ASTROAGENTS

AGENTIC AI AT THE DAWN OF LIFE

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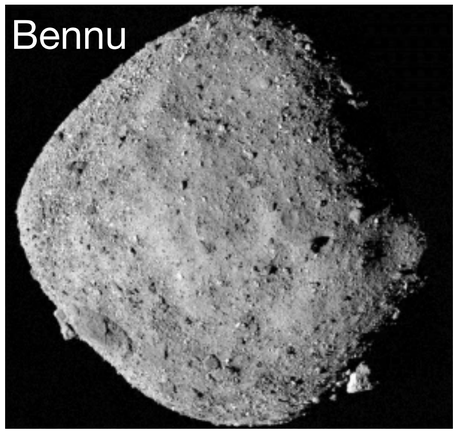
Quick overview

- Our recent works at the intersection of **Gen AI** and **astrobiology** on origins of life
  - ***LifeTracer*****:** Discriminating Abiotic and Biotic Organics in Meteorite and Terrestrial Samples (*PNAS Nexus*, in press)
  - ***AstroAgents v1*****:** A Multi-Agent AI for Hypothesis Generation from Mass Spectrometry Data (*ICLR*, Agentic workshop)
- Future collaborations with Microsoft on expanding hypothesis generation

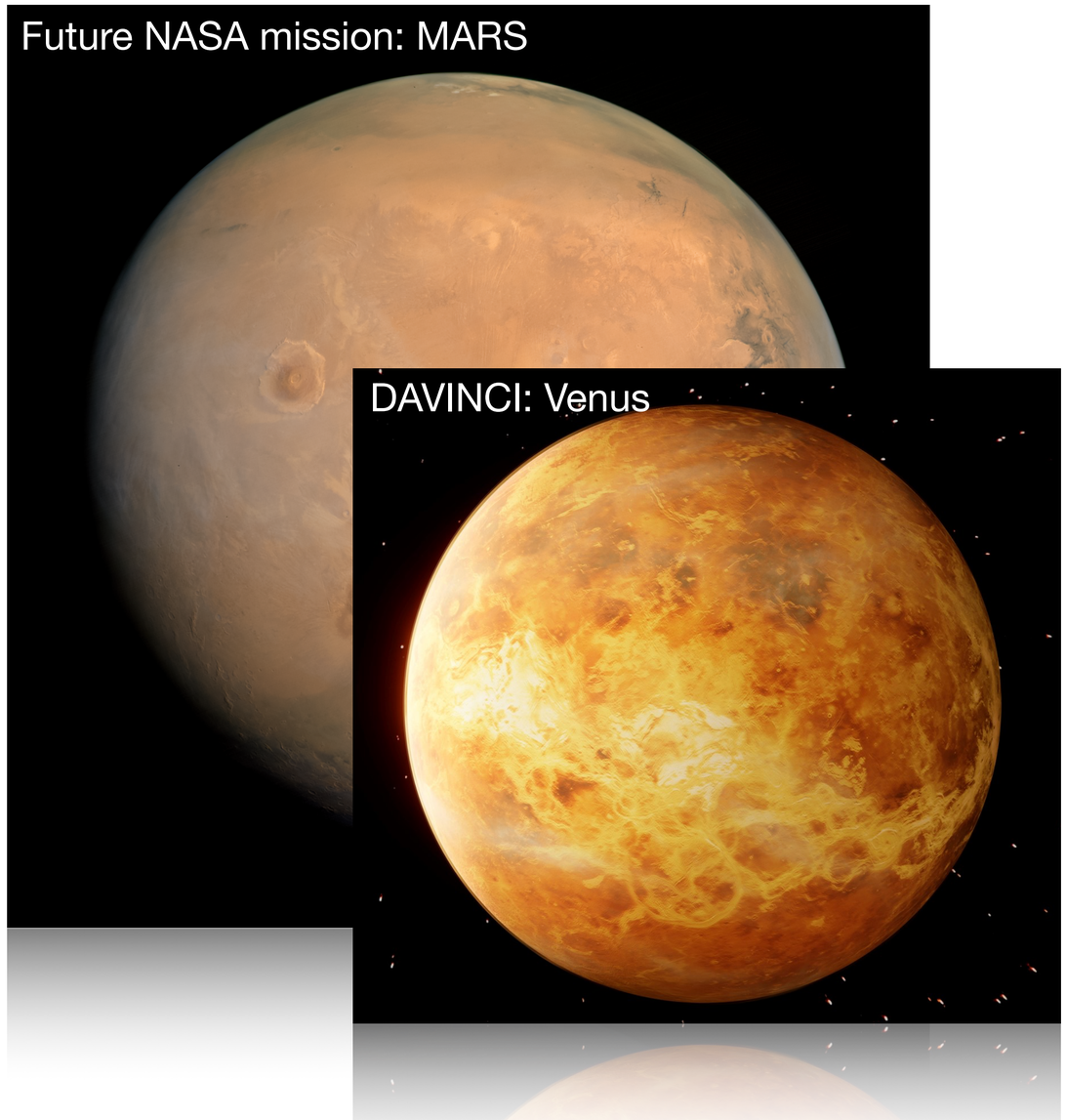
Sample return missions: **need for tools to detect alien life**



