Please note: the substantive content of the 2026 NRI Roadmap Survey begins at Question 20 with prior questions dealing with administrative and other information).
As such all submissions that are published include the responses submitted from Question 20 onwards only.
Q20.
Part 2: Research themes 2.1 NRI comprises the assets, facilities and associated expertise to support leading-edge research and innovation in Australia and is accessible to publicly and privately funded users across Australia and internationally. We are seeking your input on possible directions for future national-level investment - i.e., where the requirements are of such scale and importance that national-level collaboration and coordination are essential.
The 2021 Roadmap used a challenge framework to support NRI planning and investment. With this in mind, consider likely future research trends in the next 5 - 10 years, and with respect to one or more of the 8 challenge areas identified in the 2021 Roadmap as listed below: • describe emerging research directions and the associated critical research infrastructure requirements
 that are either not currently available at all, or not at sufficient scale and describe current national infrastructure requirements that you anticipate will no longer fit the definition of NRI in 5-10 years.
Do not limit your commentary to NCRIS funded capabilities.
Q21. Resources Technology and Critical Minerals Processing

Food and Beverage

Over the next 5–10 years, advances in AI and precision agriculture driven by biomolecular deep learning methods are set to revolutionise the food and beverage sector by driving novel crop breeding, optimising supply chains, and enabling data-driven manufacturing processes. These breakthroughs require a national-level investment in high-performance computing (HPC) that can analyse vast genomic, environmental, and industrial datasets in real time. Currently, Australia's HPC capacity and data management infrastructure are insufficient to support large-scale multi-omics research and advanced process simulation at the scale required by emerging food and beverage innovations. In addition, distributed training and robust data-sharing frameworks must be established to enable a skilled workforce to harness these tools effectively. Meanwhile, smaller or outdated HPC facilities lacking scalability will no longer meet the definition of critical national research infrastructure in the coming decade, underscoring the need for coordinated upgrades and integration of cutting-edge hardware and expertise.

Q23.

Medical Products

Al-driven drug discovery, personalised therapeutics, and precision medicine are poised to transform the development of new medical products. However, as mentioned above, these breakthroughs demand a step change in national research infrastructure (NRI), especially in high-performance computing (HPC) and data management systems. At present, Australia lacks the scale of GPU-accelerated resources needed to handle the vast and complex datasets underpinning emerging multi-omics techniques. This shortfall is even more critical given the increasing importance of secure, sovereign capabilities for sensitive health data. Moving forward, large-scale HPC clusters with integrated analytics and training support, built collaboratively across institutions, will be vital to keep pace with global competitors.

Q24.

Defence

Biomolecular deep learning will increasingly underpin defence applications, from rapid detection of biosecurity threats to designing countermeasures for emerging pathogens. These methods are used at a fundamental level in a number if disciplines and have broad reaching impact. However these advances hinge on large-scale high-performance computing (HPC) and robust data management frameworks capable of handling complex, sensitive biological datasets. Currently, Australia's computing capacity and sovereign infrastructure do not adequately support these resource-intensive algorithms, posing security and research challenges. Investing in scalable, GPU-optimised HPC resources—with the necessary training and technical support—will be essential for maintaining strategic advantage and ensuring resilience in the face of evolving threats.

Q25.

Recycling and Clean Energy

Biomolecular deep learning is central to synthetic biology and protein engineering. It can design specialised enzymes and microorganisms for waste degradation, carbon capture, and renewable fuel production. These breakthroughs require large-scale, GPU-enabled high-performance computing (HPC) and advanced data management to handle the immense complexity of multi-omics datasets and rapidly iterate enzyme or metabolic pathway designs. At present, Australia's HPC capability and storage infrastructure are insufficient for these computationally intensive tasks, limiting innovation in both materials recycling and clean energy. Targeted investment in scalable HPC systems, alongside specialised training for researchers, will be essential to maintain a competitive edge and meet national sustainability goals.

Q26. **Space**

Environment and Climate

Biomolecular deep learning will support breakthroughs in areas such as microbial degradation of pollutants, carbon sequestration, and the engineering of climate-resilient crops. However, these data-intensive methods rely on large-scale, GPU-enabled high-performance computing (HPC) systems to analyse and model complex multi-omics datasets. Australia's current HPC resources are inadequate to support the computational demands posed by this emerging research, limiting the nation's ability to address pressing environmental challenges. A coordinated, national-level approach to scalable HPC investment, combined with specialised training, will be essential to maintain global competitiveness and develop sustainable, climate-focused solutions.

Q28.

Frontier Technologies and Modern Manufacturing

Biomolecular deep learning is poised to revolutionise frontier technologies and modern manufacturing, particularly through breakthroughs in synthetic biology, enzyme engineering, and the design of next-generation materials. However, as mentioned in the previous sections, fully harnessing these opportunities requires large-scale, GPU-accelerated computing resources and advanced data management systems which are currently limiting in Australia. Addressing these problems should be a priority.

