Serapis Tasking Form

Tasking Form Part 1: *(to be completed by the Authority's Project Manager)*

To:	Lot 6 Frazer-Nash Consultancy Ltd	**From:**	The Authority

Any Task placed as a result of your quotation will be subject to the Terms and Conditions of Framework Agreement Number:

LOT 6 DSTL/AGR/SERAPIS/UND/01

VERSION CONTROL

Version 1.0

REQUIREMENT

Proposal Required by:	[dd/mm/yyyy]	**Task ID Number:**	[U92]
The Authority Project Manager:	Redacted under FOIA exemption	**The Authority Technical Point of Contact:**	Redacted under FOIA exemption
Task Title:	[Accelerating the Discovery and Synthesis of Advanced Energetic Materials using artificial intelligence]		
Required Start Date:	[01/08/2022]	**Required End Date:**	[01/08/2024]
Requisition No:	[RQ0000007526]	**Budget Range**	£2.5M

TASK DESCRIPTION AND SPECIFICATION

Serapis Framework Lot	☐ Lot 1: Collect ☐ Lot 2: Space systems ☐ Lot 3: Decide ☐ Lot 4: Assured information infrastructure ☐ Lot 5: Synthetic environment and simulation ☒ Lot 6: Understand

Statement of Requirements (SOR)

The Advanced Energetic Materials project aims to accelerate the discovery and delivery of new explosives and energetic materials for future use by UK Defence and Homeland Security.

With ever-increasing demands on energetics to meet tougher mission requirements, the UK requires new materials that are able to provide increased performance or else offer other key advantages. In addition, there is significant potential to realise other important benefits – including reductions in both manufacturing costs and environmental impact.

This high technical risk, low technology readiness level (TRL) research programme aims to harness new and under-exploited technologies, with a focus on automated processes, for the purposes of identifying new energetic materials, as well as on finding new synthesis pathways – both to those new energetic materials, and to existing ones for which significant barriers to production currently exist.

As a critical, underpinning technology, new energetic materials are required for a wide range of defence and security applications. Energetic materials (or 'energetics') are materials with a high amount of stored, but suitably accessible, chemical energy. Foremost amongst these are explosives, propellants and pyrotechnics,

with additional examples including energetic additives in the form of binders, plasticisers or bonding agents. Novel energetic molecules, Redacted under FOIA exemption are the strategic focus for this very low technology readiness level (TRL) research.

Significant 21st century advancements in automation and computing power – including the field of Artificial Intelligence (AI) – have made game-changing tools more accessible, and the chemical and biological sciences ever more receptive to adopting them. The Energetics Industry is one area where considerable potential for development exists if such tools were successfully adopted.

Redacted under FOIA exemption

The exact mechanism for success is not prescribed, however, proposals are welcome that utilise data in its current non-ideal format or that are able to generate data of suitable quality to support these ambitions.

Bids that are perceived as having high technical risk or novelty will be encouraged, and the generation of patents or publications for the benefit of national prosperity will be positively explored. The innovation in proposals will receive specific scoring criteria when assessments of the returns are undertaken.

Please note that Dstl has a duty of care to ensure research is conducted safely under our sponsorship, and that this responsibility is of utmost importance to us.

Whilst not directly expected as part of this requirement, should any practical work involving energetic materials become necessary by the Supplier on the basis that it is deemed fundamental to successful delivery, bids will need to demonstrate sufficient prior experience and suitable capability to work with energetic materials, or else will be rejected. To this end, collaborative bids with partners with the required energetics experience/ facilities are welcomed.

Where sufficient experience and capability to work safely with energetic materials is not demonstrated, practical work must instead be restricted to the study of justifiably representative, non-energetic model compounds and systems only.

Bids will be assessed by a panel which may include Government technical experts from the Centre of Excellence for Energetic Materials (CoEEM) as well as Dstl, using Proposal criteria in Section 5.

Communications will be managed through Serapis and in accordance with the standard Dstl Commercial process.

After the contract(s) have been awarded, activity will be instigated by the Authority, with a Project Kick-Off Meeting at the agreement of all parties.

Proposals are welcome that cover the full criteria of each SoR, or sub-elements thereof. However, in all cases it must be made clear which element each application applies to. **Bids that cover multiple elements must also provide a clear breakdown in terms of pricing for each element. This latter point will be important for proposals to meet the criteria for commercial assessment.**

This research topic is expected to complement the objectives contained in an SoR for theoretical characterisation and validation of energetic materials using computational chemistry. Suppliers with relevant expertise are encouraged to apply to both SoRs.

