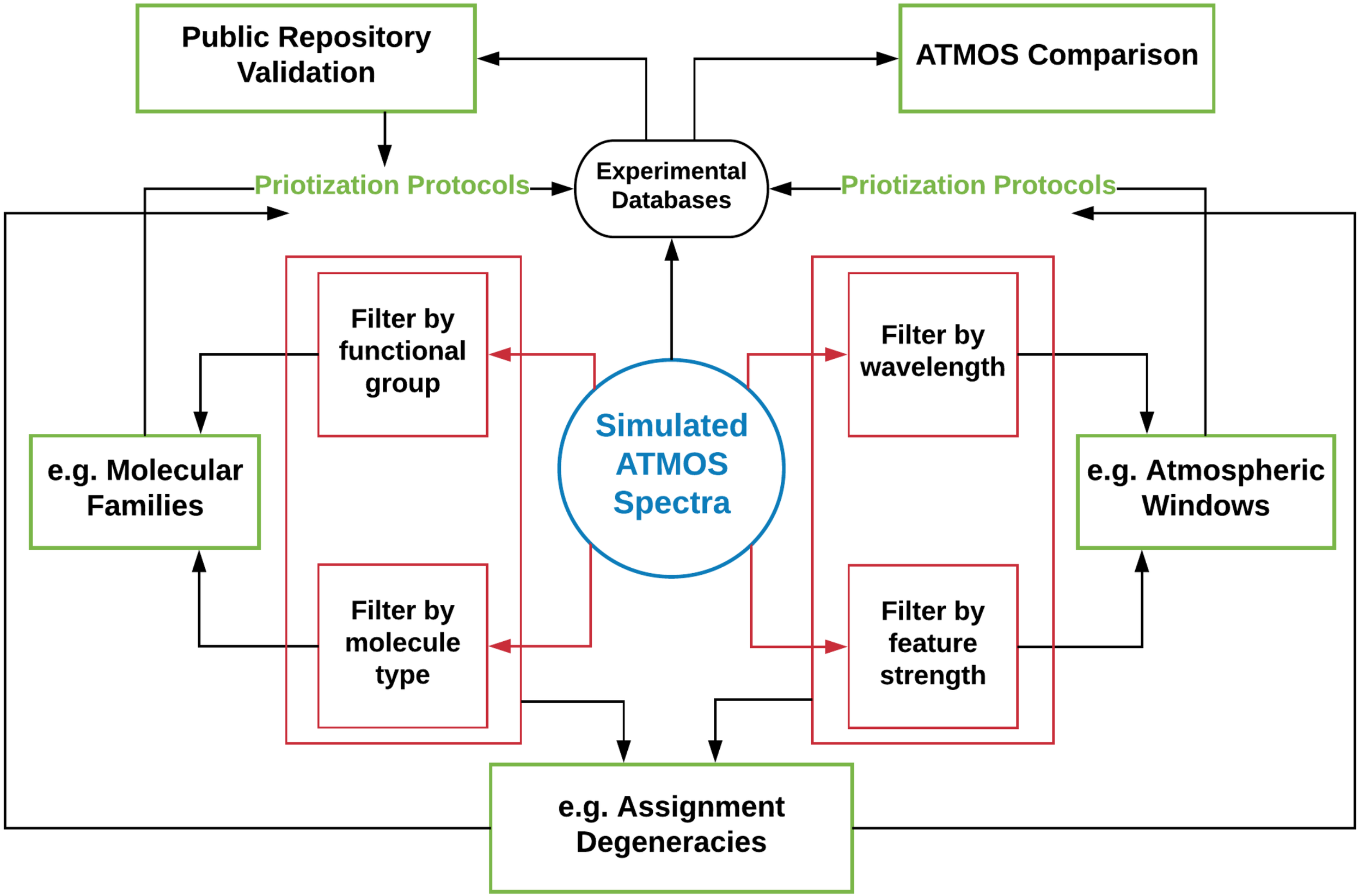


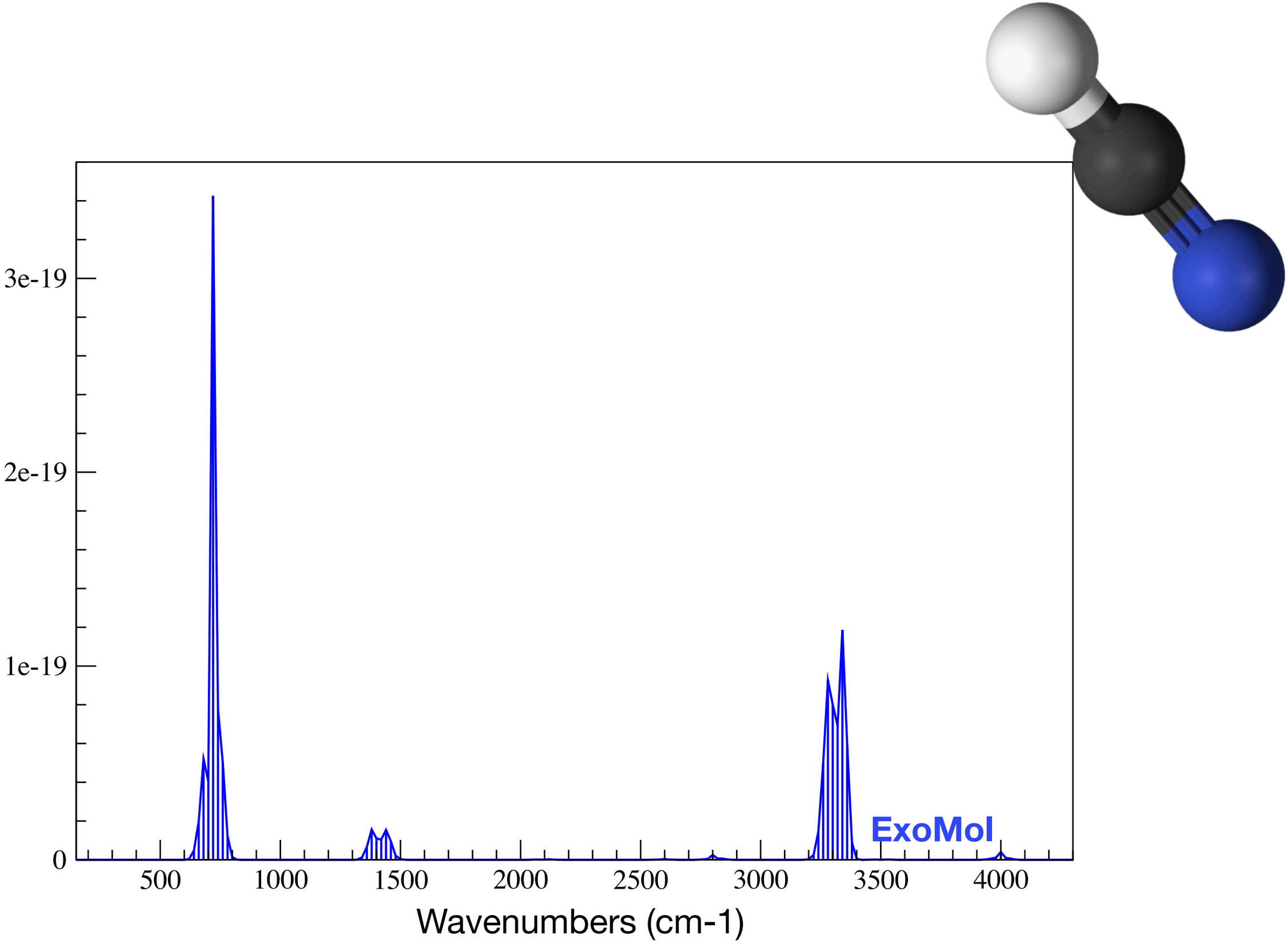
Sousa-Silva+ submitted

ATMoS: Approximate Theoretical Molecular Spectra

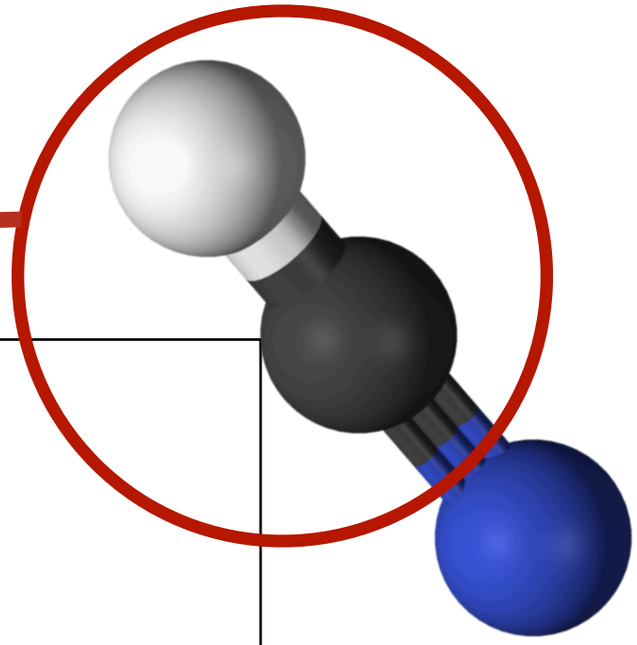


ATMoS: Approximate Theoretical Molecular Spectra




3e-19
2e-19
1e-19
0
500
1000
1500
2000
2500
3000
3500
4000
Wavenumbers (cm-1)
ExoMol