The New York Times

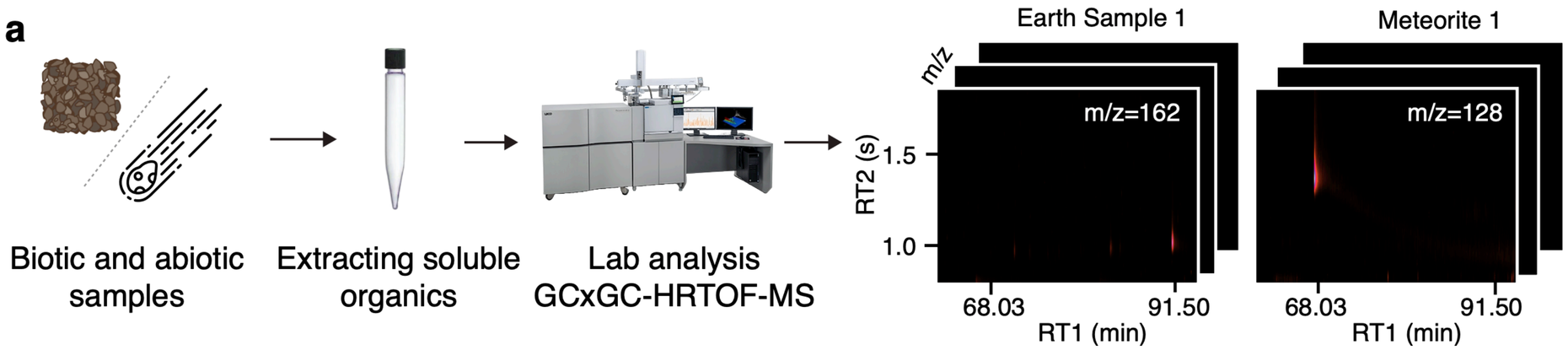
Lurking Inside an Asteroid: Life's Ingredients

Scientists studying samples that NASA collected from the asteroid Bennu found a wide assortment of organic molecules that shed light on how life arose.

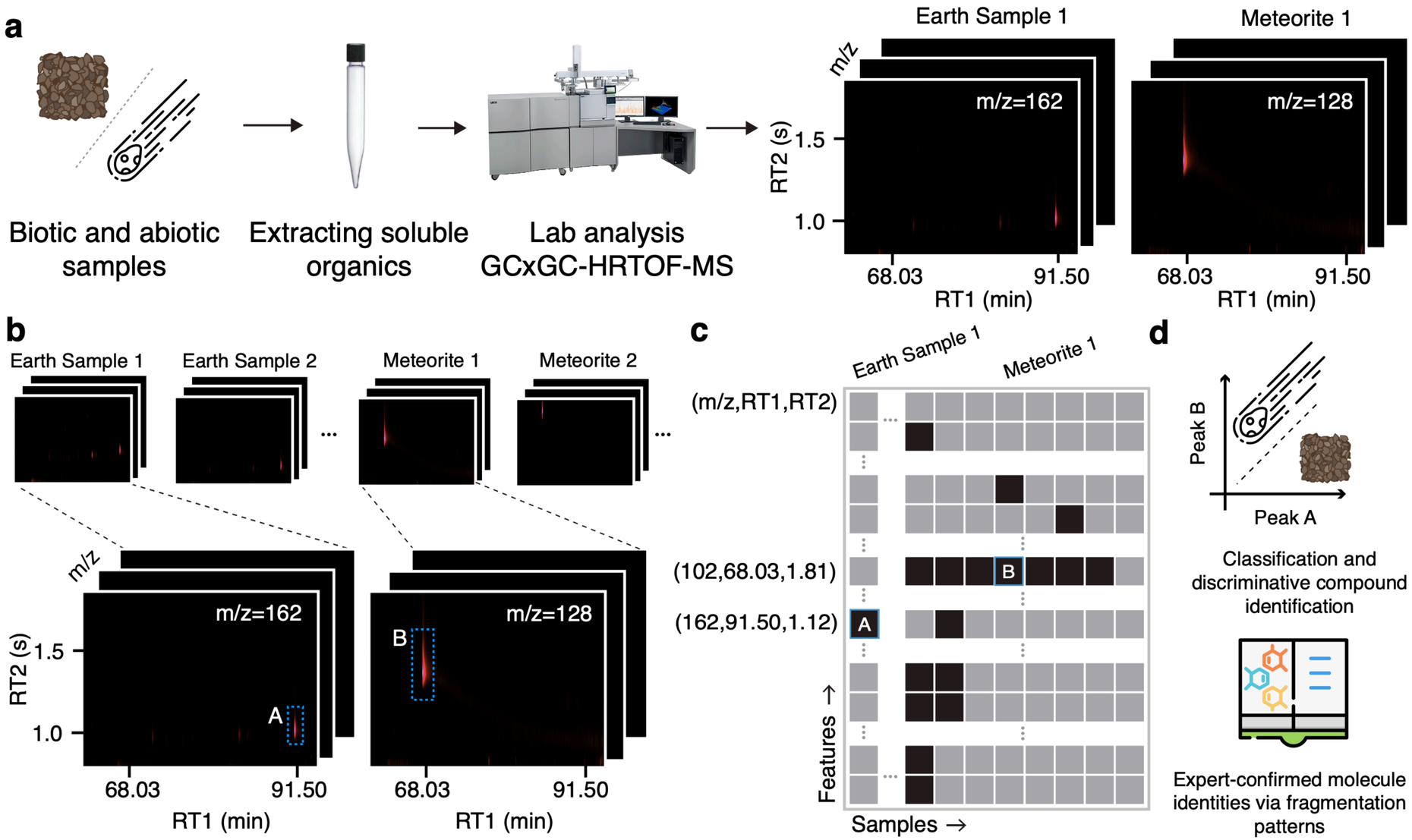


https://science.nasa.gov/mission/osiris-rex/

LifeTracer


a
Biotic and abiotic samples
Extracting soluble organics
Lab analysis GCxGC-HRTOF-MS
Earth Sample 1
Meteorite 1
m/z
m/z=162
m/z=128
RT2 (s)
1.5
1.0
68.03
91.50
RT1 (min)

