

PROCEDURA PUBBLICA DI SELEZIONE PER IL RECLUTAMENTO DI N. 1 RICERCATORE A TEMPO DETERMINATO AI SENSI DELL'ART.24, COMMA 3, LETT. A) DELLA LEGGE 240/2010 PRESSO LA SCUOLA NORMALE SUPERIORE - SETTORE SCIENTIFICO DISCIPLINARE CHIM/12 CHIMICA DELL'AMBIENTE E DEI BENI CULTURALI, BANDITA CON D.D. N.169 DEL 1°03.2022.

RELAZIONE RIASSUNTIVA

La Commissione giudicatrice della procedura pubblica di selezione sopra citata, nominata con D.D. n.397 del 25.05.2022, composta da:

- prof.ssa Nadia Marchettini, ordinario del settore concorsuale oggetto della selezione, in servizio presso l'Università degli Studi di Siena;
- prof.ssa Angela Agostiano, ordinario del settore concorsuale oggetto della selezione, in servizio presso l'Università degli studi di Bari Aldo Moro;
- prof. Julien Roland Michel Bloino, associato del settore concorsuale oggetto della selezione in servizio presso la Scuola.

ha tenuto complessivamente n. 3 riunioni telematiche iniziando i lavori il 28/07/2022 e concludendoli il 15/09/2022, come di seguito indicato:

I riunione: giorno 28/07/2022 dalle ore 15:15 alle ore 18:00

II riunione: giorno 23/08/2022 dalle ore 15:00 alle ore 16:30

III riunione: giorno 15/09/2022 dalle ore 14:00 alle ore 16:45

Nella **prima riunione** la Commissione:

- ha preliminarmente preso visione degli atti normativi e regolamentari che disciplinano lo svolgimento della procedura;
- ha proceduto alla designazione, nel proprio seno, di Presidente e Segretario attribuendo tali funzioni rispettivamente alla Prof.ssa Nadia Marchettini e al Prof. Julien Roland Michel Bloino;
- ha preso atto della durata massima dei lavori (nel limite di quattro mesi dal giorno 25/05/2022 data del decreto di nomina della Commissione);
- ha preso atto che il numero dei candidati ammessi alla selezione in possesso dei requisiti è inferiore a sei e ha proceduto a predeterminare i criteri e parametri da utilizzare per l'attribuzione di un punteggio ai titoli e alle singole pubblicazioni dei candidati successiva alla discussione pubblica;
- ha stabilito le modalità di accertamento dell'adeguata conoscenza della lingua inglese prevista dal bando contestualmente allo svolgimento della discussione pubblica, nonché i criteri e le modalità di espressione del relativo giudizio;

Il verbale n.1 contenente i criteri e parametri di valutazione adottati dalla Commissione nella seduta preliminare è stato trasmesso al responsabile del procedimento al fine di renderli noti ai candidati – come previsto dal Regolamento, tramite pubblicazione effettuata nell'apposita sezione del sito Web della Scuola dedicato alla selezione, a cura degli uffici amministrativi. Decorso sette giorni dalla data di pubblicazione dei criteri e parametri predetti, la Commissione ha potuto proseguire i lavori prendendo visione delle domande ammesse.

Nella **seconda riunione** la Commissione:

- ha preso visione dell'elenco dei candidati che hanno presentato domanda, non esclusi o non rinunciatari alla data della riunione medesima, che sono i seguenti:

Zoi Salta

Anuj Tripathi

e ognuno dei componenti della Commissione ha reso apposita dichiarazione ai sensi del D.P.R. n. 445/2000, allegata al verbale della seconda riunione, di non avere relazioni di parentela e affinità entro il IV grado incluso, con gli altri commissari e con i candidati (art.5, comma 2 del D. Lgs 1172/1948), che non sussistono le cause di astensione di cui agli artt.51 e 52 del c.p.c. e ha

La candidata presenta titoli e lavori ritenuti di buon livello scientifico e attinenti al settore scientifico-disciplinare CHIM/12. Ha esposto con chiarezza i risultati della propria ricerca, dimostrando una buona padronanza della lingua inglese.

Dopo la redazione collegiale da parte della Commissione della presente relazione riassuntiva, alle ore 16:45 del giorno 15/09/2022 il Presidente ha dichiarato chiusi i lavori, impegnandosi a consegnare gli atti concorsuali al Responsabile del procedimento, con lettera di trasmissione indirizzata al Direttore della Scuola.

Letto, approvato e sottoscritto:

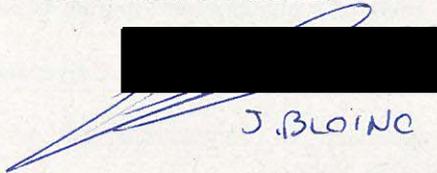
LA COMMISSIONE:

Prof.ssa Nadia Marchettini, Presidente

Prof.ssa Angela Agostiano, Componente

Prof. Julien Roland Michel Bloino Componente con funzioni anche di Segretario

PER LA COMMISSIONE:



J. BLOINO

Prof. Julien Roland Michel Bloino

ELENCO DEI TITOLI E DELLE PUBBLICAZIONI VALUTABILI

1) CANDIDATA: *Salta Zoi*

TITOLI E CURRICULUM:

TITOLI VALUTABILI

- 1 – Titolo: dottorato di ricerca in Chimica
- 2 – Titolo: attività di insegnamento “Physical Chemistry Laboratory 2”, Università di Ioannina, Grecia
- 3 – Titolo: attività di insegnamento “Computational Chemistry Laboratory”, Università di Ioannina, Grecia
- 4 – Titolo: attività di insegnamento “Modern quantum and statistical mechanics techniques for the investigation of chemical reactions”, Università di Ioannina, Grecia
- 5 – Titolo: attività di formazione o ricerca “Fellowship from Bilateral Collaboration Program Greece-Slovenia”, Università di Ioannina, Grecia
- 6 – Titolo: attività di formazione o ricerca “Research Funding Program: Heracleitus II”, Università di Ioannina, Grecia
- 7 – Titolo: attività di formazione o ricerca “Development and application of computational methods for chemical reactivity in the gas phase”, Scuola Normale Superiore, Pisa, Italia
- 8 – Titolo: relatore a congressi e convegni nazionali e internazionali: 3 internazionali e 1 nazionale

TITOLI NON VALUTABILI

- 1 – Titolo: laurea triennale (bachelor) in Scienza dei Materiali e Ingegneria perché non rientra nei criteri di valutazione prestabiliti.
- 2 – Titolo: master in Chimica, Scienza dei Materiali e Ingegneria perché non rientra nei criteri di valutazione prestabiliti.
- 3 – Titolo: organizzazione, direzione e coordinamento di gruppi di ricerca nazionali e internazionali “Participation in Prof. Kosma’s group” perché il periodo rappresentava la frequenza di un laboratorio da studente.
- 4 – Titolo: organizzazione, direzione e coordinamento di gruppi di ricerca nazionali e internazionali “Participation in Prof. Ventura’s group” perché non è specificato il periodo.
- 5 – Titolo: organizzazione, direzione e coordinamento di gruppi di ricerca nazionali e internazionali “Participation in Prof. Barone’s group” perché non è specificato il periodo.
- 6 – Titoli aggiuntivi (vedi CV) 1-5 perché la presentazione di poster non rientra nei criteri di valutazione prestabiliti
- 7 – Titoli aggiuntivi: 6-10 perché l’attività di reviewing per giornali con valutazione da pari non rientra nei criteri di valutazione prestabiliti
- 8 – Titoli aggiuntivi: 11-16 perché le attività seminariali non rientrano nei criteri di valutazione prestabiliti
- 9 – Titoli aggiuntivi: 17-19 perché le attività di mentoring non rientrano nei criteri di valutazione prestabiliti

PUBBLICAZIONI

PUBBLICAZIONI VALUTABILI

- 1 – Tutte le pubblicazioni presentate (1-12, vedi “LIST OF SUBMITTED PUBLICATIONS”) sono valutabili

PUBBLICAZIONI NON VALUTABILI

Nessuna

TESI DI DOTTORATO:

Non elencata tra i 12 lavori

PRODUZIONE SCIENTIFICA COMPLESSIVA

Il candidato presenta una produzione scientifica complessiva, risultante dal curriculum, pari a n. 23 pubblicazioni, svolta nell'arco di 16 anni effettivi. La 24° pubblicazione non è valutabile perché in fase di referaggio al momento della presentazione della domanda.