≡C-H



3e-19

2e-19

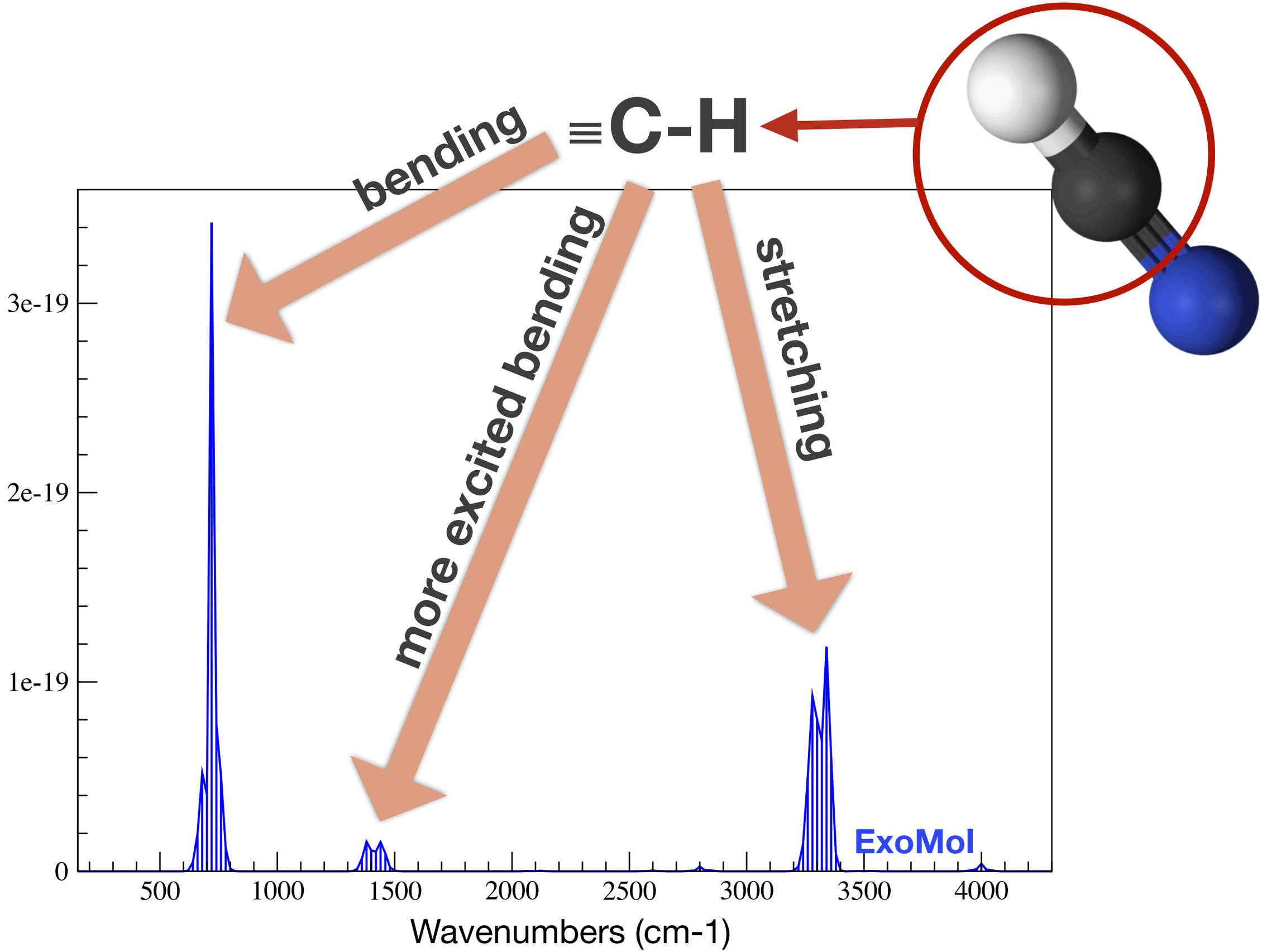
1e-19

0

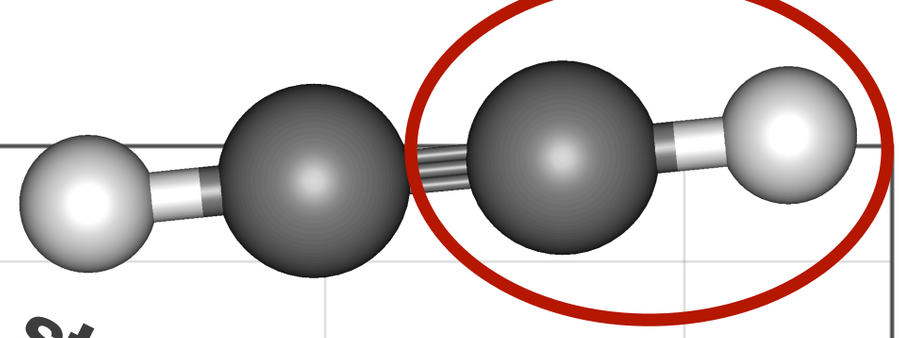
500 1000 1500 2000 2500 3000 3500 4000

Wavenumbers (cm-1)

ExoMol


≡C-H
bending
more excited bending
stretching
3e-19
2e-19
1e-19
0
500
1000
1500
2000
2500
3000
3500
4000
Wavenumbers (cm-1)
ExoMol

Acetylene (C_2H_2)



bending

bending

stretching

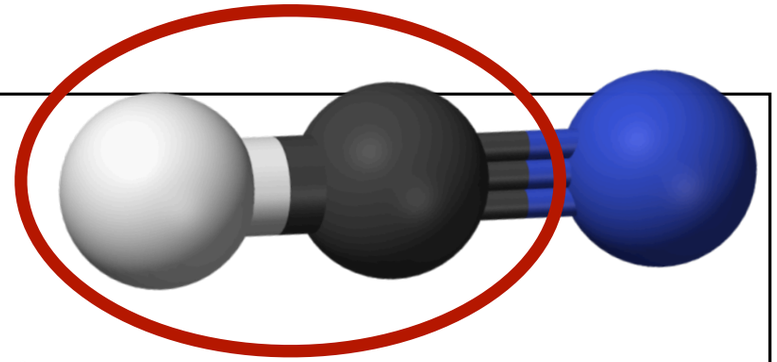
NIST

Absorbance

2.5
2.0
1.5
1.0
0.5
0.0
-0.5

500
1000
1500
2000
2500
3000
3500

Hydrogen Cyanide (HCN)