LifeTracer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m/z=162
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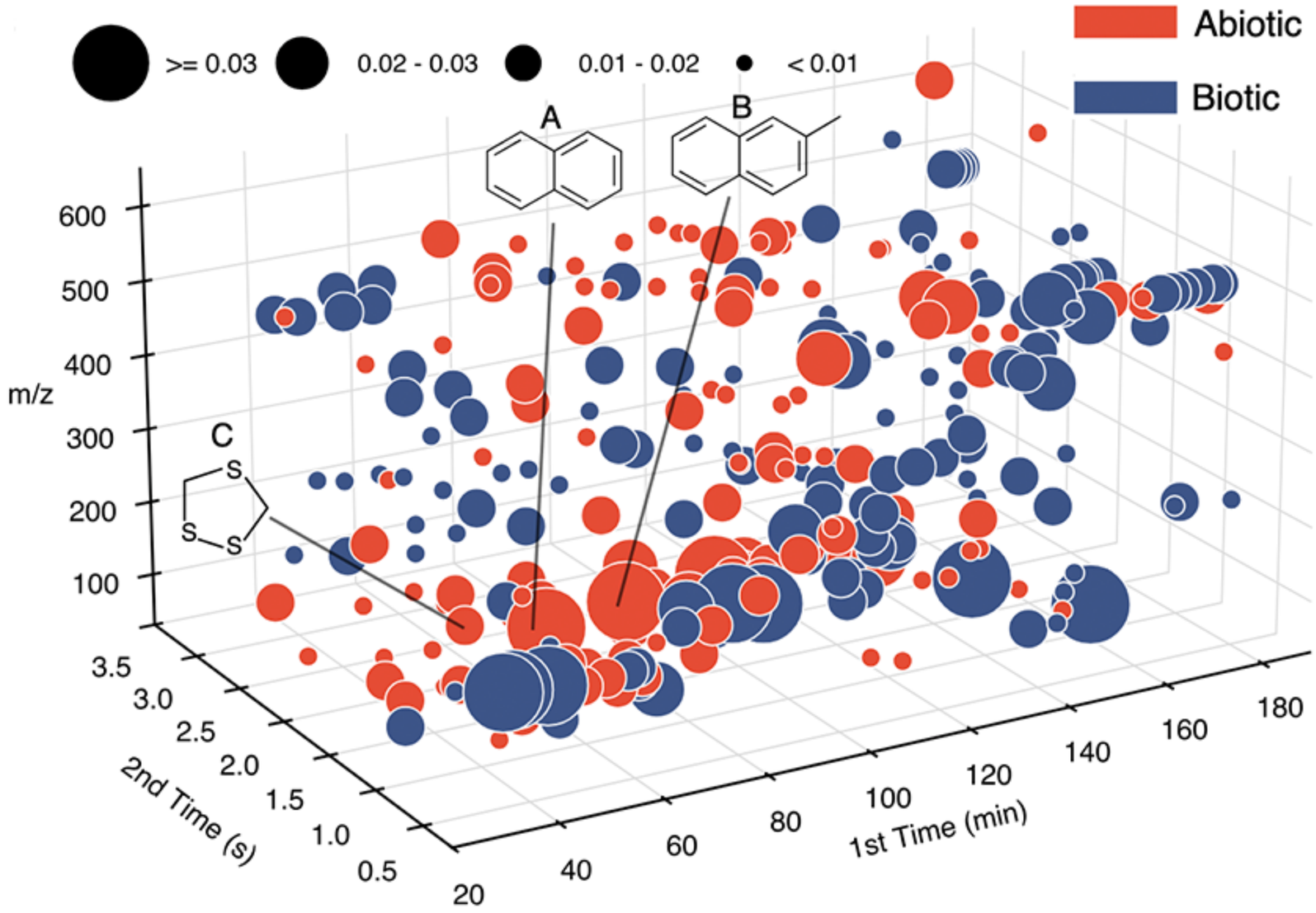
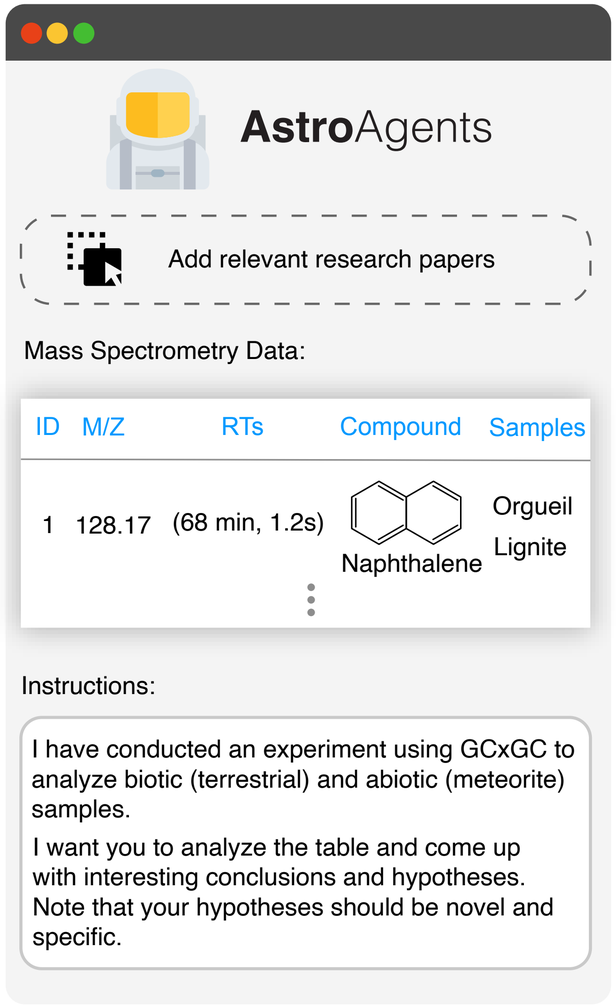
RT2 (s)
1.5
1.0
68.03
91.50
RT1 (min)
b
Earth Sample 1
Earth Sample 2
Meteorite 1
Meteorite 2
A
B
c
(m/z,RT1,RT2)
(102,68.03,1.81)
(162,91.50,1.12)
Features →
Samples →
d
Peak B
Peak A
Classification and discriminative compound identification
Expert-confirmed molecule identities via fragmentation patterns