2) CANDIDATO: Tripathi Anuj

TITOLI E CURRICULUM:

TITOLI VALUTABILI

1 – Titolo: dottorato di ricerca in chimica

2 – Titolo: attività di formazione o ricerca presso National Institute of Technology, Kurukshetra, Haryana, India

3 – Titolo: relatore a congressi e convegni nazionali e internazionali: 3 internazionali e 1 nazionale

TITOLI NON VALUTABILI

1 – Master in chimica organica perché non rientra nei criteri di valutazione prestabiliti.

PUBBLICAZIONI

PUBBLICAZIONI VALUTABILI

Nessuna

PUBBLICAZIONI NON VALUTABILI

1 – Pubblicazioni 1 a 12 (vedi "LIST OF SUBMITTED PUBLICATIONS") perché non presenti nella domanda

TESI DI DOTTORATO:

Non elencata tra i 12 lavori

PRODUZIONE SCIENTIFICA COMPLESSIVA

Il candidato presenta una produzione scientifica complessiva, risultante dal curriculum e dal documento allegato, pari a n. 26 pubblicazioni, svolta nell'arco di 6 anni effettivi.

Allegato n. 2 alla relazione riassuntiva

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**PUNTEGGIO DEI TITOLI E DELLE PUBBLICAZIONI DEI CANDIDATI
E GIUDIZIO SULL'ACCERTAMENTO DELLA CONOSCENZA DELLA LINGUA STRANIERA**

1) CANDIDATA: *Zoi Salta*

TITOLI

Titoli valutabili	Max punti 50
dottorato di ricerca di ricerca o equipollenti in chimica, conseguito all'Estero	punti 5
attività didattica a livello universitario all'Estero svolta: Università di Ioannina, Grecia	punti 2
documentata attività di formazione o di ricerca presso qualificati istituti italiani o stranieri: Università di Ioannina, Grecia e Scuola Normale Superiore (Pisa)	punti 13 di cui:
per la valorizzazione delle esperienze di mobilità	Punti 3
per gli ulteriori criteri di valutazione previsti	punti 10
documentata attività in campo clinico	punti _____
attività progettuale	punti _____
organizzazione, direzione e coordinamento di gruppi di ricerca nazionali e internazionali, o partecipazione agli stessi:	punti 0
titolarità di brevetti	punti 0
relatore a congressi e convegni nazionali e internazionali: 3 internazionali e 1 nazionale	punti 7
premi e riconoscimenti nazionali e internazionali per attività di ricerca:	punti 0
diploma di specializzazione europea riconosciuto da Board internazionali	punti _____
PUNTEGGIO COMPLESSIVO TITOLI	Punti 27

PUBBLICAZIONI

PUBBLICAZIONI VALUTABILI	Criteri/Punti				Totale max punti 50
	a) originalità ecc.	b) congruenza	c) rilev.scientif.coll.edit.	d) apporto	

				individuale	
Pubblicazione n. 1	Punti 2	Punti 4	Punti 2	Punti 1	Punti 9
Pubblicazione n.2	Punti 2	Punti 4	Punti 3	Punti 1	Punti 10
Pubblicazione n.3	Punti 2	Punti 4	Punti 2	Punti 1	Punti 9
Pubblicazione n.4	Punti 2	Punti 4	Punti 1	Punti 4	Punti 11
Pubblicazione n.5	Punti 2	Punti 4	Punti 3	Punti 4	Punti 13
Pubblicazione n.6	Punti 2	Punti 4	Punti 1	Punti 4	Punti 11
Pubblicazione n.7	Punti 2	Punti 4	Punti 3	Punti 4	Punti 13
Pubblicazione n.8	Punti 2	Punti 4	Punti 2	Punti 4	Punti 12
Pubblicazione n.9	Punti 2	Punti 4	Punti 3	Punti 4	Punti 13
Pubblicazione n.10	Punti 2	Punti 4	Punti 3	Punti 4	Punti 13
Pubblicazione n.11	Punti 2	Punti 4	Punti 3	Punti 4	Punti 13
Pubblicazione n.12	Punti 2	Punti 1	Punti 4	Punti 4	Punti 11
PUNTEGGIO COMPLESSIVO PUBBLICAZIONI					Punti 50

PUNTEGGIO TOTALE TITOLI E PUBBLICAZIONI	Punti 77
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ACCERTAMENTO CONOSCENZA LINGUA INGLESE

GIUDIZIO	Buono
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2) CANDIDATO: Anuj Tripathi

TITOLI

Titoli valutabili	Max punti 50
dottorato di ricerca di ricerca o equipollenti in chimica, conseguito all'Estero	punti 1
attività didattica a livello universitario all'Estero svolta:	punti 0
documentata attività di formazione o di ricerca presso qualificati istituti italiani o stranieri:	punti 3 di cui:
per la valorizzazione delle esperienze di mobilità	Punti 0
per gli ulteriori criteri di valutazione previsti	punti 3
documentata attività in campo clinico	punti _____
attività progettuale	punti _____
organizzazione, direzione e coordinamento di gruppi di ricerca nazionali e internazionali, o partecipazione agli stessi:	punti 0

titolarità di brevetti	punti 0
relatore a congressi e convegni nazionali e internazionali: 3 internazionali e 1 nazionale	punti 1
premi e riconoscimenti nazionali e internazionali per attività di ricerca:	punti 0
diploma di specializzazione europea riconosciuto da Board internazionali	punti _____
PUNTEGGIO COMPLESSIVO TITOLI	Punti 5

PUBBLICAZIONI

LE PUBBLICAZIONI NON SONO STATE PRESENTATE. QUINDI QUESTA PARTE NON È VALUTABILE.