bending

bending

stretching

ExoMol

3e-19
2e-19
1e-19
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2000
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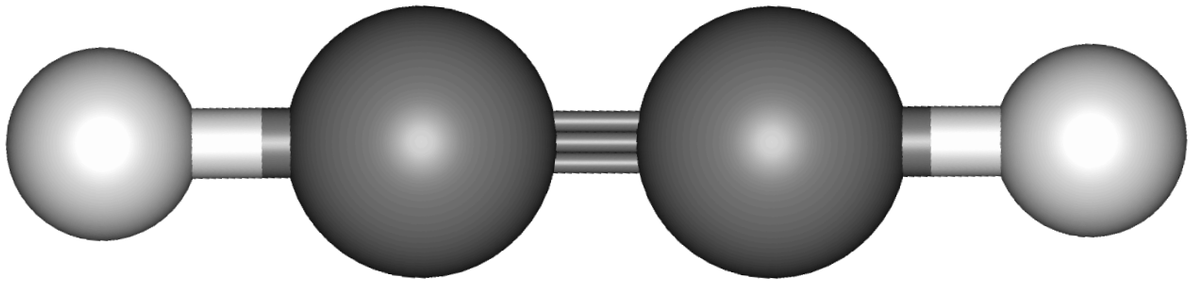
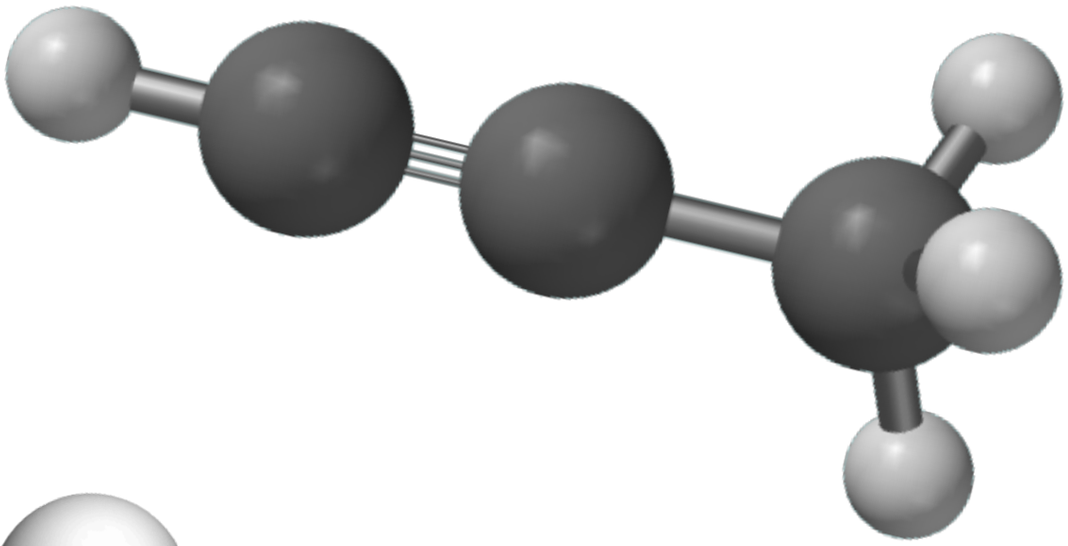
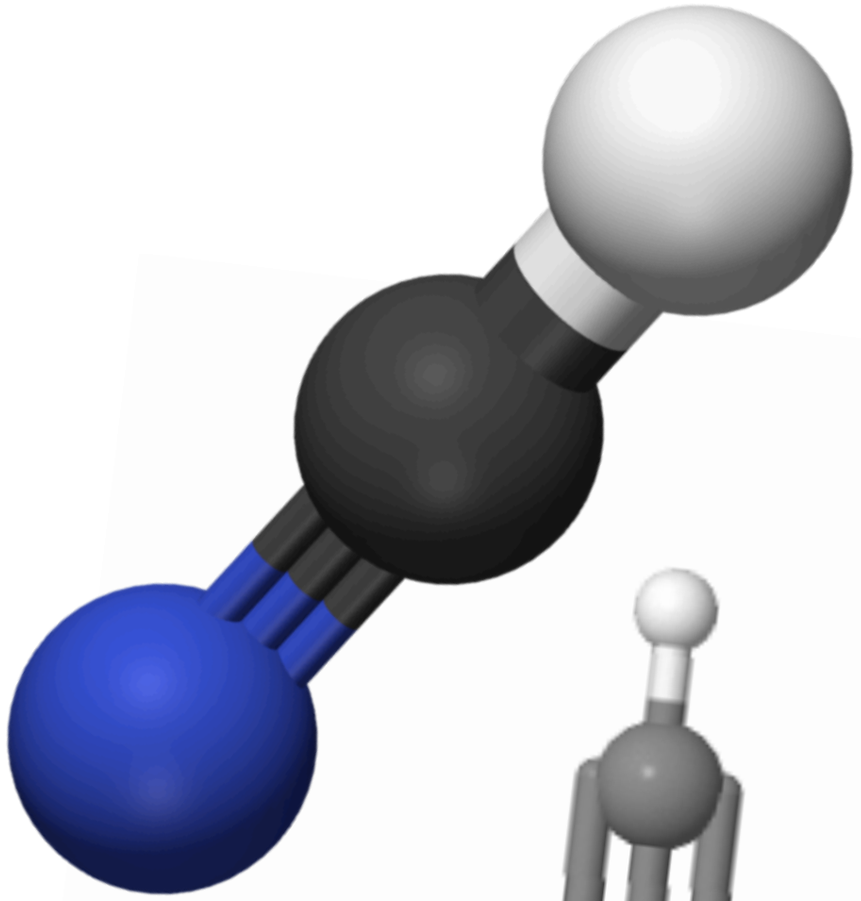
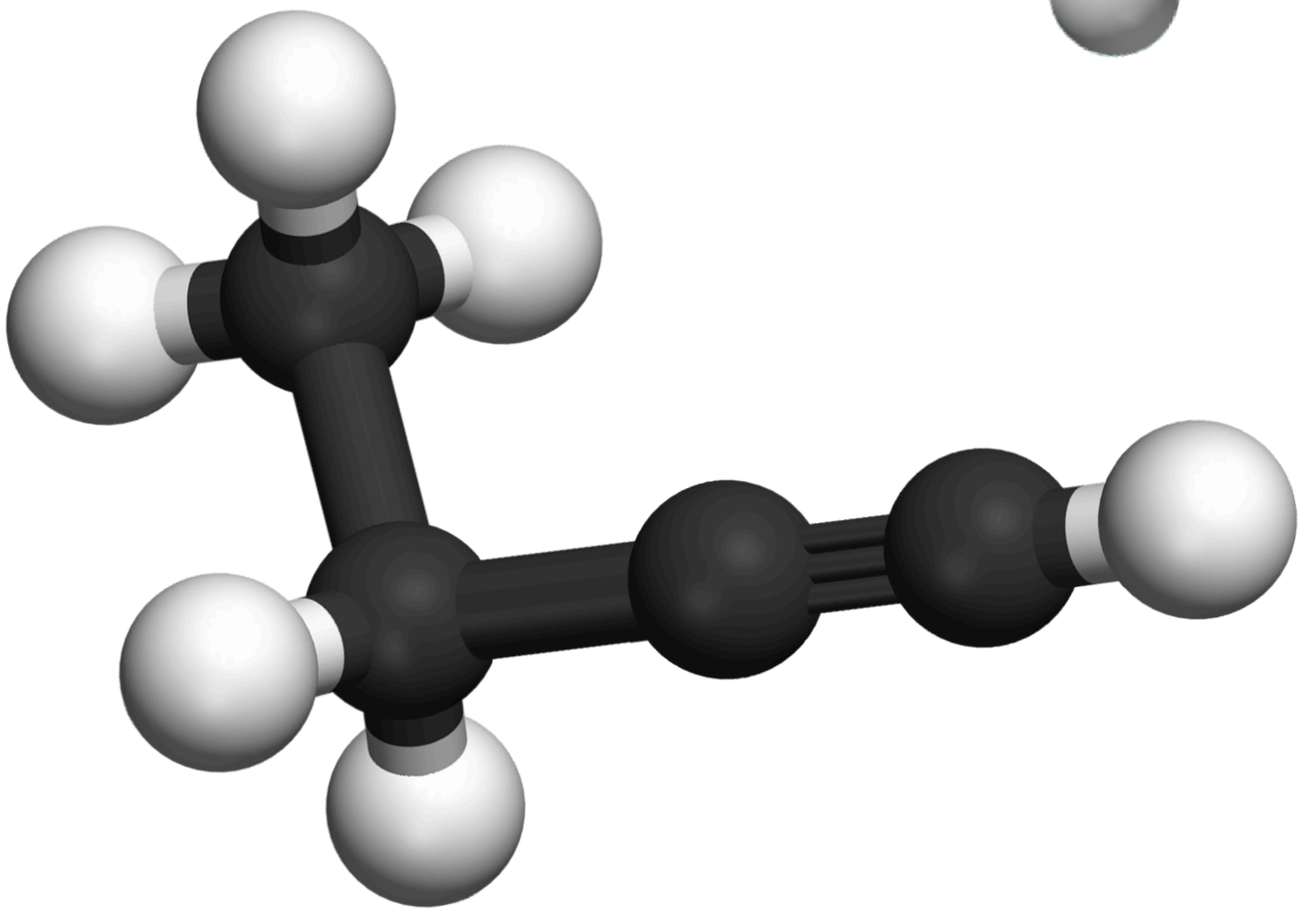
3000
3500

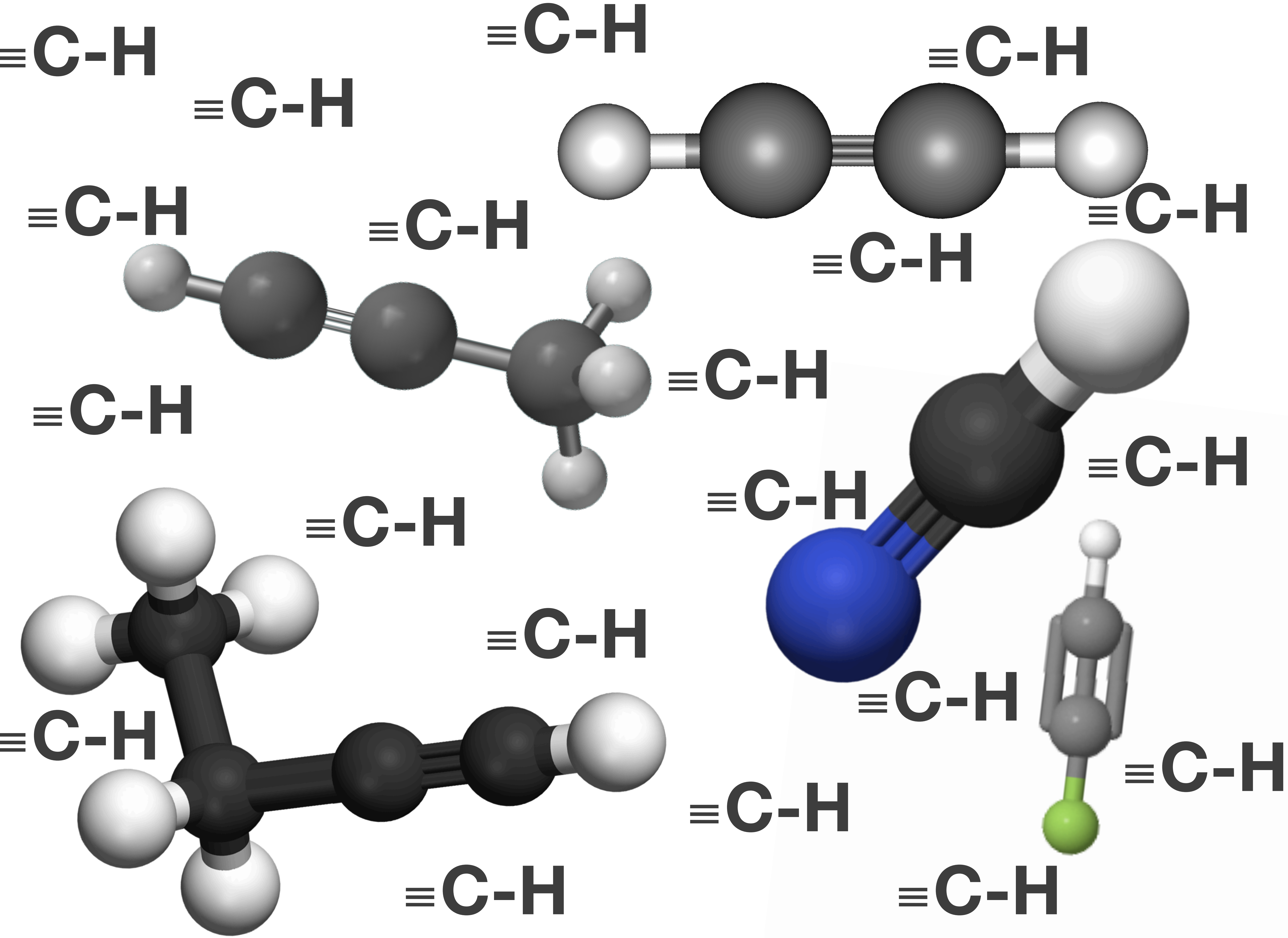
Wavenumbers (cm-1)