Discovered biosignatures by LifeTracer

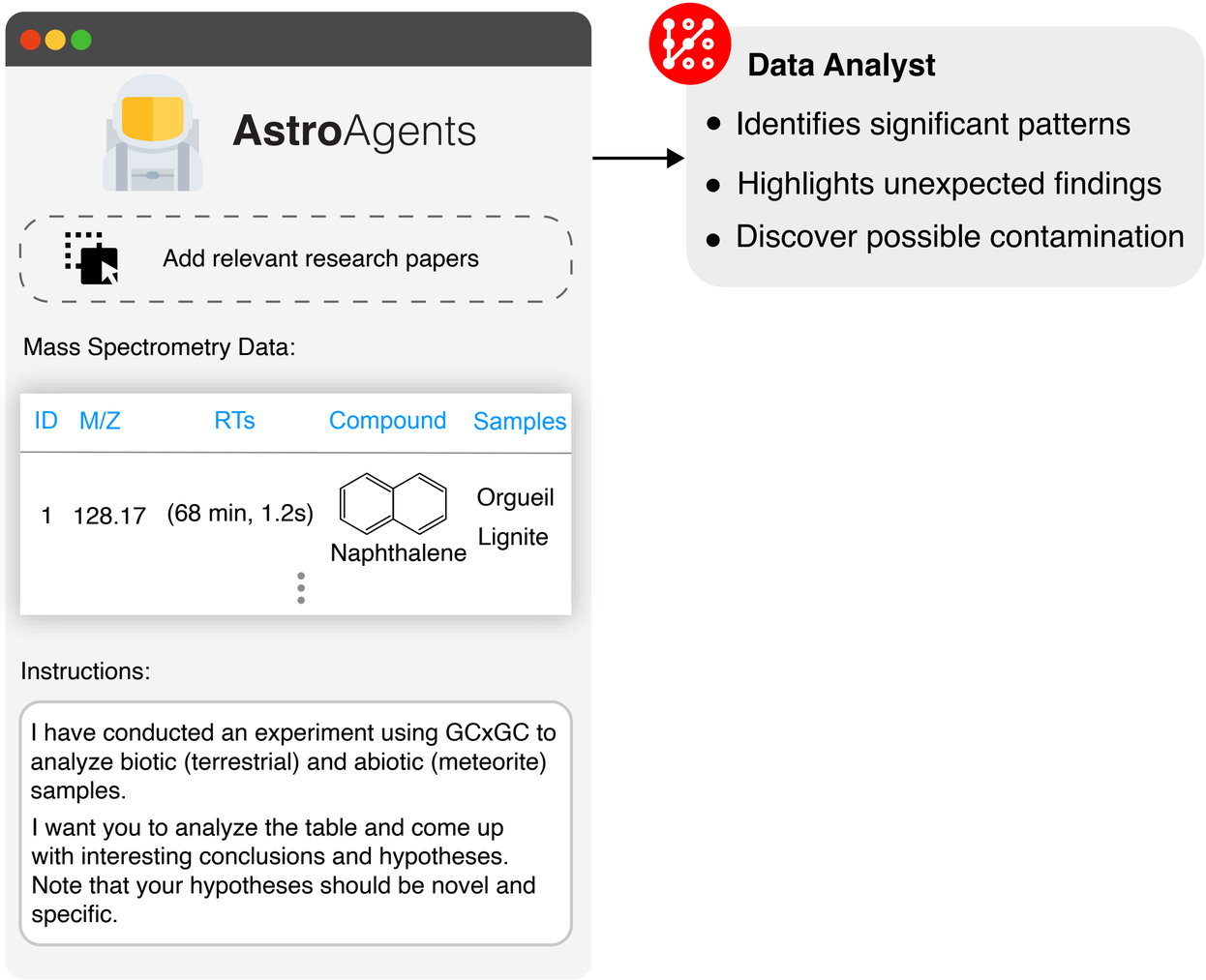


PNAS Nexus 2025, In press

AstroAgents v1



AstroAgents v1