PUBBLICAZIONI VALUTABILI	Criteri/Punti				Totale max punti 50
	a) originalità ecc.	b) congruenza	c) rilev.scientif.coll.edit.	d) apporto individuale	
Pubblicazione n. 1	Punti	Punti	Punti ____	Punti ____	Punti
Pubblicazione n.2	Punti	Punti	Punti ____	Punti ____	Punti
Pubblicazione n.3	Punti	Punti	Punti ____	Punti ____	Punti
Pubblicazione n.4	Punti	Punti	Punti ____	Punti ____	Punti
Pubblicazione n.5	Punti	Punti	Punti ____	Punti ____	Punti
Pubblicazione n.6	Punti	Punti	Punti ____	Punti ____	Punti
Pubblicazione n.7	Punti	Punti	Punti ____	Punti ____	Punti
Pubblicazione n.8	Punti	Punti	Punti ____	Punti ____	Punti
Pubblicazione n.9	Punti	Punti	Punti ____	Punti ____	Punti
Pubblicazione n.10	Punti	Punti	Punti ____	Punti ____	Punti
Pubblicazione n.11	Punti	Punti	Punti ____	Punti ____	Punti
Pubblicazione n.12	Punti	Punti	Punti ____	Punti ____	Punti
PUNTEGGIO COMPLESSIVO PUBBLICAZIONI					Punti 0

PUNTEGGIO TOTALE TITOLI E PUBBLICAZIONI	Punti 5
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ACCERTAMENTO CONOSCENZA LINGUA INGLESE

GIUDIZIO	Buono
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CURRICULUM VITAE ¹

DR. ZOI SALTA

I Part – Personal details

Name and Surname	<i>Zoi Salta</i>
Date of birth	██████████
Place of birth	██████████
Nationality	██████████
Current academic/work position, specifying if permanent/tenured position	<i>Research Fellow on “Development and application of computational methods for chemical reactivity in the gas phase”, Faculty of Sciences, Scuola Normale Superiore, Pisa, Italy</i>
Languages spoken	<i>Greek (native), English (excellent), Italian (good), German (good)</i>

II Part – Academic titles

Title name and type	Achievement date	Institute and Country	Final grade	Thesis title and notes
B.Sc. in Materials Science and Engineering	22/07/2005	Department of Materials Science and Engineering, University of Ioannina, Ioannina, Greece	Very Good (6.92/10)	Computational study of structural, electronic and oscillatory properties of metallic nanowires of copper (Cu).
M.Sc. in Chemistry and Materials Science and Engineering	11/04/2008	Department of Chemistry, University of Ioannina, Ioannina, Greece	Very Good	Computational study of structural, spectroscopic and thermodynamic properties of halogenated nitro-organic compounds and their formation-dissociation reaction pathways in the Atmosphere.
Ph.D. in Chemistry	06/02/2015	Department of Chemistry, University of Ioannina, Ioannina, Greece	Excellent	Computational study of the nitroderivatives of methyl thiyl radical (CH ₃ S) – Structural, spectroscopic and energetic properties and modeling of their formation reactions in Atmospheric Chemistry.

¹ The present CV describes in detail the qualification held by the candidate that are deemed relevant for the assessment procedure. The CV is organised following a scheme that can be modified/integrated by the candidate who wishes to adapt it to its own activity. All the space available can be integrated as needed.

III Part – Other qualifications

III.1 – Teaching activity in Italian or foreign universities:

Dates	Institute and Country	Short description of the teaching activity ²
Fall semester of the academic years 2008 – 2011	Department of Chemistry, University of Ioannina, Ioannina, Greece	Non-tenure professor: Physical Chemistry Laboratory 2: “Electrochemistry, Chemical Kinetics and Physical Chemistry of Polymers”, Bachelor’s degree course in Chemistry
From 19/10/2016 to 03/02/2017	Department of Chemistry, University of Ioannina, Ioannina, Greece	Non-tenure professor: “Computational Chemistry Laboratory”, Master’s degree course in Chemistry
From 15/03/2018 to 30/09/2018	Department of Chemistry, University of Ioannina, Ioannina, Greece	Non-tenure professor: “Modern quantum and statistical mechanics techniques for the investigation of chemical reactions”, Bachelor’s degree course in Chemistry

III.2 – Certified study or research activity in Italian or foreign institutions

Dates	Institute and Country	Short description of the study/research activity ³
from 2005 to 2008	Department of Chemistry, University of Ioannina, Ioannina, Greece	M.Sc. Scholarship – Fellowship from the Bilateral Collaboration Program Greece-Slovenia, Ministry of Higher Education, Science and Technology of Slovenia – General Secretariat for Research and Technology of Greece
from 2010 to 2013	Department of Chemistry, University of Ioannina, Ioannina, Greece	Ph.D. Scholarship – Fellowship from the European Union (European Social Fund – ESF) and Greek national funds through the Operational Program "Education and Lifelong Learning" of the National Strategic Reference Framework (NSRF) - Research Funding Program: Heracleitus II . Investing in knowledge society through the European Social Fund
From 01/06/2018 to date	Faculty of Sciences, Scuola Normale Superiore, Pisa, Italy	Postdoctoral Fellowship on “Development and application of computational methods for chemical reactivity in the gas phase”

III.3 – Clinical activities (only for those recruitment fields that require it):

Dates	Institute and Country	Short description of the activity ⁴
dal ___/___/____ dal ___/___/____		

² Please list in detail all the relevant elements for assessment, e.g.: name of the course or lectures held, total teaching hours, type of course (e.g.: Bachelor’s degree course, PhD course, Master’s degree course, Summer School), type of contract (e.g.: teaching appointment, visiting professor, researcher appointment), etc.

³ Please list in details all the relevant elements for assessment, e.g.: type of contract or academic position (e.g.: research grant, fixed-term researcher contract, PhD scholarship/grant.), subject, procedures, etc.

⁴ Please list in detail all the relevant elements for assessment. If irrelevant, please leave blank.

III.4 - Projects (only for those recruitment fields that require it):

Dates	Institute and Country	Short description of the activity ⁵
from ___/___/___ to ___/___/___		

III.5 - Organisation, supervision and coordination of national and international research groups or participation in any research group:

Dates	Research group/programme ⁶	Role and short description of the activity ⁷
From 01/09/2005 to 01/06/2018	Computational Chemistry Laboratory, Division of Physical Chemistry, Department of Chemistry, University of Ioannina, Ioannina, Greece	Participation in Prof. Kosma's group as a principal investigator of reaction mechanisms in atmospheric chemistry
From 01/09/2017 to date	Computational Chemistry and Biology Group, CCBG, DETEMA, Facultad de Química, Universidad de la República, 11400 Montevideo, Uruguay	Participation in Prof. Ventura's group as a researcher in the application of computational chemistry in complex reaction mechanisms
From 01/06/2018 to date	SMART Laboratory – Multidisciplinary Approaches for Research and Technology, Faculty of Sciences, Scuola Normale Superiore, Pisa, Italy	Participation in Prof. Barone's group as a theoretical investigator of reaction mechanisms and their kinetics, in the earth's atmosphere and in astrochemical environments.

III.6 – Ownership of patents (only for those recruitment fields that require it)⁸:

Title	Description	Submission No.	License No.	Name of the owner	Name of the inventor	Date of submission

⁵ Please list in detail all the relevant elements for assessment. If irrelevant, please leave blank.

⁶ Please state the name of the research group and/or programme, specifying if national or international, the name of any private/public funding body and any call or other relevant detail.

⁷ Please list in detail all the relevant elements for assessment, e.g.: any organisation, supervision or coordination role within the research programme (PI-principal investigator, local supervisor, etc.) and any activities.

⁸ Please fill every space; in case the candidate does not own any patent, please leave blank.