≡C-H
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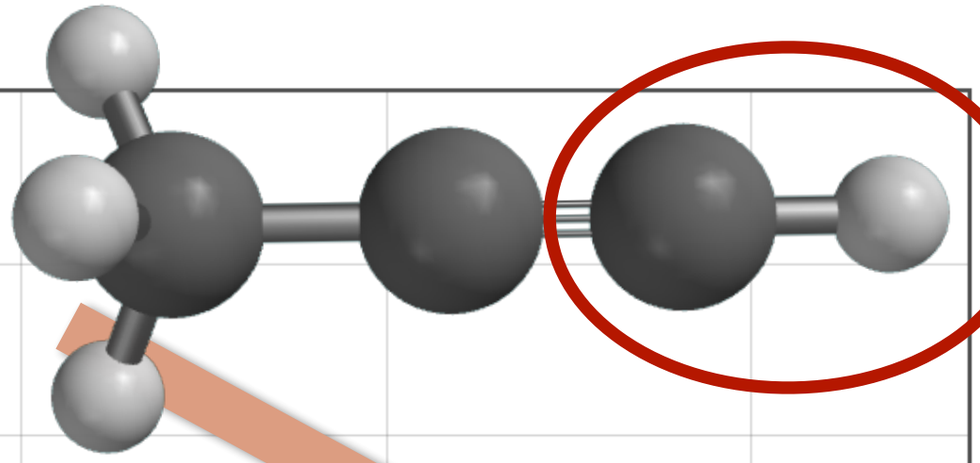
≡C-H

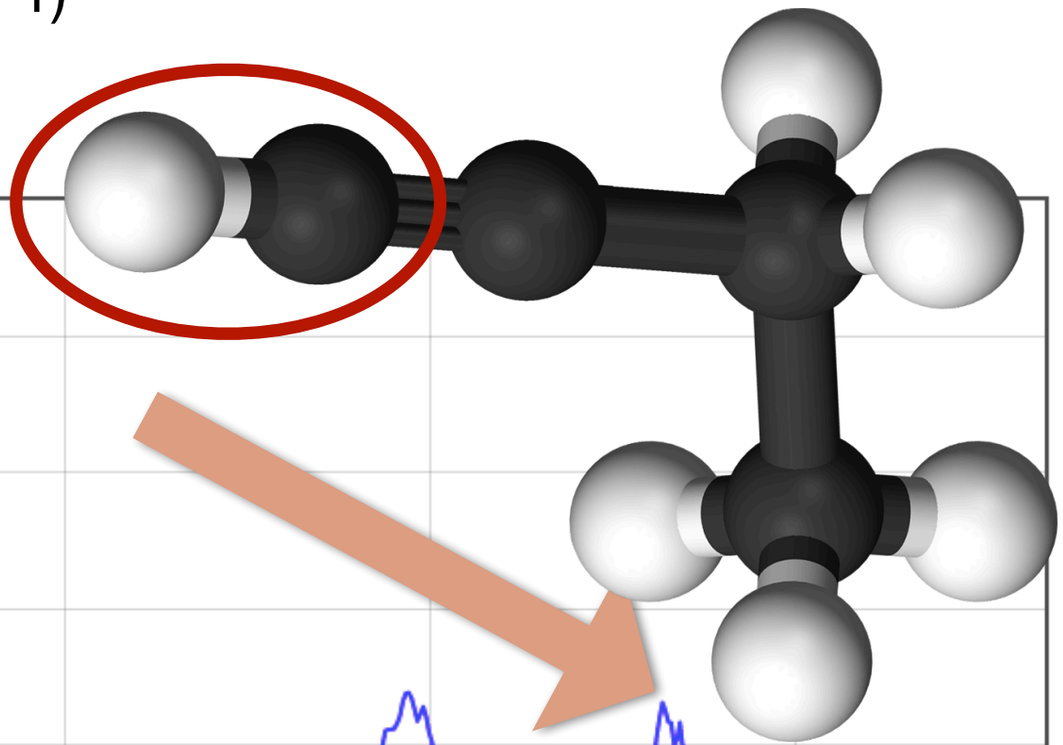
NIST

Propyne



Wavenumbers (cm-1)

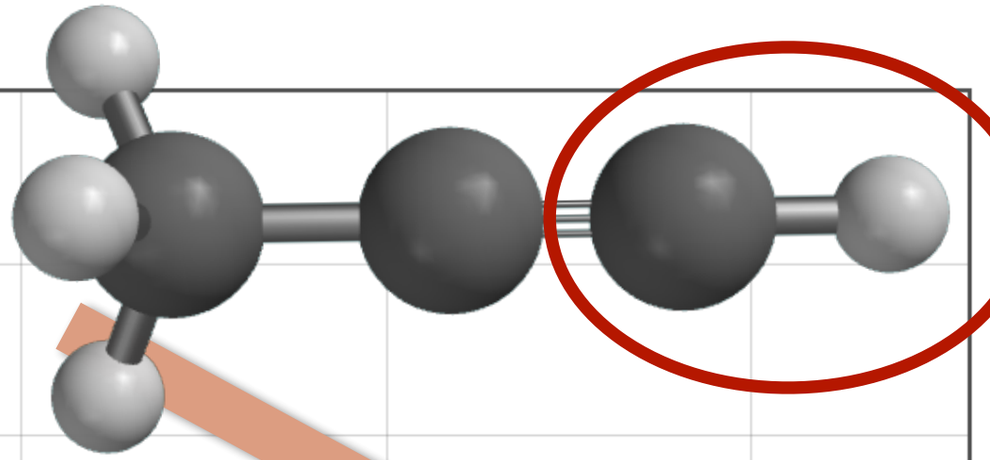
1-Butyne



NIST

NIST

Propyne



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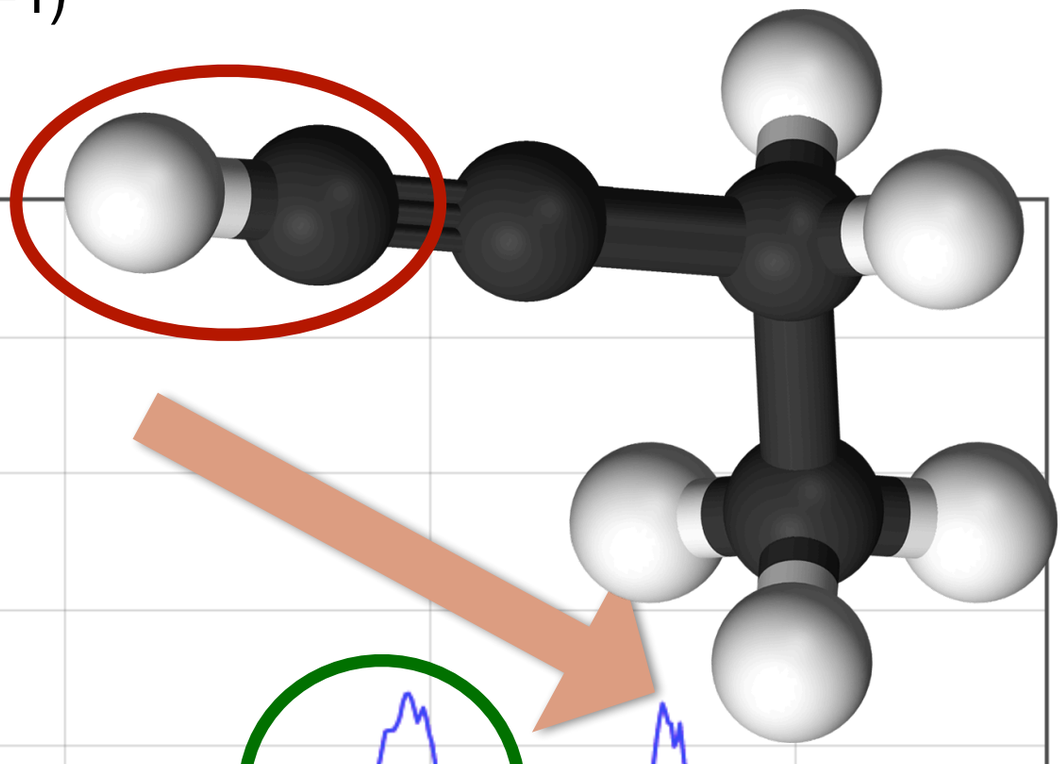


NIST

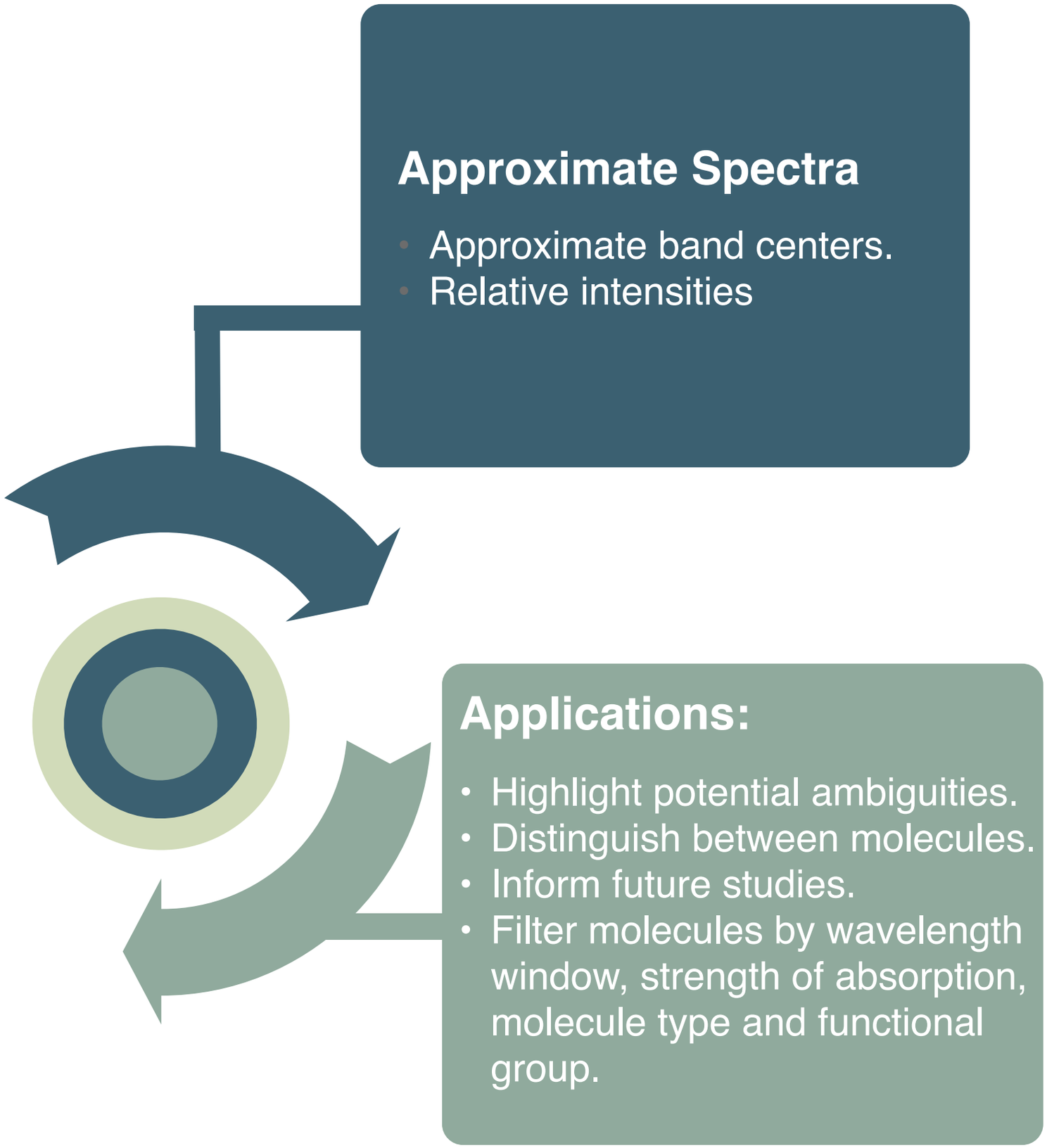
ATMoS:

Approximate

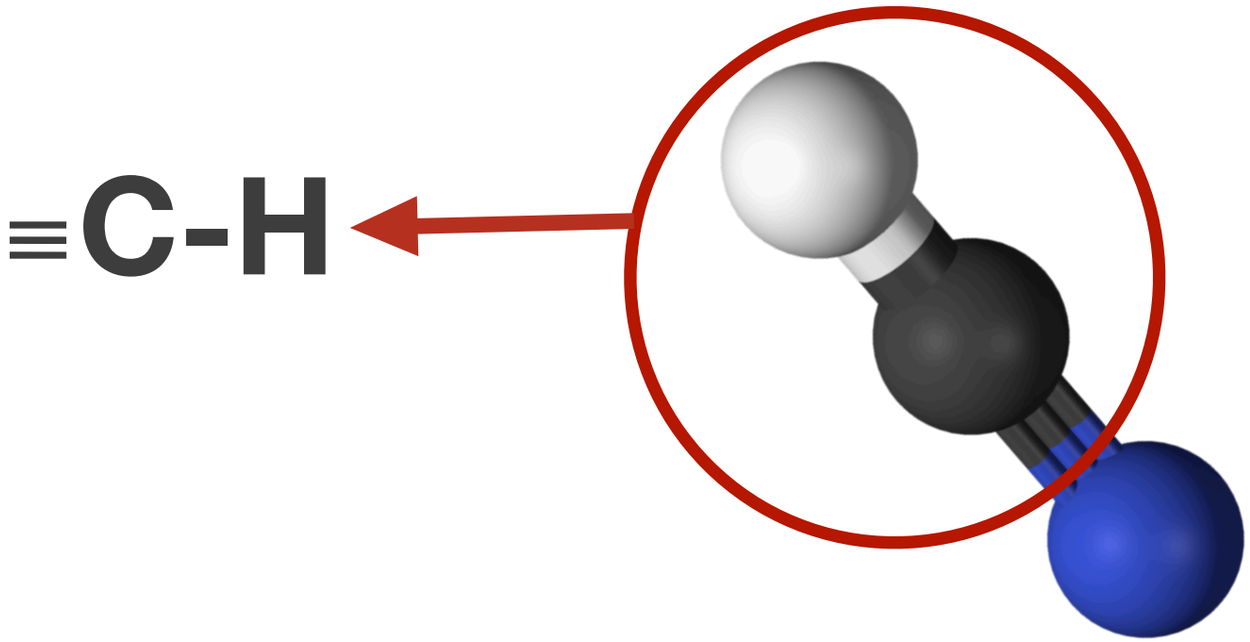
Theoretical

Molecular

Spectra



ATMoS 1.1: Muted functionals



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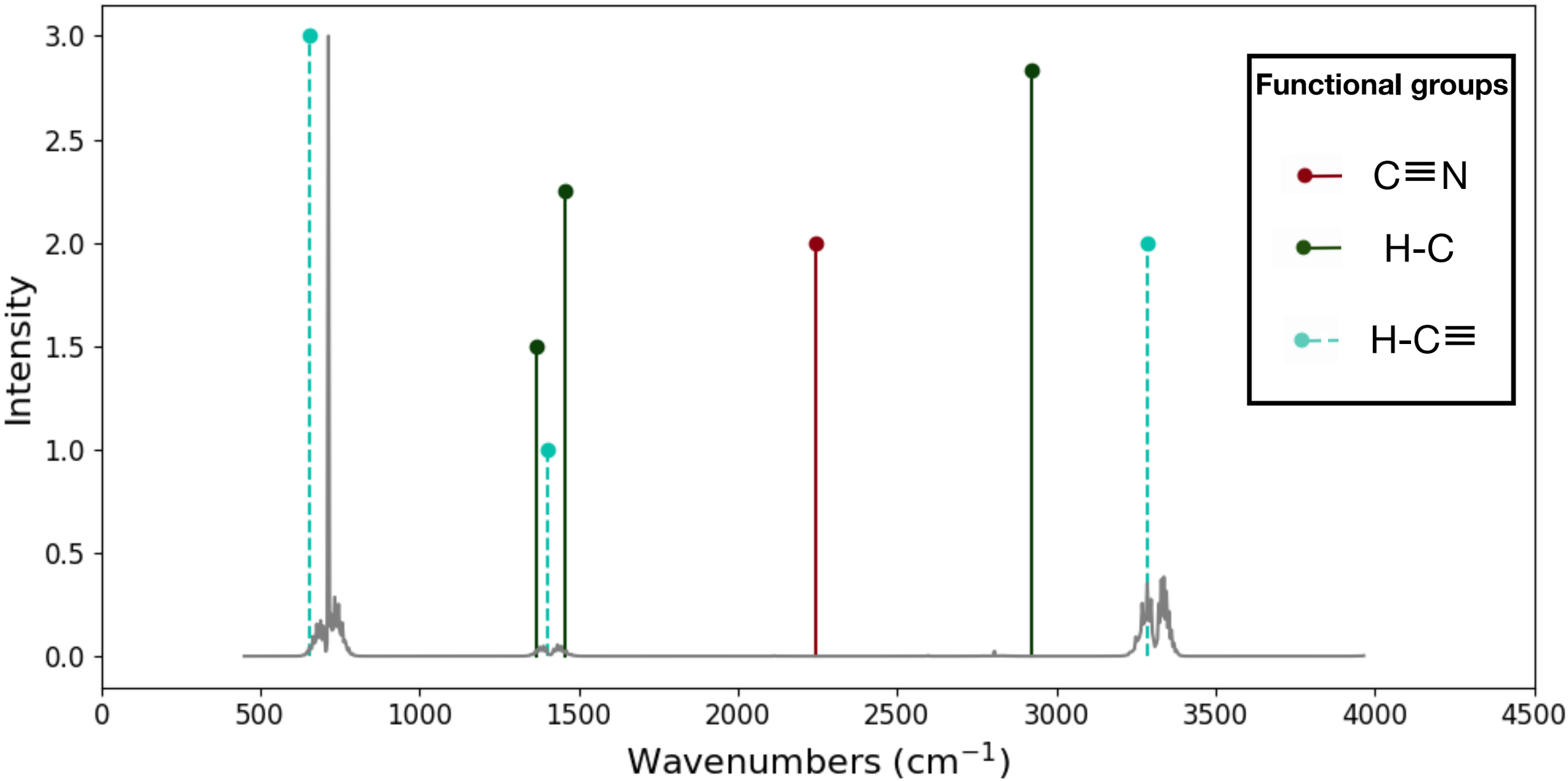
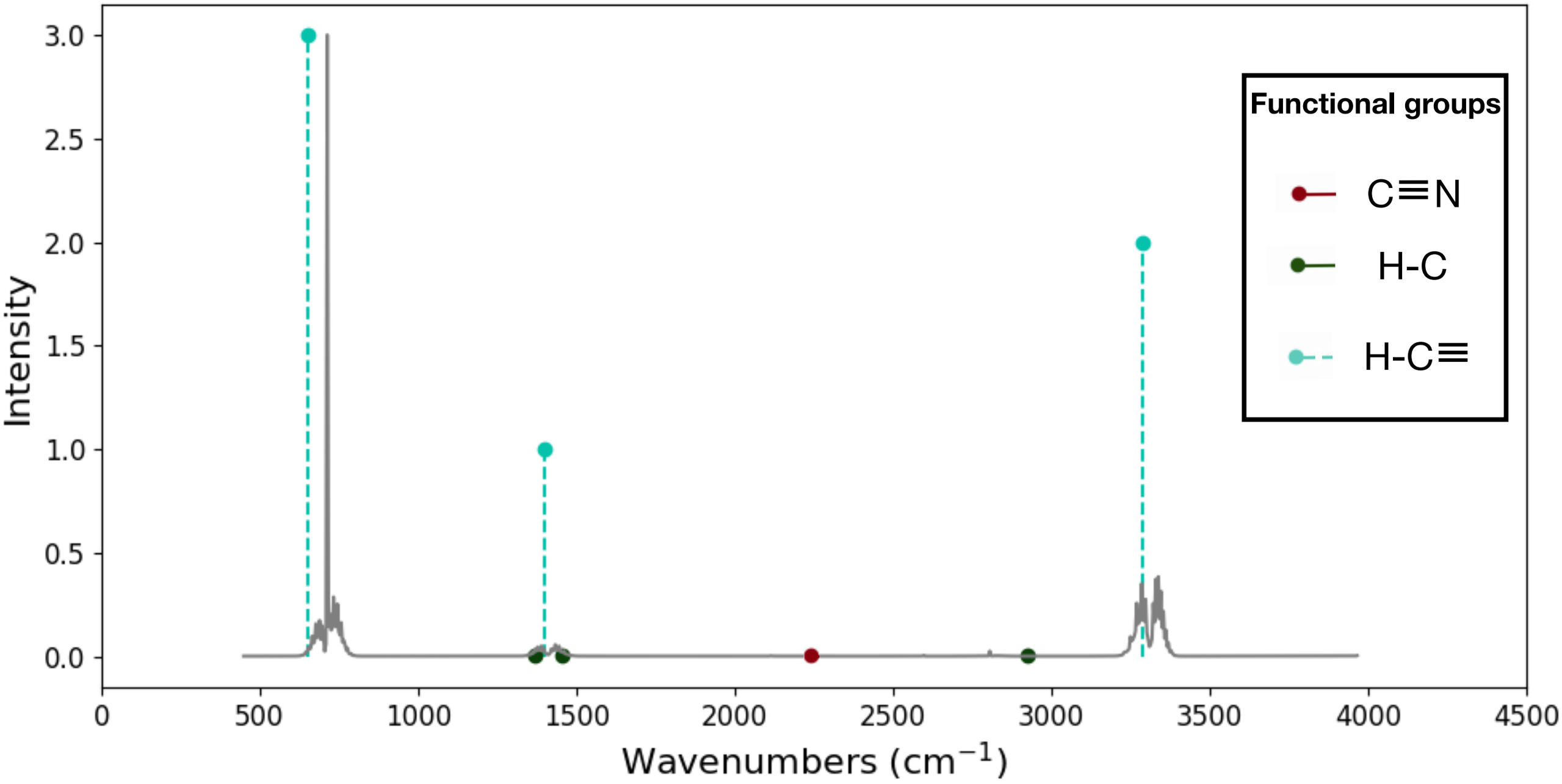
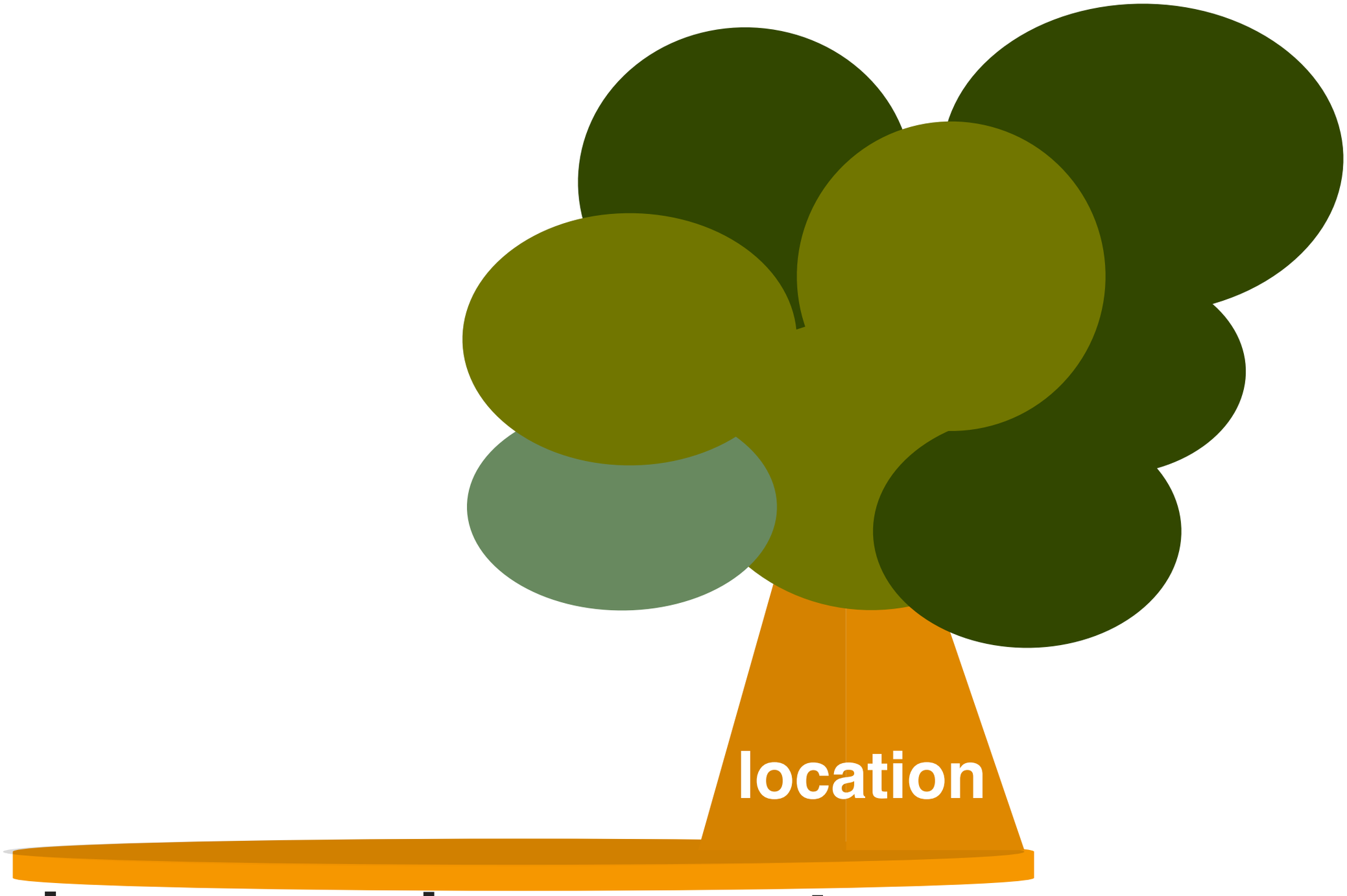