Please note that any novel discoveries that offer distinct military advantage may necessitate a significant increase in classification level of this work as the project progresses. Therefore any suppliers who intend to resource PhD students to support contract delivery need to be aware that a Research Worker Form will need to be completed. Individuals who are eligible (provided they meet the requirements of the checks) are from the following list:

- UK nationals
- Irish citizens
- From the EU, EAA, or Switzerland and has the appropriate EU Settlement Scheme status to study and/or work in the UK at the organisation detailed
- from outside the UK, the Republic of Ireland, EU, EEA or Switzerland and has the appropriate immigration status (in accordance with the requirements of the UK Visas & Immigration) to study and/or work in the UK at the organisation detailed
- not going to be studying or working in the UK

The following focus areas have been identified as possible solutions to known issues. **These are only intended as examples for research and should not be viewed as a barrier to innovative ideas or novel applications of technologies.**

AI for discovery

Redacted under FOIA exemption

Redacted under FOIA exemption

Integration of any or all of these processes with systems for automated practical experimentation would be welcome.

Dstl will consider support for the procurement of necessary licences and software where explicitly identified and justified as part of the bid. These must be agreed with Dstl during the contracting stage. This would enable researchers to develop their algorithms using the best available data, and to search within datasets where relevant materials are identified.

It is expected that the contracted research will largely take place *in silico* and will focus on the identification of materials or synthesis routes not known in the context of energetics. These 'new' entities may be known chemicals or routes that have no existing energetic test data, or they may be conceptual and completely un-trialled for any application. Additionally, researchers may uncover materials that present energetic characteristics only once transformed in structure or scale from their common occurrences.

Once again, these approaches are included here only as examples of the means for enhancing the discovery process for new energetic materials. This document does not intend to specify all acceptable AI approaches that may be used to that end. **Alternative and unorthodox approaches are welcome where their feasibility is suitably justified within bids.** Whatever the precise discovery route, the intended outcome of this research is the identification of new energetic molecules or routes to them, combined with theoretical validation of energetic performance or pathway viability**.**

References

[1] K. Walch, "The Increasing Use Of AI In The Pharmaceutical Industry," 26 December 2020 - https://www.forbes.com/sites/cognitiveworld/2020/12/26/the-increasing-useof-ai-in-the-pharmaceutical-industry/ [Accessed 09 November 2021].

[2] J. Vamathevan, D. Clark, P. Czodrowski and et al., "Applications of machine learning in drug discovery and development," *Nature Reviews Drug Discovery,* no. 18, pp. 463-477 (2019).

[3] Q. Zhao, H. Yang, J. Liu, H. Zhou, H. Wang and W. Yang, "Machine learningassisted discovery of strong and conductive Cu alloys: Data mining from discarded experiments and physical features," Materials & Design, vol. 197, no. 109248 (2021).

[4] J. Mavračić et al.; "ChemDataExtractor 2.0: Autopopulated Ontologies for Materials Science", J. Chem. Inf. Model. 2021, 61, 9, 4280–4289 (2021).

[5] M. Krallinger et al.; "Information Retrieval and Text Mining Technologies for Chemistry", Chem. Rev. 2017, 117, 12, 7673–7761 (2017).

[6] 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane https://doi.org/10.1002/prep.19970220502

Procurement Strategy

☒ Lot Lead to recommend ☐Single Source / Direct Award

Pricing:

☒ Firm Pricing ☐ Ascertained Costs* ☐ Other*

Firm Pricing shall be in accordance with DEFCON 127 and DEFCON 643

Ascertained Costs shall be in accordance with DEFCON 653 or DEFCON 802.

*only at Authority's discretion

Task IP Conditions

Task IP Conditions (Follow the NIPPY guide to identify your information and IP requirements for each deliverable)	**Summary of the Authority's rights in foreground IP (IP generated by the supplier in performance of the contract)**
DEFCON 703 ☒	Vests ownership with the Authority

DEFCON 705 Full Rights ☐	Enables MOD to share in confidence as GFI or IRC under certain types of agreements. Can be shared in confidence within UK Government.
OTHER IP DEFCONS: 14* ☐, 15* ☐, 16* ☐, 90* ☐, 91* ☐, 126* ☐	Generally only suitable for deliverables at TRL 6 and above.
BESPOKE IP Clause ☐ *	Details to be added and agreed by IP Group
* Do not use without IPG advice and approval	
Please state in this text box if MOD or the customer has a requirement a) that one or more Other Government Departments is able to share confidentially with their own suppliers, b) to publish but you do not think there is a requirement to own or control the deliverable, or c) to share under a procurement Memorandum of Understanding (MOU).* *If any of these three issues applies, please contact IPG for advice before completing this form. *Listing research MOUs is not required, but can be a helpful courtesy to the supplier.*	