III.7 – Speeches⁹ in national and international conferences and congresses:

Date of the conference/congress	Organising body and place of the conference	Conference/Congress title <i>(please specify if national or international)</i>	Speech title <i>(please specify if invited speaker)</i>
Date 06/04/2014	Metropolitan Hotel, Athens, Greece	International Conference of Computational Methods in Sciences and Engineering 2014	S-OO Bond Dissociation Energies and Enthalpies of Formation of the Thiomethyl Peroxyl Radicals CH ₃ S(O) _n OO (n=0,1,2).
Date 05/09/2018	University of Sapienza, Rome, Italy	15 th Eurasia Conference on Chemical Sciences (International)	Computational Characterization of the Herbicide Metolachlor: Structure, Conformational Analysis and Monohydroxylated Photo Degradation Products.
Date 14/02/2019	Centro Congressi Federico II, Naples, Italy	Winter Modeling 2019 Special Edition (National)	Molecular Modeling Tools for Reactivity and Kinetics
Date 24/06/2019	Centre national de la recherche scientifique (CNRS), Orléans, France	11 th International Conference on Chemical Kinetics	H-abstraction from DMS by an excess of OH in the absence of O ₂ .

III.8 – National and international awards for research activities:

Date of issue	Name/Title of the award <i>(please specify if national or international)</i>	Awarding body and Country	Notes

III.9 – European specialisation diplomas recognised by international boards (only for those recruitment fields that require it):

Date	Institute and Country	Short description ¹⁰

III.10 – Any additional title or qualification¹¹:

Name of the title or qualification	Dates	Short description
1 - 14 th International Density Functional Theory Conference - Applications in Physics, Chemistry, Biology, Pharmacy, Athens, Greece	29/8 – 2/9 2011	Poster presentation: “The atmospheric reactions between the alkylperoxy radicals RO ₂ (R=CH ₃ , CH ₃ SCH ₂ etc) and NO. Thermochemistry using DFT methods.”

⁹ Please fill this section only if you have participated in conferences/congresses as speaker. Any different kind of participation (as listener, for poster presentation etc.) shall be listed in the following section III.10.

¹⁰ Please list in detail all the relevant elements for assessment, e.g.: scientific field, title of the thesis, final grade. In case the candidate does not hold this kind of diploma, please leave blank.

¹¹ E.g. participation in editorial committees of scientific journals, supervision or tutoring activities for doctoral theses, participation in organisational committees of conferences/congresses, scientific divulgation activities, participation in academic selection committees, scientific reviewing activities, organisation of relevant exhibitions, participation in congresses/conferences not as speaker. The Selection Committee will decide on the relevance of any additional title/qualification.

2 - 12 th Eurasia Conference on Chemical Sciences, Corfu, Greece	16/4 – 21/4 2012	Poster presentation: “Ab initio and DFT investigation of the structural and thermochemical properties of the peroxy nitrates $\text{CH}_3\text{S}(\text{O})_n\text{OONO}_2$ and the $\text{CH}_3\text{S}(\text{O})_n\text{OO}$ decomposition radicals ($n=0,1,2$).”
3 - 22 nd Panhellenic Chemistry Conference Meeting, Thessaloniki, Greece	2/12 – 4/12 2016	Poster presentation: “Water complexes of halogenated nitromethanes. A computational study of structure and properties.”
4 - 5 th Chemistry Conference Meeting, Department of Chemistry, University of Ioannina, Ioannina, Greece	29/9 – 30/9 2017	Poster presentation: “Physicochemical and computational study of 3-Methyl-1,3-thiazolidine-2-thione complexes with dihalogens (I_2 , IBr , ICl , BrBr , BrCl) for the design of novel drugs in thyroid disease treatments.”
5 - 5 th Chemistry Conference Meeting, Department of Chemistry, University of Ioannina, Ioannina, Greece	29/9 – 30/9 2017	Poster presentation: “Atmospheric degradation of the peroxy radical $\text{CF}_3\text{OCH}_2\text{O}_2$. A computational study of the reactions with HO_2 and NO .”
6 - ACS Earth and Space Chemistry (ACS Publications)	Since 15/01/2020	Scientific Reviewing Activity
7 - Journal of Molecular Structure (Elsevier)	Since 20/01/2020	Scientific Reviewing Activity
8 - Atmospheric Environment (Elsevier)	Since 01/09/2020	Scientific Reviewing Activity
9 - ACS Omega (ACS Publications)	Since 28/12/2020	Scientific Reviewing Activity
10 - Journal of Physical Chemistry A (ACS Publications)	Since 24/03/2021	Scientific Reviewing Activity
11 - “Computational Study of the Formation of Halogenated N-organic Compounds and of Nitroderivatives of the Methylthiyl Radical (CH_3S) in the Atmosphere”, Jožef Stefan Institute, Ljubljana, Slovenia.	18/11/2011	Invited Lecture
12 - “Computational Study of the Peroxyl Nitroderivatives of the Methylthiyl Radical (CH_3S)- Modeling of Formation Reactions in Atmospheric Chemistry”, Graduate Conference Meeting, Department of Chemistry, University of Ioannina, Ioannina, Greece	15/03/2013	Invited Lecture
13 - “Molecular Modeling Tools for Reactivity and Kinetics”, Undergraduate Seminar (Seminari sulle Frontiere della Chimica) for the Chemistry Course of Scuola Normale Superiore, Faculty of Sciences, Scuola Normale Superiore, Pisa, Italy	17/07/2020	Invited Lecture
14 - “Molecular Modeling Tools for Reactivity and Kinetics”, Undergraduate Seminar (Seminari sulle Frontiere della Chimica) for the Chemistry Course of Scuola Normale Superiore, Faculty of Sciences, Scuola Normale Superiore, Pisa, Italy	13/10/2021	Invited Lecture

15 - "Mechanisms and Kinetics in the Earth's Atmosphere", Postgraduate Seminar for the Astrochemistry Course of the PhD program "Molecular Sciences for Earth and Space (MOSES)", Scuola Superiore Meridionale, Naples, Italy	09/03/2022	Invited Lecture
16 - "Molecular Modeling Tools for Reactivity and Kinetics – Case Examples of Environmental Interest", Undergraduate Seminar (Seminari sulle Frontiere della Chimica) for the chemistry course of Scuola Normale Superiore, Faculty of Sciences, Scuola Normale Superiore, Pisa, Italy	30/03/2022	Invited Lecture
17 - Master dissertation: "Water-Assisted Degradation of Chloroalcohols in Gas Phase." Division of Physical Chemistry Department of Chemistry, University of Ioannina, Ioannina, Greece	2017 - 2018	Second-supervisor with tutoring activities of <u>George Petsis</u> for his M.Sc. degree in Chemistry
18 - PhD thesis: "Physicochemical and computational study of Iodine Dihalogen complexes (I ₂ , IBr, ICl) as model compounds for the design of novel drugs in thyroid disease treatments." Division of Physical Chemistry Department of Chemistry, University of Ioannina, Ioannina, Greece	2017 - 2018	Second-supervisor with tutoring activities of <u>Christos Lygdas</u> for his Ph.D. degree in Chemistry
19 - PhD thesis on the subject: "Computational Quantum Chemistry for Atmospheric Monitoring and Environmental Sustainability." IUSS University School for Advanced Studies, Pavia and Faculty of Sciences, Scuola Normale Superiore, Pisa, Italy	2022 - present	Second-supervisor with tutoring activities of <u>Nadjib Rais</u> for his Ph.D. degree in Sustainable Development and Climate Change

IV Part – Authored or co-authored scientific publications

No.	Type of scientific product	Author/s	Publication title	Title of the journal/book/dictionary containing the article/contribution/entry and its code	Year of publication
1 -	<i>Article</i>	Lesar, A., Salta, Z., Kovacic, S., Kosmas, A.M.	Theoretical characterization of halogenated methylperoxy nitrites	Chemical Physics Letters 446, 268–275. doi:10.1016/j.cplett.2007.08.062 ISSN:0009-2614	2007