ATMoS 1.1: Muted functionals

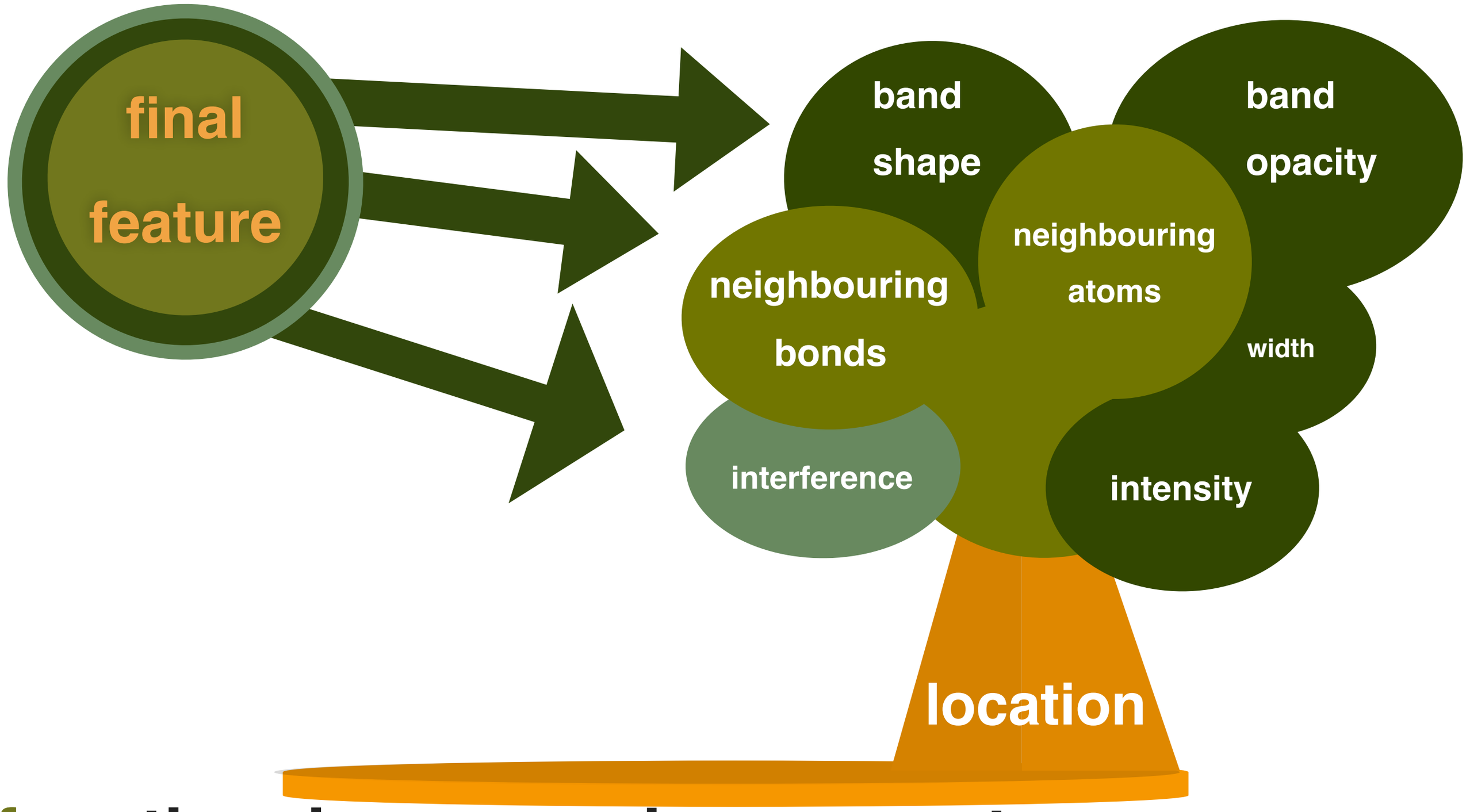


ATMoS 1.2

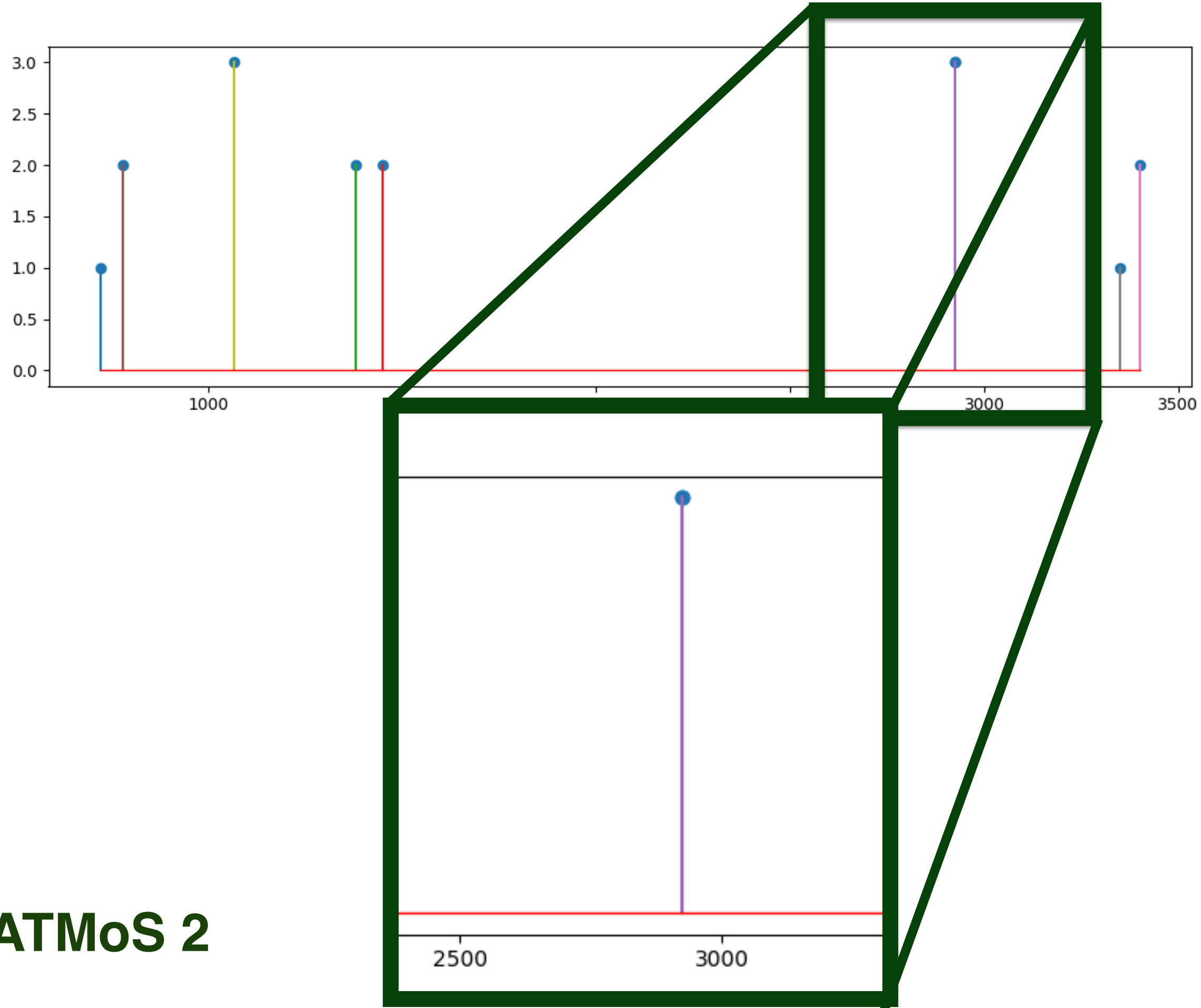


functional group enhancement

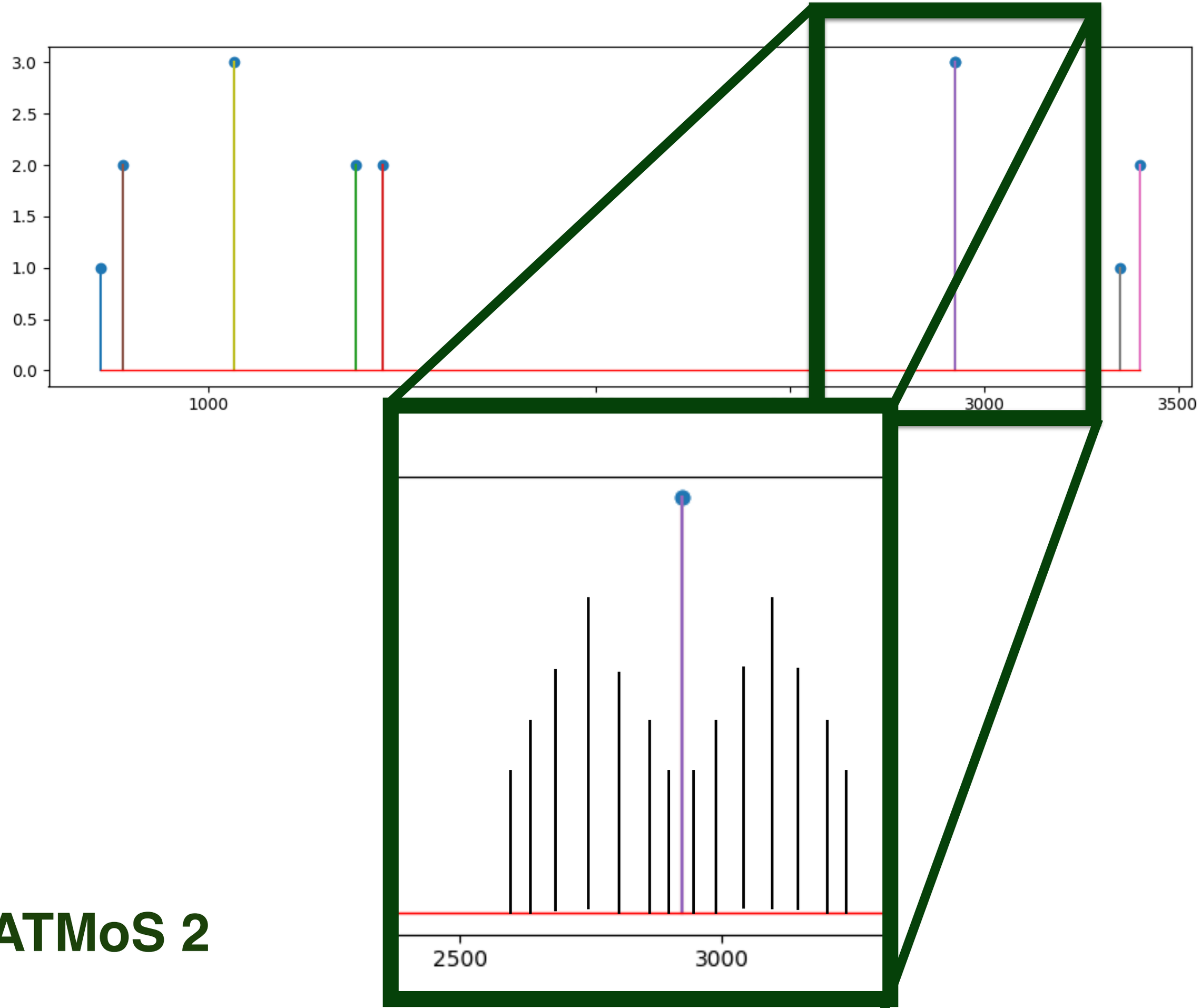