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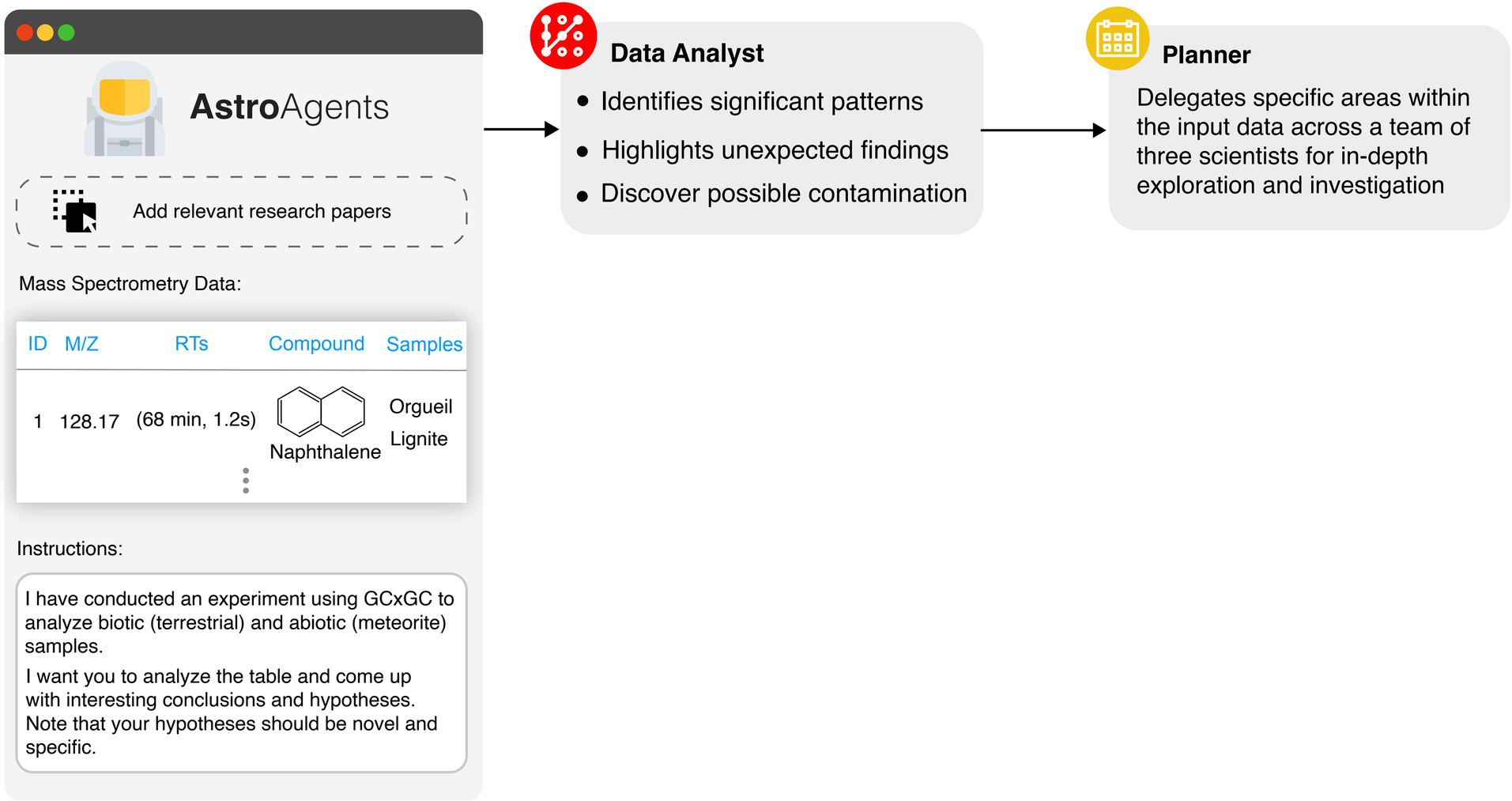

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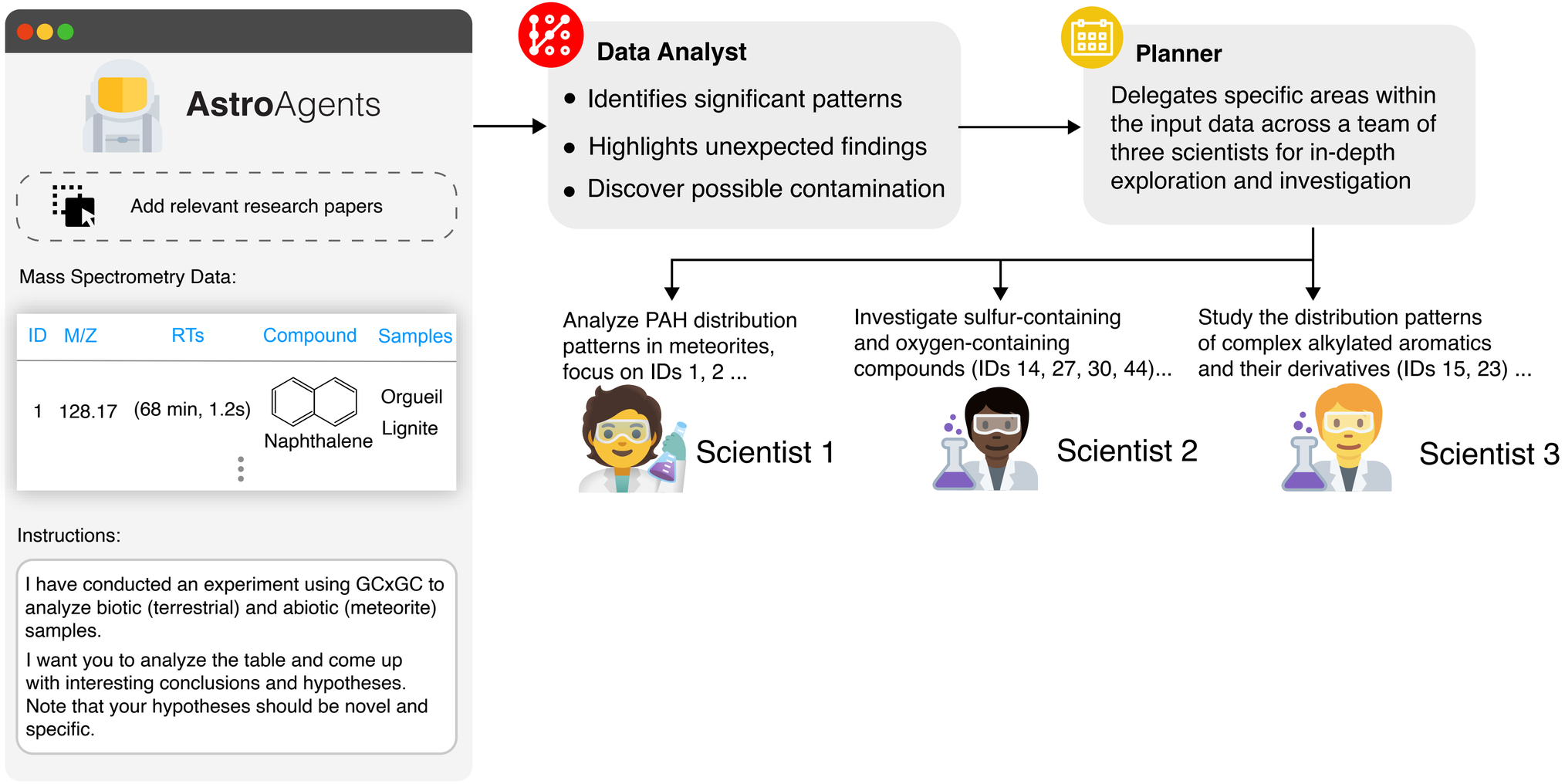