			$CX_nY_{3-n}OONO$ (X, Y=H, F, Cl)		
2 -	Article	Kosmas, A.M., Salta, Z., Lesar, A.	Effect of Halogenation on the Mechanism of the Atmospheric Reactions between Methylperoxy Radicals and NO. A computational Study	Journal of Physical Chemistry A 113, 3545–3554. doi:10.1021/jp808895a ISSN:1520-5215	2009
3 -	Article	Kosmas, A.M., Mpellos, C., Salta, Z., Drougas, E.	Structural and heat of formation studies of halogenated methyl hydro-peroxides	Chemical Physics 371, 36–42. doi:10.1016/j.chemphys.2010.03.026 ISSN:1873-4421	2010
4 -	Article	Salta, Z., Kosmas, A.M., Lesar, A.	Computational investigation of the peroxy radicals $CH_3S(O)_nOO$ and the peroxy nitrates $CH_3S(O)_nOONO_2$ ($n=0, 1, 2$)	Computational and Theoretical Chemistry 1001, 67–76. doi:10.1016/j.comptc.2012.10.007 ISSN:2210-271X	2012
5 -	Article	Salta, Z., Kosmas, A.M.	Computational Study of the Reaction of the Methylsulfonyl Radical, $CH_3S(O)_2$, with NO_2	International Journal of Quantum Chemistry 114, 1430–1437. doi:10.1002/qua.24700 ISSN: 1097-461X	2014
6 -	Article	Salta, Z., Kosmas, A.M., Lesar, A.	S-OO bond dissociation energies and enthalpies of formation of the thiomethyl peroxy radicals $CH_3S(O)_nOO$ ($n=0,1,2$)	AIP Conference Proceedings Series 1618, 916–919. doi:10.1063/1.4897882 ISSN:1551-7616	2014
7 -	Article	Salta, Z., Kosmas, A.M.	Computational investigation of the formation and isomerization pathways of CH_3SNO_2 and the S–N bond dissociation energies of $CH_3S(O)_nNO_2$ ($n=0,1,2$) species	Structural Chemistry 27 (4), 1149–1156. doi:10.1007/s11224-015-0737-y ISSN:1040-0400	2016
8 -	Article	Salta, Z., Papayannis, D.K., Kosmas, A.M.	Computational study of the hydrogen bonding interactions in the $[CH_2XNO_2 \cdot H_2O]$ clusters (X=H, F, Cl, Br, I)	Computational and Theoretical Chemistry 1115, 63–68. doi:10.1016/j.comptc.2017.05.028 ISSN:2210-271X	2017
9 -	Article	Salta, Z., Kosmas, A.M., Ventura, O.N.	Computational characterization of the herbicide metolachlor and its mono-hydroxylated photodegradation products	Theoretical Chemistry Accounts 137(11), 151. doi:10.1007/s00214-018-2353-6 ISSN:1432-2234	2018
10 -	Article	Salta, Z., Kosmas, A.M., Ventura, O.N., Barone, V.	Computational Evidence Suggests That 1-Chloroethanol May Be an Intermediate in the Thermal Decomposition of 2-Chloroethanol into Acetaldehyde and HCl	Journal of Physical Chemistry A 123, 1983–1998. doi:10.1021/acs.jpca.8b11966 ISSN:1520-5215	2019
11 -	Article	Petsis, G., Salta, Z., Kosmas, A.M., Ventura, O.N.	Theoretical study of the microhydration of 1-chloro and 2-chloro ethanol as a clue for their	International Journal of Quantum Chemistry 119 (17), e25931. doi:10.1002/qua.25931	2019

			relative propensity toward dehalogenation	ISSN: 1097-461X	
12 -	Article	Salta, Z., Liaska, S., Papayannis, D.K., Lesar, A., Kosmas, A.M.	Computational studies on the reactions of the peroxy radical $\text{CF}_3\text{OCH}_2\text{O}_2^\cdot$ with HO_2^\cdot and NO^\cdot	Computational and Theoretical Chemistry 1163, 112510. doi:10.1016/j.comptc.2019.112510 ISSN:2210-271X	2019
13 -	Article	Ventura, O.N., Kieninger, M., Salta, Z., Kosmas, A.M., Barone, V.	Enthalpies of formation of the benzyloxyl, benzylperoxyl, hydroxyphenyl radicals and related species on the potential energy surface for the reaction of toluene with the hydroxyl radical	Theoretical Chemistry Accounts 138(10), 115. doi:10.1007/s00214-019-2500-8 ISSN:1432-2234	2019
14 -	Article	Salta, Z., Lupi, J., Tasinato, N., Barone, V., Ventura, O.N.	Unraveling the role of additional OH-radicals in the H-Abstraction from Dimethyl sulfide using quantum chemical computations	Chemical Physics Letters 739, 136963. doi:10.1016/j.cplett.2019.136963 ISSN:0009-2614	2020
15 -	Article	Salta, Z., Kosmas, A.M., Ventura, O.N.	Kinetics and thermodynamics of the hydroxylation products in the photodegradation of the herbicide Metolachlor	Pure and Applied Chemistry, vol. 92, no. 3, pp. 473-484. doi:10.1515/pac-2018-1205. ISSN:1365-3075	2020
16 -	Article	Salta, Z., Lupi, J., Barone, V., Ventura, O.N.	H-Abstraction from Dimethyl Sulfide in the Presence of an Excess of Hydroxyl Radicals. A Quantum Chemical Evaluation of Thermochemical and Kinetic Parameters Unveils an Alternative Pathway to Dimethyl Sulfoxide	ACS Earth and Space Chemistry 4, 3, 403-419. doi:10.1021/acsearthsp.acechem.9b00306 ISSN:2472-3452	2020
17 -	Article	Salta, Z., Tasinato, N., Lupi, J., Bousseffi, R., Balbi, A., Puzzarini, C., Barone, V.	Exploring the Maze of $\text{C}_2\text{N}_2\text{H}_5$ Radicals and Their Fragments in the Interstellar Medium with the Help of Quantum-Chemical Computations	ACS Earth and Space Chemistry 4, 5, 774-782. doi:10.1021/acsearthsp.acechem.0c00062 ISSN:2472-3452	2020
18 -	Article	Salta, Z., Kosmas, A.M., Segovia, M.E., Kieninger, M., Ventura, O.N., Barone, V.	A reinvestigation of the deceptively simple reaction of toluene with OH, and the fate of the benzyl radical: a combined thermodynamic and kinetic study on the competition between OH-addition and H-abstraction reactions	Theoretical Chemistry Accounts, 139:112. doi:10.1007/s00214-020-02626-8 ISSN:1432-2234	2020
19 -	Article	Salta, Z., Kosmas, A.M., Segovia, M.E., Kieninger, M., Tasinato, N., Barone, V., Ventura, O.N.	Reinvestigation of the Deceptively Simple Reaction of Toluene with OH and the Fate of the Benzyl Radical: The "Hidden" Routes to Cresols and Benzaldehyde	Journal of Physical Chemistry A 124, 5917-5930. doi:10.1021/acs.jpca.0c03727 ISSN:1520-5215	2020