ATMoS 1.2



functional group enhancement



ATMoS 2



ATMoS 2

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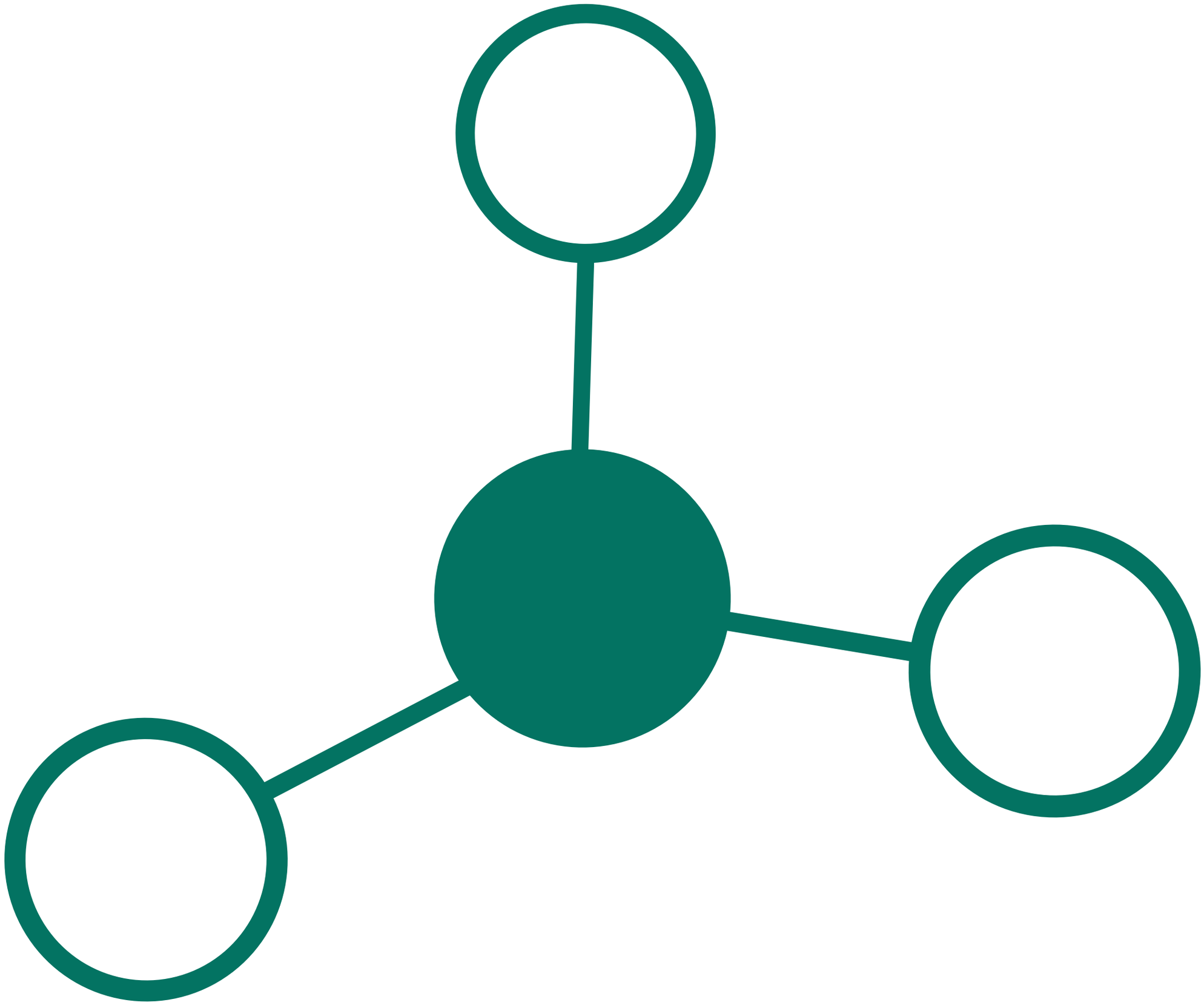