Q29.

2.2 The 2024 statement of National Science and Research Priorities (NSRPs) includes outcomes linked to each priority to assist in identifying critical research needed in the next 5 to 10 years.

Consider the priority statements and, with respect to one or more of the 5 priority areas as listed below:

- describe emerging research directions and the associated critical research infrastructure requirements that are either not currently available at all, or
- not at sufficient scale and describe current national infrastructure requirements that you anticipate will no longer fit the definition of NRI in 5-10 years.

Do not limit your commentary to NCRIS funded capabilities, and where relevant, refer to the underpinning outcomes and research identified in the NSRPs document.

Q30.

Transitioning to a net zero future

Q31.

Supporting healthy and thriving communities

Medicine is currently experiencing a pivotal 'compute moment', characterised by rapid breakthroughs enabled by advanced computational analysis of complex biological datasets. Biomolecular deep learning is uncovering previously inaccessible discoveries, accelerating research and delivering tangible benefits in clinical practice. However, Australia's lack of suitable computational infrastructure—particularly GPU-enabled high-performance computing, fast storage solutions, and secure management of sensitive medical data—is significantly hindering progress and placing Australian researchers at a marked global disadvantage. Immediate investment in scalable HPC tailored for medical applications will not only enhance Australia's scientific competitiveness but also deliver substantial economic returns. Given escalating healthcare costs and our ageing population, the relative affordability and high-impact potential of this technology represent a strategic, cost-effective solution with enduring benefits.

Q32

Q33.

Protecting and restoring Australia's environment

Deep learning in bio molecular science is accelerating bio engineering and our understanding of biology at a fundamental level. This knowledge and capability to engineer biology is essential for Australian researchers to harness to ensure we can protect our unique flora and fauna and respond rapidly to climate change and environmental pressures. Limitations in HPC currently are throttling these capabilities. Investment in HPC for biological AI is essential.

Q34.

Building a secure and resilient nation

Currently there are significant gaps in Australia's Al-capable HPC- we currently have limited sovereign capability. This is particularly evident for my field of biomolecular Al. Investing in this space would improve our nation's security and resilience by enhancing its ability to respond rapidly to emerging threats, safeguarding sensitive research, and foster domestic innovation. Large-scale GPUs and advanced data processing capabilities allow for: rapid threat detection and response, sovereignty over critical research and data, accelerated R&D and innovation and in enhancing collaboration. Australia needs sovereign capabilities in biomolecular Al technology to ensure our population is able to meet it's needs in regards to health, manufacturing, defense and the environment.

Q35.

2.3 The case for a new NRI capability, or enhancements to existing capabilities, typically emerges through advocacy from research communities clustering around rigorously identified needs and goals. Such a concept could respond to a requirement for novel or expanded capacity within a domain, or across domains, and must be such that it could only be made available with national-level investment.

If you have identified such a requirement, briefly describe the need, the proposed infrastructure capability, the medium-term goals, impacted research communities, and the timeframe over which you advocate its establishment. Your response can include links to relevant existing reports.