20 -	Article	Puzzarini, C., Salta, Z., Tasinato, N., Lupi, J., Cavallotti, C., Barone, V.	A twist on the reaction of the CN radical with methylamine in the interstellar medium: new hints from a state-of-the-art quantum-chemical study	Monthly Notices of the Royal Astronomical Society 496 (4), 4298–4310. doi:10.1093/mnras/sta1652 ISSN:1365-2966	2020
21 -	Article	Salta, Z., Segovia, M.E., Katz, A., Tasinato, N., Barone, V., Ventura, O.N.	Isomerization and Fragmentation Reactions on the [C ₂ SH ₄] Potential Energy Surface: The Metastable Thione S-Methylide Isomer	Journal of Organic Chemistry 86, 2941–2956. doi:10.1021/acs.joc.0c02835 ISSN:1520-6904	2021
22 -	Article	Barone, V., Lupi, J., Salta, Z., Tasinato, N.	Development and Validation of a Parameter-Free Model Chemistry for the Computation of Reliable Reaction Rates	Journal of Chemical Theory and Computation 17, 4913–4928. doi:10.1021/acs.jctc.1c00406 ISSN:1549-9626	2021
23 -	Article	Ceselin, G., Salta, Z., Bloino, J., Tasinato, N., Barone, V.	Accurate Quantum Chemical Spectroscopic Characterization of Glycolic Acid: A Route Toward its Astrophysical Detection.	Journal of Physical Chemistry A 126, 2373–2387. doi:10.1021/acs.jpca.2c01419 ISSN:1520-5215	2022
24 -	Article	Salta, Z., Vega-Tejido, M., Katz, A., Tasinato, N., Barone, V., Ventura, O.N.	Dipolar 1,3-cycloaddition of formaldehyde-S-methylide (CH ₂ SCH ₂) to ethylene and acetylene. A comparison with (valence) isoelectronic O ₃ , SO ₂ , CH ₂ OO and CH ₂ SO.	Journal of Computational Chemistry, Manuscript ID number: JCC-22-0207 (under review)	2022

Research Fields and Current Research Interests

- Development and implementation of computational protocols, based on the combination and interaction of different theoretical methods and programs, for the simulation, validation and evaluation of chemical reactions
- Theoretical studies on the chemical reactivity of important species in environmental chemistry, with the use of state-of-the-art computational protocols and methods. Determination of thermochemical, spectroscopic and kinetic properties of neutral and radical species participating in formation and degradation mechanisms, in gas phase, microsolvation and small clusters
- Chemical transformation of nitrogen, sulfur and halogen species in gas phase and using water clusters, upon reaction with the most prominent atmospheric oxidants (OH, Cl, NO_x). Studies on interhalogen species and the halogen bond, especially in relation to their implications in biological and environmental systems
- Elucidation of proposed reaction mechanisms of closed-shell and radical species identified in the atmospheric degradation of important greenhouse gases and ozone-depleting compounds that are among the factors driving the global climate change

LIST OF SUBMITTED PUBLICATIONS¹

I, the undersigned, **Salta Zoi**, born in [REDACTED], on [REDACTED], resident in [REDACTED]
Italy

SUBMIT

the following publications, in the maximum number of 12 established by the call, for the purpose of evaluation in the context of the selection procedure of No. **1 fixed-term researcher - Type a)** – in the Academic recruitment field **03/A2 – Models and methods for Chemistry**, Academic discipline **CHIM/12 – Chemistry for the environment and for cultural heritage**:

No.	Type of scientific product	Author/s	Publication title	Title of the journal/book/dictionary containing the article/contribution/entry and its code	Year of publication
1 -	Article	Lesar, A., Salta, Z., Kovacic, S., Kosmas, A.M.	Theoretical characterization of halogenated methylperoxy nitrites $CX_nY_{3-n}OONO$ (X, Y=H, F, Cl).	Chemical Physics Letters 446, 268–275. doi:10.1016/j.cplett.2007.08.062 ISSN:0009-2614	2007
2 -	Article	Kosmas, A.M., Salta, Z., Lesar, A.	Effect of Halogenation on the Mechanism of the Atmospheric Reactions between Methylperoxy Radicals and NO. A computational Study.	Journal of Physical Chemistry A 113, 3545–3554. doi:10.1021/jp808895a ISSN:1520-5215	2009
3 -	Article	Kosmas, A.M., Mpellos, C., Salta, Z., Drougas, E.	Structural and heat of formation studies of halogenated methyl hydro-peroxides.	Chemical Physics 371, 36–42. doi:10.1016/j.chemphys.2010.03.026 ISSN:1873-4421	2010
4 -	Article	Salta, Z., Kosmas, A.M., Lesar, A.	Computational investigation of the peroxy radicals $CH_3S(O)_nOO$ and the peroxy nitrates $CH_3S(O)_nOONO_2$ ($n=0, 1, 2$).	Computational and Theoretical Chemistry 1001, 67–76. doi:10.1016/j.comptc.2012.10.007 ISSN:2210-271X	2012
5 -	Article	Salta, Z., Kosmas, A.M.	Computational Study of the Reaction of the Methylsulfonyl Radical, $CH_3S(O)_2$, with NO_2 .	International Journal of Quantum Chemistry 114, 1430–1437. doi:10.1002/qua.24700 ISSN: 1097-461X	2014
6 -	Article	Salta, Z., Kosmas, A.M., Ventura, O.N.	Computational characterization of the herbicide metolachlor and its mono-hydroxylated photodegradation products.	Theoretical Chemistry Accounts 137(11), 151. doi:10.1007/s00214-018-2353-6 ISSN:1432-2234	2018
7 -	Article	Salta, Z., Kosmas, A.M., Ventura, O.N., Barone, V.	Computational Evidence Suggests That 1-Chloroethanol May Be an Intermediate in the Thermal Decomposition of 2-Chloroethanol into Acetaldehyde and HCl.	Journal of Physical Chemistry A 123, 1983–1998. doi:10.1021/acs.jpca.8b11966 ISSN:1520-5215	2019

¹ Please see art. 3, par. 2. c) of the call for selection for the list of valid publications and the submittal procedure.

8 -	Article	Salta, Z., Lupi, J., Tasinato, N., Barone, V., Ventura, O.N.	Unraveling the role of additional OH-radicals in the H-Abstraction from Dimethyl sulfide using quantum chemical computations.	Chemical Physics Letters 739, 136963. doi:10.1016/j.cplett.2019.136963 ISSN:0009-2614	2020
9 -	Article	Salta, Z., Lupi, J., Barone, V., Ventura, O.N.	H-Abstraction from Dimethyl Sulfide in the Presence of an Excess of Hydroxyl Radicals. A Quantum Chemical Evaluation of Thermochemical and Kinetic Parameters Unveils an Alternative Pathway to Dimethyl Sulfoxide.	ACS Earth and Space Chemistry 4, 3, 403–419. doi:10.1021/acsearthsp.acechem.9b00306 ISSN:2472-3452	2020
10 -	Article	Salta, Z., Tasinato, N., Lupi, J., Boussessi, R., Balbi, A., Puzzarini, C., Barone, V.	Exploring the Maze of C ₂ N ₂ H ₅ Radicals and Their Fragments in the Interstellar Medium with the Help of Quantum-Chemical Computations.	ACS Earth and Space Chemistry 4, 5, 774–782. doi:10.1021/acsearthsp.acechem.0c00062 ISSN:2472-3452	2020
11 -	Article	Salta, Z., Kosmas, A.M., Segovia, M.E., Kieninger, M., Tasinato, N., Barone, V., Ventura, O.N.	Reinvestigation of the Deceptively Simple Reaction of Toluene with OH and the Fate of the Benzyl Radical: The “Hidden” Routes to Cresols and Benzaldehyde.	Journal of Physical Chemistry A 124, 5917–5930. doi:10.1021/acs.jpca.0c03727 ISSN:1520-5215	2020
12 -	Article	Salta, Z., Segovia, M.E., Katz, A., Tasinato, N., Barone, V., Ventura, O.N.	Isomerization and Fragmentation Reactions on the [C ₂ SH ₄] Potential Energy Surface: The Metastable Thione S-Methylide Isomer.	Journal of Organic Chemistry 86, 2941–2956. doi:10.1021/acs.joc.0c02835 ISSN:1520-6904	2021