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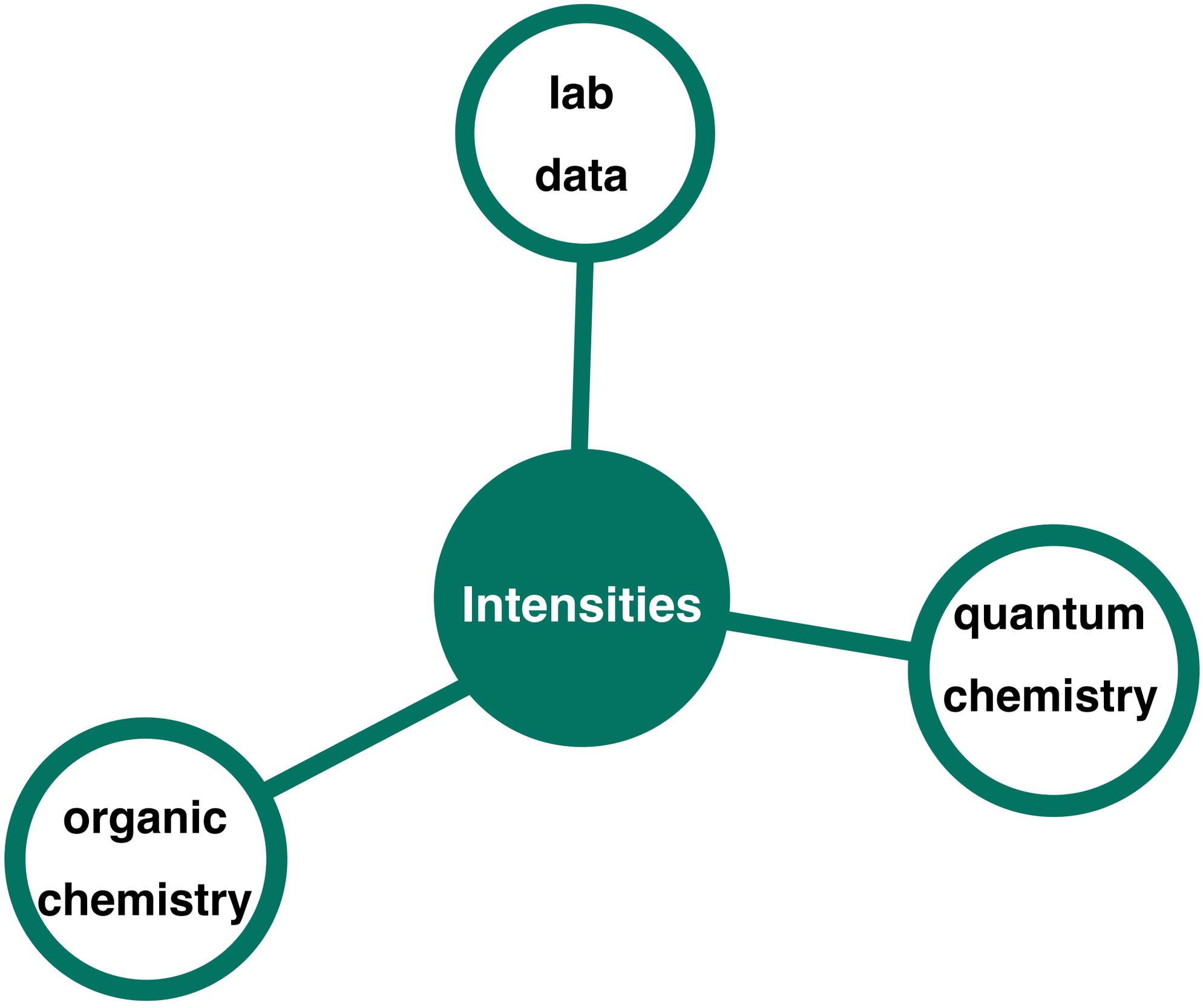
lab
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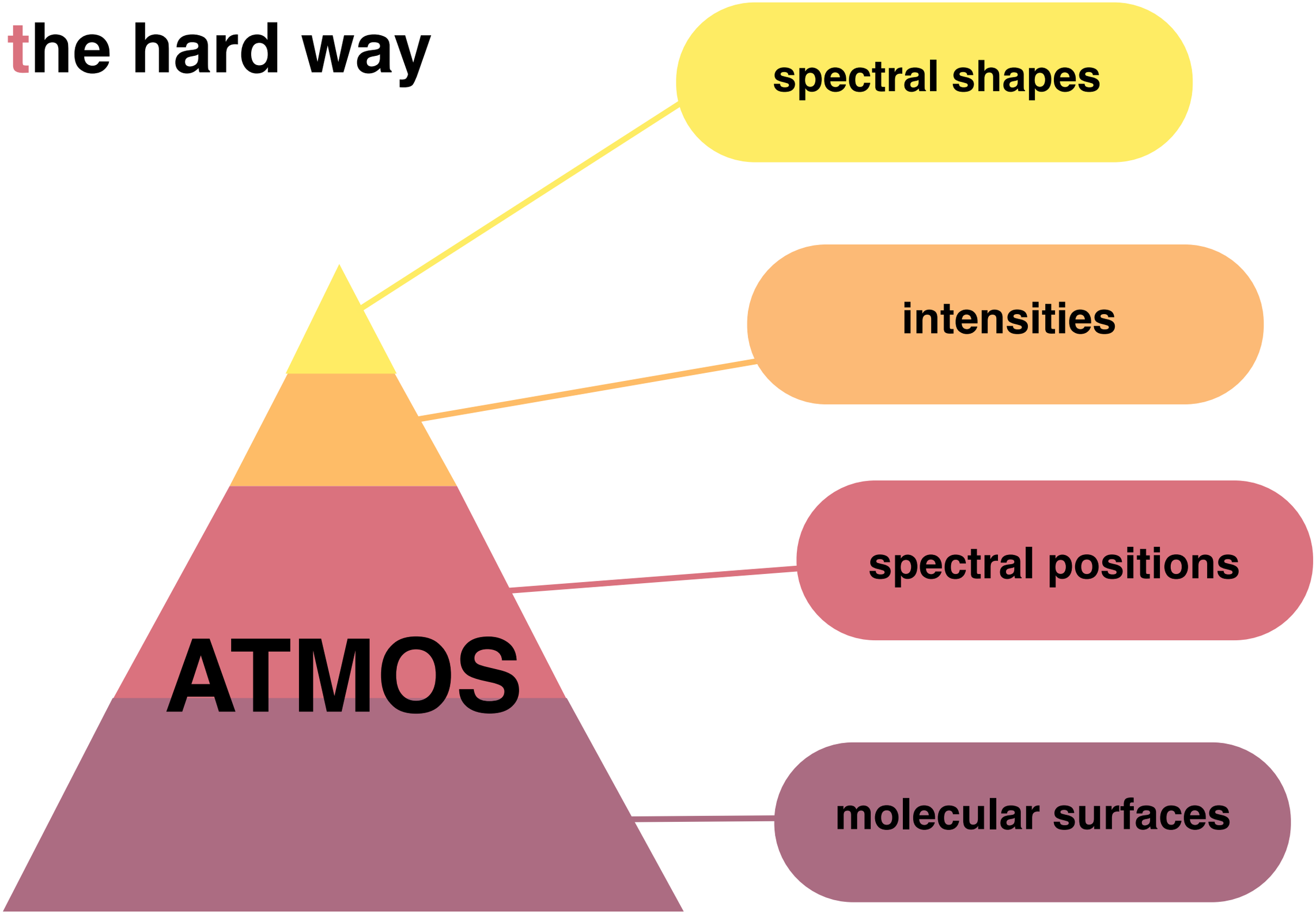
Intensities
organic
chemistry
quantum
chemistry

the hard way

ATMoS 2

the hard way



ATMoS 2

ATMoS:

Approximate

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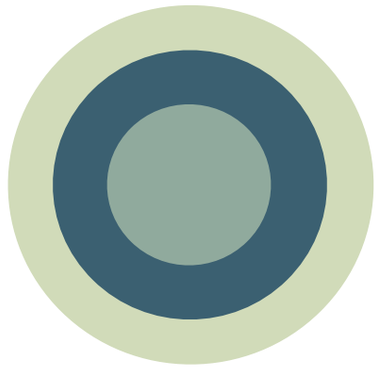
Spectra



ATMoS:

Approximate

Theoretical

Molecular

Spectra

Approximate Spectra

- Approximate band centers.
- Relative intensities
- Artificial band shapes (e.g. line functions).
- Band shapes with rigid-rotor approximation.
- Functional group enhancement.

Molecular Analysis and Triage:

- Highlight ambiguities.
- Distinguish between molecules.
- Filter molecules by wavelength window and strength of absorption.

Enhancements

- Modified functional group position and intensities.
- Bespoke functional groups.
- Rigid rotor approximation.
- Quantum chemistry for absolute intensities.

END