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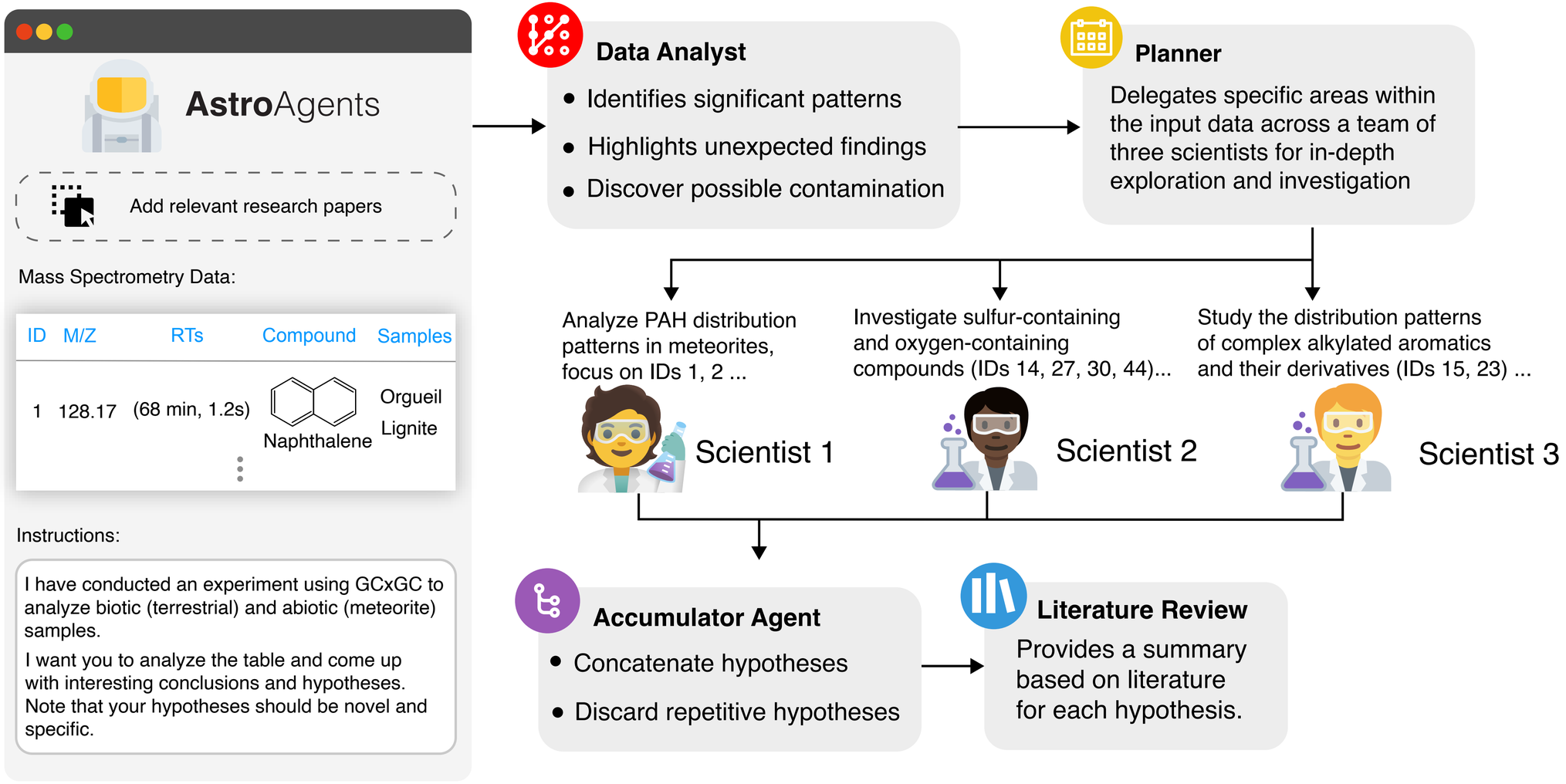