Al and HPC in Biomolecular Science Al and HPC are transforming biomolecular science, with breakthroughs in structural biology enabling accurate protein modelling and de novo protein design. These advances are driving progress across medicine, biotechnology, agriculture, and engineering. As the field evolves toward integrative multi-omics and the development of powerful biological foundation models, robust computational infrastructure is rapidly becoming indispensable. Deep Learning style computing relies heavily on resource-intensive computing powered predominantly by NVIDIA GPUs which Australian HPC Infrastructure is currently ill equipped to handle. Australia's existing HPC resources fall far short of the demands posed by rapidly advancing biomolecular AI technologies. Currently Tier 1 and Tier 2 infrastructure can not adequately support even small-scale research, let alone the training of a single protein model. Sovereign capability remains limited, and commercial platforms are prohibitively expensive and often restrict access during peak demand. To safeguard strategic research and intellectual property, Australia must strengthen resilience against global market and policy fluctuations. Targeted investment in Al-capable HPC is therefore essential to maintain scientific competitiveness, accelerate biomolecular research, and foster meaningful translational and industry partnerships. Australia faces several infrastructure bottlenecks and should prioritize funding the following areas: Computational Power: Al-driven structural biology requires significant GPU resources that are currently scarce in Australia. Many structural biology tools require hours of GPU use for a single inference. Investing in infrastructure that can be continually upgraded or expanded is crucial to keep pace with the rapid evolution of these technologies. Fast Storage: Large-scale biological AI depends on vast datasets, making fast storage vital for efficiency. Rapid data access reduces the time GPUs sit idle, lowering costs and maximising hardware utilisation. This accelerates AI workflows and ensures more can be achieved with the same GPU resources. Democratised Access: Limited availability of computing resources across institutions hinders collaboration and slows critical research progress, with only a few institutions able to access suitable hardware. This not only inflates costs for existing funded projects but also impedes the adoption and training of Al-driven methods in Australia, placing the nation at a global disadvantage. A coordinated national strategy integrating Tier 1 and Tier 2 infrastructure hubs will reduce duplication, streamline support, and optimise hardware utilisation. Training: Al in structural biology has emerged rapidly, leaving many researchers unprepared. There is a pressing need for training in Al-driven modelling, data management, and computational workflows. Infrastructure availability is the first step, but hands-on practice is essential to develop expertise and drive innovation. Specialised tools and pipelines tailored to Australian needs will spur partnerships with startups and industry, while distributed training pipelines and dedicated support teams will democratise adoption, future-proof national research capabilities, and maximise returns on infrastructure investment. Equipping a broad range of researchers with these skills will have far-reaching benefits, from designing climate-resilient crops to creating novel therapeutics for emerging pathogens. Medium-Term Goals (2-5 Years) •Build Sovereign Capability: Mitigate reliance on overseas providers by establishing local infrastructure that safeguards sensitive research and IP. •Accelerate Translational Research: Foster collaborations between academia, startups, and industry to develop next-generation therapeutics, agricultural solutions, and bioengineering applications. •Future-Proof National Research: Ensure that HPC capacity can scale with the advent of more advanced AI models (e.g., biological foundation models, integrative multi-omics). Impacted Research Communities •Biological and Medical Sciences: From vaccine design, disease research and personalised medicine. Agriculture and Environmental Studies: Breeding climate-resilient crops and managing ecological challenges.
 Biotechnology and Engineering: Developing new enzymes, materials, and industrial processes. •Cross-Disciplinary Endeavours: Integrating AI expertise into bioinformatics, genomics, chemistry. Timeframe for Establishment Australia needs to begin upgrading its HPC capacity immediately to remain competitive. We already lag behind both Europe and the US and many countries in Asia in supporting biomolecular Al. Within three years, fundamental infrastructure upgrades should be in place, with five years as a horizon for more comprehensive adoption, training programs, and industry collaboration. Al and HPC are transforming structural biology and influencing a host of disciplines and industries, yet Australia's infrastructure is falling behind. Enhancing computational capacity, data management, and workforce training is crucial for maintaining a competitive edge, bolster sovereign capability, protect intellectual property, and catalyse new partnerships. A well-coordinated national strategy will establish Australia as a global leader in Al-driven biomolecular science, and by strengthening our AI HPC capabilities over the next few years, Australia can secure a leadership position in Al-driven biomolecular science, delivering tangible benefits across academia, industry, and the broader economy, including pressing challenges in human health, agriculture, and biotechnology. Data from early adopters shows that this technology delivers a strong return on investment, highlighting its transformative impact and reinforcing the case for broader adoption. (see https://australian-structural-biology-computing.github.io/website/ for the more).

Q36.

Part 3: Industry perspectives

This section is seeking input specifically from industry-based respondents. Other respondents can skip this section.

Recommendation 6 of the <u>2021 Roadmap</u> related to improvements in industry engagement with NRI. To complement work on this topic that has occurred since then, we are seeking additional advice on NRI requirements as perceived by current or potential industry-based users.

Q37

3.1 Have you (or your organisation) interreacted with or used Australia's NRI?

Yes

No

Q38.

3.2 If so, please briefly outline the NRI capabilities you (or your organisation) have interacted with or used. Do not limit your response to NCRIS capabilities.

Q39.	
3.3 Please indicate your (one or more) primary reasons for interacting with NRI:	
This question was not displayed to the respondent.	
Q40.	
3.4 If you answered no, please indicate your (one or more) primary reasons:	
☐ I did not know about it	
Other facilities suit my needs better	
☐ I would like to, but cannot get access due to geographical location	
☐ I would like to, but believed that access was only available to academic researchers	

Q41.

Part 4: Other comments

Other (please specify)

I am not aware of any capability that meets my needs

4.1 Please elaborate on any of your above responses or add any other comments relevant to the development of the 2026 Roadmap. Your response can include reference or links to existing reports that you recommend be considered during the 2026 Roadmap development process.

Further detail about infrastructure requirements are outlined in the Australian Computational Structural Biology Infrastructure Roadmap, about to be released. (https://australian-structural-biology-computing.github.io/website/). This roadmap has been prepared by subject matter experts in consultation with the structural biology community across Australia.

Q49.

4.2 Optional Document Attachment.

Note: Our strong preference is that answers are provided against the relevant questions in the survey. However, this file upload option is available for submissions in file format, where needed. Please ensure the document includes your name or organisation.