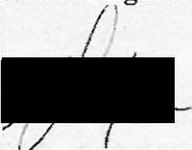
To this end, under my own responsibility, pursuant to art. 46 and art. 47 of Presidential Decree 445/2000 and subsequent amendments, and aware of the legal sanctions under article 76 of the same Presidential Decree in case of false declarations, I hereby

DECLARE

- that every copy of the publications listed above – to upload exclusively on PICA platform – is conform to the original in my possess and that all the works listed have been published as provided by current regulations (and certified in the application form)

Date 29/4/2022

Readable signature



Annex 1 - Resume template

PROFESSIONAL SCIENTIFIC CURRICULUM ¹
(to be uploaded on the PICA IT procedure)

DOTT./DOTT. SSA: ANUJ TRIPATHI
(NAME AND SURNAME)

PART I - GENERAL INFORMATION

Name and surname	Anuj Tripathi
Date of birth	07/07/1987
Place of birth	
Citizenship	
Academic/job position currently held, specifying whether permanent/tenured	Visiting Researcher(Tenured)
Language skills	ENGLISH, HINDI

Part II - ACADEMIC QUALIFICATIONS

Type of title and denomination	Date of achievement	Institution and State	Judgment/ final evaluation (is planned)	Thesis title and any notes
Ph.D. in Chemistry (Computational Chemistry)	08/02/2021	National Institute of Technology Kurukshetra, India	completed	Tuning of Optical and Charge transport properties in linear and star-shaped thiophene based organic materials: A DFT Insight
Masters (Organic Chemistry)	02/08/2014	University of Allahabad	completed	Application of some important oxidizing and reducing agents in organic chemistry

etc. (specify these data for each academic qualification obtained)

PART III - OTHER SECURITIES HELD

III.1 - Teaching activities at university level in Italy or abroad:

Period (start date and end date)	Institution and State	Brief description of the teaching activity carried out ²
from ___ / ___ / ___ to ___ / ___ / ___		
from ___ / ___ / ___ to ___ / ___ / ___		

etc. (specify these data for each period of teaching activity carried out)

¹ This professional scientific curriculum contains the overall and detailed list of the qualifications held by the candidate, considered useful for the evaluation, according to a model scheme that can be modified / integrated by the candidate adapting it to the peculiarities of his scientific-professional activity. The spaces available in the scheme for the various categories of titles listed can be integrated by the candidate according to their needs.

² Indicate in detail the elements useful for the evaluation such as the name of the course or lessons held and the number of hours of frontal teaching, the type of training activity in which the teaching activity was carried out (degree course, doctorate, master, summer school etc.), the employment contract / relationship on the basis of which the teaching activity was held (teaching assignment, visiting professor, researcher contract, etc.) etc.

III.2 - Documented training or research activities at qualified Italian or foreign institutes:

Period (start date and end date)	Institution and State	Brief description of the training/research activity carried out ³
28/10/2015- 25/09/2018	National Institute of Technology (NIT), Kurukshetra, Haryana, India	Designing of new thiophene and their heteroatomic based organic molecule and studying their linear optical properties. Comparative Computational study of the designed molecules using DFT and TDDFT methodology. Detailed study of charge transport properties of the designed molecules.

etc. (specify these data for each period of training or research carried out)

III. 3 - Activities in the clinical field (only in relation to the competition sectors in which these specific skills are required):

Period (start date and end date)	Institution and State	Brief description of the activity carried out ⁴
from __ / __ / __ / __ / _ / _ / _ / _ /		

Etc. (specify these data for each activity in the clinical field carried out)

III. 4 - Implementation of project activities (only in relation to the insolvency sectors in which it is planned):

Period (start date and end date)	Institution and State	Brief description of the activity carried out ⁵
from __ / __ / __ / _ / _ / _ /		

Etc. (specify these data for each project activity carried out)

III. 5 - Organization, direction and coordination of national and international research groups, or participation in them:

Period (start date and end date)	Research group/programme ⁶	Role held and brief description of the activity ⁷
from __ / __ / __ / _ / _ / _ /		
from __ / __ / __ / _ / _ / _ /		

etc. (specify such data for each research group/programme concerned)

III. 6 - Ownership of patents (in relation to the insolvency sectors in which it is envisaged):⁸

³ Indicate in detail the elements useful for the evaluation such as the employment / contractual relationship or the academic position on the basis of which the training / research activity was carried out (eg research grant, fixed-term researcher contract, scholarship / exchange during PhD, etc.), the object of the activity, the methods of carrying out, etc.

⁴ Indicate in detail the elements useful for the evaluation. If you have not carried out these activities, leave the blank/unfilled spaces.

⁵ Indicate in detail the elements useful for the evaluation. If you have not carried out these activities, leave the blank/unfilled spaces.

⁶ Indicate the name of the group and / or the research program concerned, specifying whether it is national or international, the possible public/private funding body and any competitive call under which the program has been funded, and any other useful element.

⁷ Indicate in detail the elements useful for the evaluation such as the role of organization, direction, coordination, participation that you have within the group / research program indicated (eg. PI-principal investigator or local unit manager etc.) and the activities carried out.

⁸ Indicate the data in the spaces indicated; if you are not a patent holder, leave the blank/unfilled spaces.

Title	Description	N°deposit	Concession number	Holder's name	Inventor name	Filing date

Etc. (specify such data for each patent)

III. 7 - Speaker⁹ at national and international congresses and conferences:

Day(s) of the congress/conference	Organizing body and venue	Title of the congress/conference, (specifying whether national or international)	Title of speech as <u>rapporteur</u> (specifying whether it was by invitation)
15 th -17 th March 2018	CSIR-Indian Institute of Petroleum Dehradun, India	International Conference on Advances in Analytical Sciences (ICAAS) (international)	A DFT study on Electronic excitations and Charge transfer properties in benzotrithiophenes (BTTs) (oral presentation)
20 th January 2018	Department of Chemistry, National Institute of Technology Kurukshetra, India	Multifunctional Materials Analytical Techniques and Diverse Applications (MMAD18) (international)	Impact of replacement of central benzene ring in Anthracene by Heterocyclic ring on electronic excitations and reorganization energies (poster presentation)
9 th -10 th March 2019	Department of Physics, National Institute of Technology Kurukshetra, India	Nanoscience and Instrument Technology (NCNIT) (national)	A DFT study of Optoelectronic and Charge Transport properties on Truxene, Isotruxene and their heteroatom (N, O, Si, S) analogs (poster presentation)
9 th -11 th February, 2017	Department of Chemistry, Sacred Heart College (Autonomous), Thevara, Kochi, India.	New Trends in Applied Chemistry (NTAC -2017) (international)	Comparative computational study of C-C and C-N bonding croconines molecules

etc. (specify these data for each activity of speaker at congresses and conferences)

III. 8 - National and international awards and recognitions for research activities:

Date/year of achievement	Title/name of the award or recognition (specifying whether national or international)	Transferring Body/Institution and State	Any notes

etc. (specify these data for each award/recognition for research activities achieved)

III. 9 - European specialization diploma recognized by international boards (in relation to the competition sectors in which it is envisaged):

⁹ Reference is made here exclusively to interventions carried out as a speaker at congresses / conferences. Participations in a different capacity (with posters, as a simple auditor, etc.) may be indicated under the following point III.10.