DELIVERABLES

Ref	Title	Due by	Format	Expected classification (subject to change)	Information required in deliverable	IPR DEFCON
D-1	Quarterly Progress and Technical Review (QPTR 1)	T+3, T+6, T+9, T+12, T+15, T+18, T+21 months.	Presentation from Supplier (remote or in-person meeting)	UK OFFICIAL	Presentation pack to include but not limited to: • Update on technical progress • Progress report against project schedule. • Review of risk management plan. • Commercial aspects. • Review of deliverables. • Risks/issues. • GFA and supplier performance	703
D-2	Knowledge shares	T+3, T+6, T+9, T+12, T+15, T+18, T+21 months.	Presentation / workshop	UK OFFICIAL	Technical seminars to support understanding of developed models/ utilised tools. This will enhance SQEP within Dstl and enhance ability of staff to utilise outputs effectively after completion of the contract.	703
D-3	Year-End Report	T+12 months	Report	UK OFFICIAL	Full year-end report, to include: • Project background • Summary of Yr1 work • Conclusions • Recommendations for follow-on research, with plans for following year • Identification and summary of IP (potential or actual) arising in-year. • Progress versus deliverables	703

					• Recommendations for any potential parallel research	
D-4	Final report	T+24 months	Report & presentation	UK OFFICIAL	Full final report, to include: • Project background • Summary of Yr1 & Yr2 work • Conclusions • Recommendations for follow-on research • Copies of relevant publications arising or pending • Identification and summary of IP (potential or actual) arising • Progress versus deliverables • Any other technical issues or findings that Dstl should reasonably be made aware of Additional presentation, to include: • Brief summary of each year's work • Overall progress and conclusions • Demonstration of system and/or technology outputs • Recommendations for future work • Summary of publications and IP (submitted or pending) arising	703
D-5	Technical output	T+24 months	Negotiable	UK OFFICIAL SENSITIVE	This will constitute the technical output of the contract and will vary depending on which element a proposal aims to meet. This deliverable will include: [redacted] This will ensure that MOD will retain control of aspects valuable to national security interests and future exploitation for advantage over adversaries.	703
D-6	Applied model(s)	T+24 months	Source code	UK OFFICIAL	[redacted]	703*

					Redacted under FOIA exemption [redacted]	
D-7	Configuration files/ documentation	T+24 months	YAML or similar	UK OFFICIAL	Redacted under FOIA exemption [redacted]	703

DELIVERABLE: ACCEPTANCE / REJECTION CRITERIA

Unless otherwise stated below, Standard Deliverable Acceptance / Rejection applies. This is 30 business days, in accordance with DEFCON 524 Rejection, and DEFCON 525 Acceptance.

Standard Deliverable Acceptance / Rejection:-

Yes ☒ (DEFCON 524 Rejection, and DEFCON 525 Acceptance)

No ☐ (if no, please state details of applicable criteria below)

Government Furnished Assets (GFA)

ISSUE OF EQUIPMENT/RESOURCES/INFORMATION/FACILITIES - NONE

QUALITY STANDARDS

☐ **ISO9001** (Quality Management Systems)

☐ **ISO14001** (Environment Management Systems)

☐ **ISO12207** (Systems and software engineering — software life cycle)

☐ **TickITPlus** (Integrated approach to software and IT development)

☐ **Other:** (Please specify in free text below)

SECURITY CLASSIFICATION OF THE WORK

The highest classification of this SOR

OFFICIAL ☒ OFFICIAL-SENSITIVE ☐ SECRET ☐ TOP SECRET ☐ STRAP ☐ SAP ☐

The highest expected classification of the work carried out by the contractor

OFFICIAL ☐ OFFICIAL-SENSITIVE ☒ SECRET ☐ TOP SECRET ☐ STRAP ☐ SAP ☐

The highest expected classification of Deliverables/Output

OFFICIAL ☐ OFFICIAL-SENSITIVE ☒ SECRET ☐ TOP SECRET ☐ STRAP ☐ SAP ☐

Is a Security Aspects Letter (SAL) required? *(A Security Aspects Letter (SAL) will be required for each Task above Official-Sensitive and above)*

Yes ☒ No ☐

TASK CYBER RISK ASSESSMENT. *(In accordance with DEF STAN 05-138 and the Risk Assessment Workflow)*

Cyber Risk Level	[Very Low]
Risk Assessment Reference	[RAR-749976163]

ADDITIONAL TERMS AND CONDITIONS APPLICABLE TO THIS CONTRACT

Please ensure all completed forms are copied to DSTLSERAPIS@dstl.gov.uk when sending to the Lot Lead.