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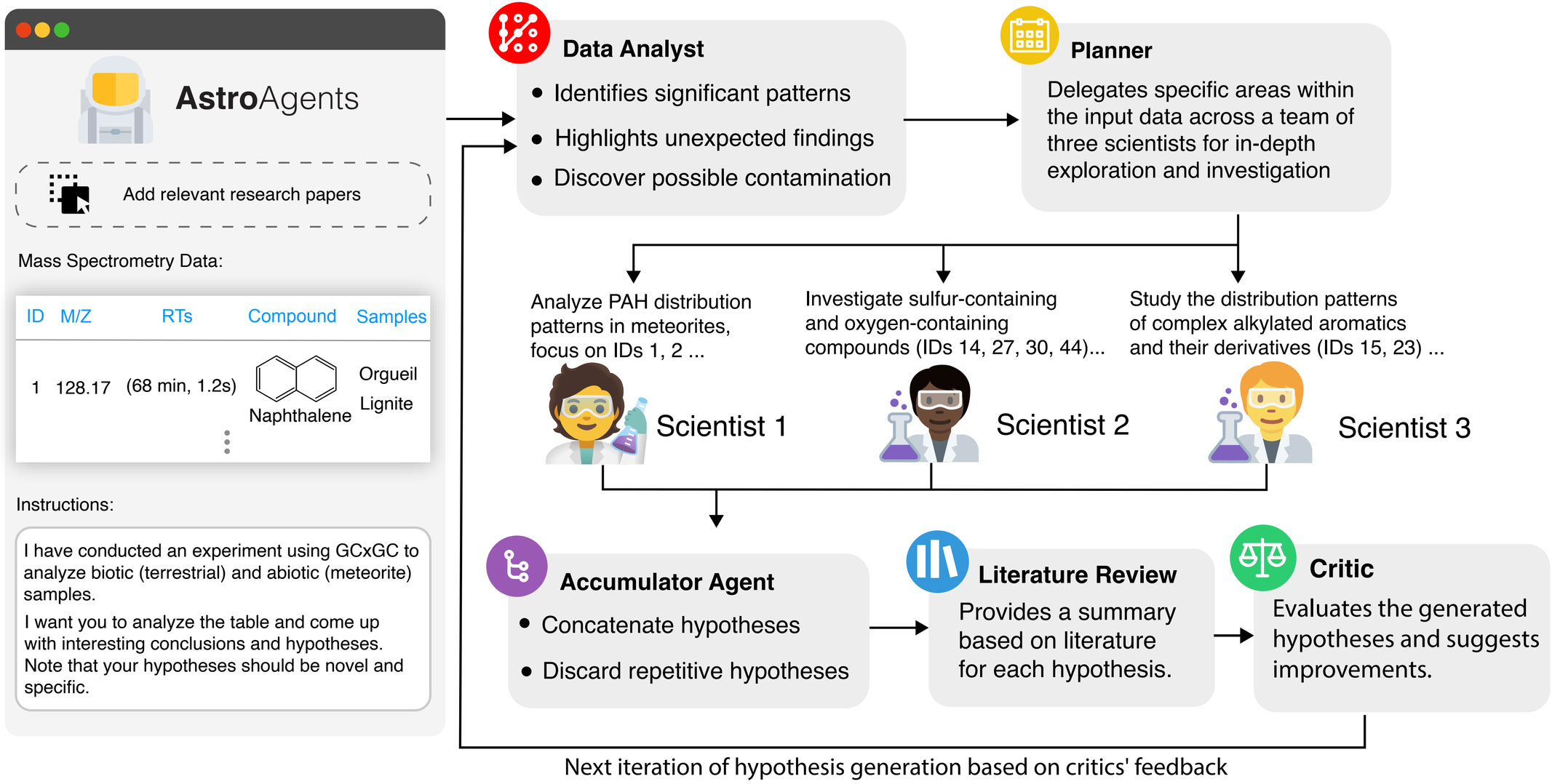


Human expert evaluations

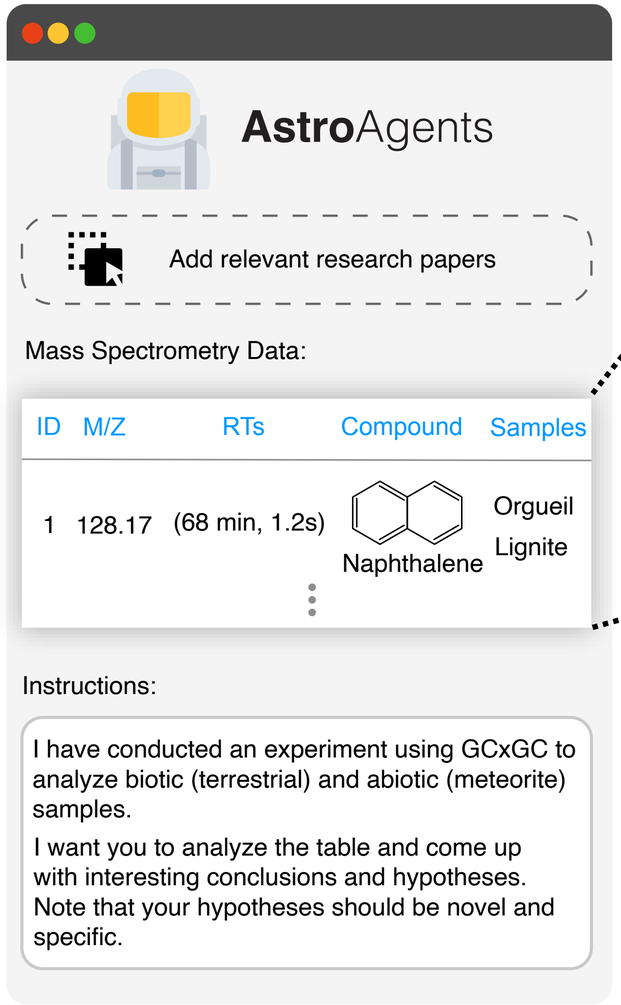
- **Claude Sonnet 3.5** (48 hypotheses)
  - fewer logical errors
  - stronger consistency with the literature
  - scored higher on **clarity**
- **Gemini 2.0 Flash** (101 hypotheses)
  - higher **novelty** scores
  - but more logical errors

Criteria	Claude Sonnet 3.5	Gemini 2.0 Flash
Novelty	2.75 ± 0.75	4.26 ± 1.87
Consistency with the literature	7.60 ± 1.91	6.19 ± 2.88
Clarity and precision	7.20 ± 2.30	5.92 ± 2.86
Empirical Support	6.75 ± 2.63	5.79 ± 2.86
Scope & Generalizability	7.60 ± 1.91	6.01 ± 2.80
Predictive Power	7.60 ± 1.91	5.86 ± 2.68
Overall Average	6.58 ± 1.74	5.67 ± 0.64

#	Statement	Key Datapoints	Evaluation Score
1	**Gemini 2.0 Flash:** The presence of 1H-Phenalen-1-one or 9H-Fluoren-9-one (ID 44, MW 180) exclusively in Orgueil and LEW 85311, and the presence of Biphenyl (ID 43, MW 154) also in the same meteorites, suggests a unique chemical environment or alteration history shared by these samples, potentially indicating a similar formation region within the early solar system. Given their related structures, this may indicate a similar source.	1H-Phenalen-1-one or 9H-Fluoren-9-one (ID 44, MW 180): Orgueil, LEW 85311; Biphenyl (ID 43, MW 154): Orgueil, LEW 85311.	*Novelty: 7/10* *Literature: 9/10* *Clarity/Precision: 9/10* *Empirical Support: 9/10* *Generalizability: 9/10* *Predictive Power: 8/10*