Tasking Form Part 2: *(To be completed by the Lot Lead)*

To: The Authority	From: The Lot Lead

Proposal Reference **017046-98063L U92 Discovery and Synthesis of Advanced Energetic Materials Using AI - Frazer-Nash Proposal** **(attached)**

Delivery of the requirement:

The proposal shall include, but not be limited to:

- A full technical proposal that meets the individual activities that are detailed in Statement of Requirements (Part 1 to Tasking Form).
- Breakdown of individual Deliverables, with corresponding Intellectual Property rights applied.
- Breakdown of Interim Milestone Payments, with corresponding due dates.
- A work breakdown structure/project plan with key dates and deliverables identified.
- A list of required Government Furnished Assets from the Authority, including required delivery dates.
- A clear identification of Dependencies, Assumptions, Risks and Exclusions which underpin your Technical Proposal.
- Sub-Contractors Personnel Particulars Research Worker Form and security clearances (if applicable)

PRICE BREAKDOWN

You are to use the costs detailed in Item 2 Table I in the Schedule of Requirement and at Annex E Table 2 of the Serapis Framework Agreement. Please also provide a price breakdown which should include, but is not limited to: Lot Lead Rates, Sub-contractors costs and rates, travel and subsistence. In support of your Proposal you are requested to provide clear details of all Dependencies, Assumptions, Risks and Exclusions that underpin your price.

Offer of Contract: *(to be completed and signed by the Contractor's Commercial or Contract Manager)*

Total Proposal Price in £	£1,976,325.61		(ex VAT)
Start Date:	24/10/2022	**End Date:**	31/10/2024

Lot Leads Representative	Name	Redacted under FOIA exemption
	Tel	Redacted under FOIA exemption
	Email	Redacted under FOIA exemption
	Date	06/10/2022
Position in Company	Serapis Lot 6 Project Manager	
Signature	Redacted under FOIA exemption	

Core Work – Breakdown

Notes:

1. Prices in this proposal are based on our current agreed rates which are valid until the end of June 2023 only. Any work beyond this date will therefore be subject to review and amended to include any agreed rates uplift as set out under Clause 8 (Variation in Price) in the Serapis Framework Agreement.
2. The Y3 and Y4 suffix in Role column of the TMS and SD tables below denote Serapis Y3 and Y4 rates have been used and relates to bullet 1.
3. H2FY22/FY23/FY24 suffixes refer to internal rate changes over Financial Years.

Lot Lead Rates for Task Management Services (TMS)

Team Member Name	Role	Activity Type	Rate (£)	Total Hours	LMS recovery per role per hour ('d' element)	Total LMS recovery due (£) ('d' x total hours)	Total TMS Cost (£) (Rate x total hours)
Redacted under FOIA exemption							
		Total		Redacted under FOIA exemption			£238,564.62

Work Delivered By Sub-Contractor(s)						
Name of Sub-Contractor	**Supplier Type**	**Activity Description**	**Team Member Role**	**Rate (£)**	**Total Hours**	**Total Cost (£)**
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
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				Total	[redacted]	**£1,687,942.65**

Travel, Subsistence, Materials & Equipment

Travel & Subsistence

Supplier Name	Spend Type	Description / Rationale	Unit Cost (£)	Quantity	Total Cost (£)
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
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			Travel & Subsistence Total		£9,150.00

Materials & Equipment

Supplier Name	Spend Type	Description / Rationale	Unit Cost (£)	Quantity	Total Cost (£)
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
			Materials & Equipment Total		£40,668.34
		Travel, Subsistence, Materials & Equipment Total			£49,818.34

Core Work – Milestone breakdown costs

Proposed Milestones Payments.

Milestone M1						
Description	**TMS cost (£)**	**Self-Delivery cost (£)**	**Sub-contractor cost (£)**	**Total milestone cost (£)**	**Milestone due date**	**DEFCON**
EMR Delivery Pre-Contract Activities	£24,997.38	£0.00	£0.00	£24,997.38	24/10/2022	N/A
Travel/Subsistence				£0.00		
Materials/Equipment				£0.00		N/A
Milestone LMS recovery (£)	£3,434.84		Total cost	£24,997.38		

Milestone M2						
Description	**TMS cost (£)**	**Self-Delivery cost (£)**	**Sub-contractor cost (£)**	**Total milestone cost (£)**	**Milestone due date**	**DEFCON**
EMR Delivery Quarterly Review	£11,054.58	£0.00	£322,530.34	£333,584.92	31/01/2023	703
Travel/Subsistence				£1,143.75		
Materials/Equipment				£0.00		703
Milestone LMS recovery (£)	£1,518.97		Total cost	£334,728.67		

Milestone M3						
Description	**TMS cost (£)**	**Self-Delivery cost (£)**	**Sub-contractor cost (£)**	**Total milestone cost (£)**	**Milestone due date**	**DEFCON**
EMR Delivery Quarterly Review	£46,350.55	£0.00	£319,114.99	£365,465.54	28/04/2023	703
Travel/Subsistence				£1,143.75		
Materials/Equipment				£0.00		703
Milestone LMS recovery (£)	£6,368.88		Total cost	£366,609.29		

Milestone M4						
Description	**TMS cost (£)**	**Self-Delivery cost (£)**	**Sub-contractor cost (£)**	**Total milestone cost (£)**	**Milestone due date**	**DEFCON**
EMR Delivery Quarterly Review	£25,434.76	£0.00	£259,257.91	£284,692.67	31/07/2023	703
Travel/Subsistence				£1,143.75		
Materials/Equipment				£0.00		703
Milestone LMS recovery (£)	£3,494.90		Total cost	£285,836.42		

Milestone M5

Description	TMS cost (£)	Self-Delivery cost (£)	Sub-contractor cost (£)	Total milestone cost (£)	Milestone due date	DEFCON
EMR Delivery Year End Report	£25,149.85	£0.00	£119,054.25	£144,204.10	31/10/2023	703
Travel/Subsistence				£1,143.75		
Materials/Equipment				£0.00		703
Milestone LMS recovery (£)	£3,455.76		Total cost	£145,347.85		

Milestone M6

Description	TMS cost (£)	Self-Delivery cost (£)	Sub-contractor cost (£)	Total milestone cost (£)	Milestone due date	DEFCON
EMR Delivery Quarterly Review	£23,902.75	£0.00	£179,392.19	£203,294.94	31/01/2024	703
Travel/Subsistence				£1,143.75		
Materials/Equipment				£20,334.17		703
Milestone LMS recovery (£)	£3,284.40		Total cost	£224,772.86		

Milestone M7

Description	TMS cost (£)	Self-Delivery cost (£)	Sub-contractor cost (£)	Total milestone cost (£)	Milestone due date	DEFCON
EMR Delivery Quarterly Review	£25,051.75	£0.00	£178,964.60	£204,016.35	30/04/2024	703
Travel/Subsistence				£1,143.75		
Materials/Equipment				£20,334.17		703
Milestone LMS recovery (£)	£3,442.28		Total cost	£225,494.27		

Milestone M8

Description	TMS cost (£)	Self-Delivery cost (£)	Sub-contractor cost (£)	Total milestone cost (£)	Milestone due date	DEFCON
EMR Delivery Quarterly Review	£24,942.00	£0.00	£198,740.23	£223,682.23	31/07/2024	703
Travel/Subsistence				£1,143.75		
Materials/Equipment				£0.00		703
Milestone LMS recovery (£)	£3,427.20		Total cost	£224,825.98		

Milestone M9						
Description	**TMS cost (£)**	**Self-Delivery cost (£)**	**Sub-contractor cost (£)**	**Total milestone cost (£)**	**Milestone due date**	**DEFCON**
EMR Delivery Final Report	£31,681.00	£0.00	£110,888.14	£142,569.14	31/10/2024	703
Travel/Subsistence				£1,143.75		
Materials/Equipment				£0.00		703
Milestone LMS recovery (£)	£4,353.18		Total cost	£143,712.89		
Total LMS (All Milestones)	**£32,780.41**	**Total Cost (All Milestones)**		**£1,976,325.61**		

Tasking Form Part 3:

To be completed by the Authority's Commercial Officer and copied to the Authority's Project Manager.

1. **Acceptance of Contract:**		
Authority's Commercial Officer	Name	Redacted under FOIA exemption
	Tel	Redacted under FOIA exemption
	Email	Redacted under FOIA exemption
	Date	26/10/2022
Requisition Number		RQ0000018856
Contractor's Proposal Number		017046/98063L/CH1
Purchase Order Number		DSTL0000009222
Signature		Redacted under FOIA exemption
Please Note: Task authorisation to be issued by the Authority's Commercial Officer or Contract Manager. Any work carried out prior to authorisation is at the Contractor's own risk.		