#			
5	**Claude 3.5 Sonnet:** The detection of possible terpenes exclusively in soil samples indicates that complex branched isoprenoid structures require enzymatic biosynthesis and are not readily formed through abiotic processes in space, making them reliable biomarkers.	IDs 4, 17, and 18 (possible terpenes) were found only in soil samples (Iceland Soil, Atacama, Utah soil, GSFC soil)	*Novelty: 3/10* *Literature: 10/10* *Clarity/Precision: 10/10* *Empirical Support: 10/10* *Generalizability: 10/10* *Predictive Power: 10/10*

Expanding hypotheses generation for origin of life

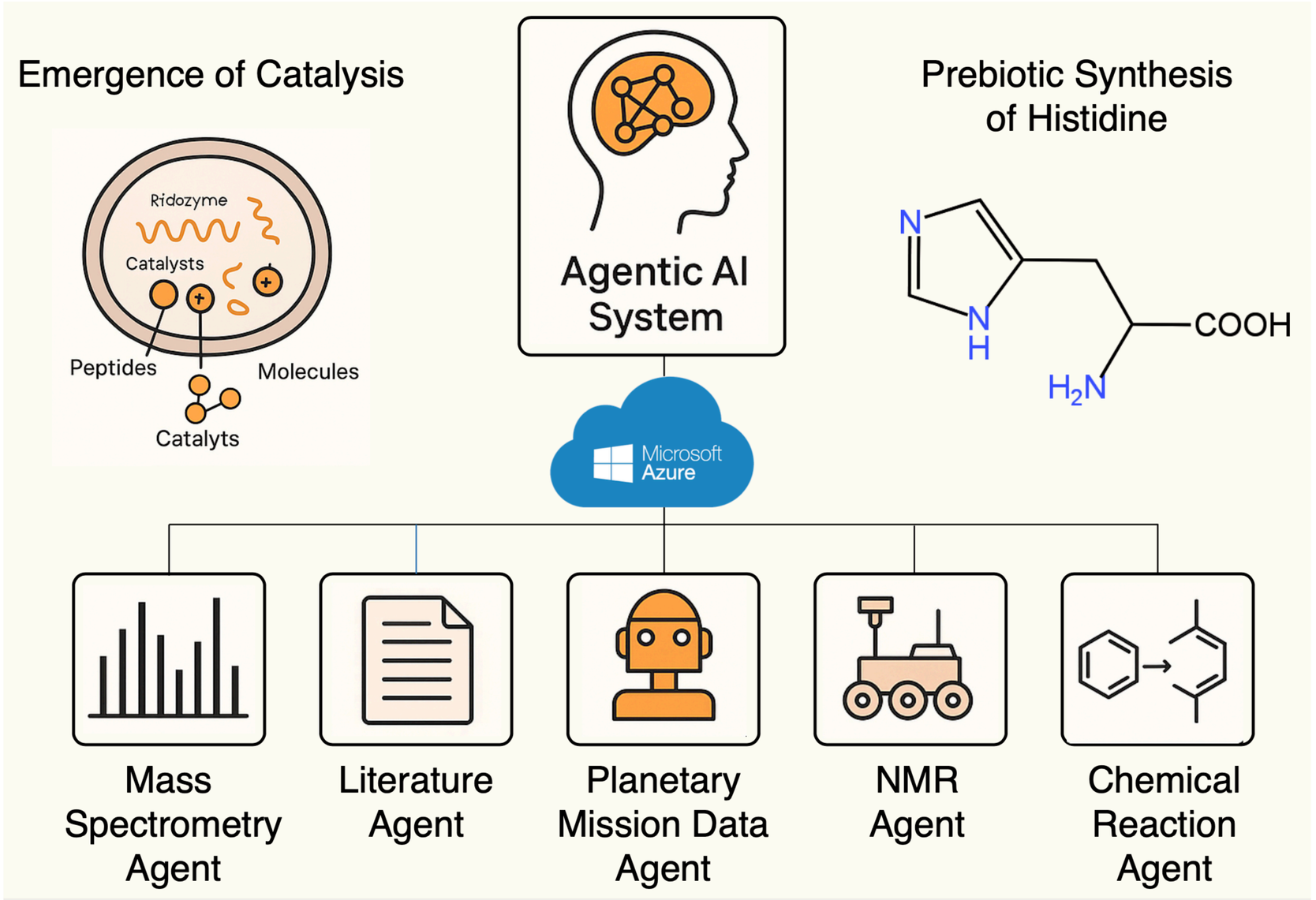


ID	M/Z	RT1	RT2	TENTATIVE ID	SAMPLES
1	128	4078.14	2.168	Naphthalene	Orgueil ALH 83100 LON 94101 Aguas Zarcas Murchison Jbilet Winselwan LEW 85311 Green River Shale Lignite
2	142	4757.92	1.840	2-Methylnaphthalene	Orgueil ALH 83100 LON 94101 Murchison Jbilet Winselwan LEW 85311 Green River Shale

+

- **From single-source to multi-source:** Moving beyond just mass spectrometry to integrate mission archives, chemical databases, and peer-reviewed literature.
- **Instruments included:** Bringing in data streams from SHERLOC (Perseverance rover) and MOMA (ExoMars rover).
- **Comprehensive evidence base:** Unifying chemical knowledge, experimental results, and planetary data for stronger, AI-driven hypothesis generation.

Expanding hypotheses generation for origin of life



Expanding hypotheses generation for origin of life

- Excited about the opportunity to collaborate with the Microsoft Discovery team and leverage their tools to advance AstroAgents++.
- Use **in-silico** simulation to test, rank, and refine hypotheses.
- **Fuse multi-modal evidence**: Interstellar medium, star & planet formation, meteorites, prebiotic chemistry, and early biological activity.
- Wet-lab testing of generated hypotheses.

Thank you!

LifeTracer

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