Date of achievement	Institution and State	Brief description ¹⁰

etc. (specify these data for each Diploma you may have)

III. 10 - Any additional securities held:¹¹

Type/denomination of the title or activity carried out	Date or period of performance	Brief description
1 - ...		
2 - ...		
3 - ...		

etc. (indicate the additional securities held, indicating for each of them, the elements useful for any evaluation)

Part IV - SCIENTIFIC PUBLICATIONS OF WHICH HE IS AUTHOR/CO-AUTHOR

N.	Type of scientific product (article, monograph, contribution in volume, etc.)	Author(s)	Product Title (of article/contribution in volume/voice... and reference (ISBN) the in and	Title of the magazine/volume/dictionary containing the article/contribution/entry and reference (ISSN-DOI-ISBN)	Year of publication
1 -	Article	A. Tripathi, V. Kumar, Ch. Prabhakar	Impact of internal (donor/acceptor) moieties and π -spacer in triphenylamine-based dyes for DSSCs	J Photochem. Photobiol. A: Chem. 426, 113738	2022
2 -	Article	A. Tripathi, V. Kumar, Ch. Prabhakar	Stability, optical and charge transport properties of saddle-shaped cyclooctatetrathiphene isomers	J. Sulfur Chem doi.org/10.1080/17415993.2021.1993851	2021
3 -	Article	A. Tripathi, A. Ganjoo, Ch. Prabhakar	Influence of internal acceptor and thiophene based π -spacer in D-A- π -A systems on photophysical and charge transport properties for efficient DSSCs: A DFT insight.	Sol. Energy, 209, 194-205	2020
4 -	Article	A. Tripathi, Ch. Prabhakar	Enhanced charge transport properties in heteroatomic (NH, O, Se) analogs of benzotrithiophene isomers: a DFT insight.	Mol. Sim., 46(7), 548-556	2020
5 -	Article	A. Tripathi, Ch. Prabhakar	Optical and charge transport properties of Chalcogens (O, S and Se) based acene molecules.	J. Mol. Struct., 1203, 127397(1-8)	2020

¹⁰ Indicate in detail the elements useful for the evaluation such as the scientific field, the title of the thesis, the judgment reported, etc. If you have not obtained this title, leave the blank/unfilled spaces.

¹¹ E.g. participation in editorial committees of scientific journals, supervisor or tutor activities for doctoral theses, etc., participation in organizing committees of congresses / conferences, participation in scientific dissemination activities, participation in competition commissions / final exams for the achievement of qualifications academics, scientific evaluation/referencing assignments, participation in the organization of relevant scientific exhibitions/exhibitions, participation in congresses/conferences not as a speaker, etc. The Commission will be able to trace these titles back to those listed in the previous points and consider them worthy of evaluation.

Format 2

LIST OF SUBMITTED PUBLICATIONS¹

I, the undersigned, (surname and name) Tripathi Anuj born in [REDACTED] resident in [REDACTED] (Prov. ____)
Address; [REDACTED]

SUBMIT

the following publications, in the maximum number of 12 established by the call, including my doctoral thesis (if submitted), for the purpose of evaluation in the context of the selection procedure of No. 1 fixed-term researcher - Type a) – in the Academic recruitment field _____, Academic discipline _____:

No.	Type of scientific product (article, monography, contribution in volume etc.)	Author/s	Publication title (of the article/contribution in volume/entry...) and its code (ISBN)	Title of the journal/book/dictionary containing the article/contribution/entry and its code (ISSN-DOI-ISBN)	Year of publication
1 -	Article	A. Tripathi, V. Kumar, Ch. Prabhakar	Impact of internal (donor/acceptor) moieties and π -spacer in triphenylamine-based dyes for DSSCs	<i>J Photochem. Photobiol. A: Chem.</i> 426, 113738	2022
2 -	Article	A. Tripathi, V. Kumar, Ch. Prabhakar	Stability, optical and charge transport properties of saddle-shaped cyclooctatetrathiophene isomers	<i>J. Sulfur Chem</i> doi.org/10.1080/17415993.2021.1993851	2021
3 -	Article	A. Tripathi, A. Ganjoo, Ch. Prabhakar	Influence of internal acceptor and thiophene based π -spacer in D-A- π -A systems on photophysical and charge transport properties for efficient DSSCs: A DFT insight.	<i>Sol. Energy</i> , 209, 194-205	2020
4 -	Article	A. Tripathi, Ch. Prabhakar	Enhanced charge transport properties in heteroatomic (NH, O, Se) analogs of benzotrithiophene isomers: a DFT insight.	<i>Mol. Sim.</i> , 46(7), 548-556	2020
5 -	Article	A. Tripathi,	Optical and charge transport properties of	<i>J. Mol. Struct.</i> ,	2020

¹ Please see art. 3, par. 2. c) of the call for selection for the list of valid publications and the submittal procedure.

		Ch. Prabhakar	Chalcogens (O, S and Se) based acene molecules.	1203, 127397(1-8)	
6 -	Article	A. Tripathi, Oleg K, Khidmet S, Ch. Prabhakar	A DFT study on optical, electronic and charge transport properties of star-shaped benzo[1,2-b:3,4-b',5,6-b''] trithiophene oligomers.	<i>J. Phys. Org. Chem.</i> , 33(3), e4037.	2020
7 -	Article	A. Tripathi, Ch. Prabhakar	Optoelectronic and charge transport properties of truxene, isotruxene and its heteroatomic (N, O, Si and S) analogs: A DFT Study (Wiley).	<i>J. Phys. Org. Chem.</i> 32(6), e3944	2019
8 -	Article	A. Tripathi, Ch. Prabhakar	ptoelectronic properties of benzotrithiophene isomers: A density functional theory study.	<i>J. Chin. Chem. Soc.</i> 66(8), 891- 898	2019
9 -	Article	A. Tripathi, Ch. Prabhakar	Impact of heteroatom (S and N) positions and change in central ring of anthracene with heterocyclic ring on charge transport and optical properties in anthratetrathiazole (ATTz).	<i>J. Sulfur Chem.</i> 40, 361-376	2019
10 -	Article	A. Tripathi, Ch. Prabhakar	A comparative computational study of C-N and C-C bonding visible to NIR absorbing croconines.	<i>J. Mol. Struct.</i> 1155, 561- 567	2018
11 -	Article	A. Tripathi, Ch. Prabhakar	Impact of replacement of central benzene ring in anthracene by heterocyclic ring on electronic excitations and reorganization	<i>J. Chin. Chem. Soc.</i> 65(8), 918-924	2018

			energies in anthratetrathiophene molecules.		
12 -	Article	A. Tripathi, Promila Ch. Prabhakar	Visible to NIR absorbing C-N and C-C bonding squaraines: A computational study.	<i>J. Phys. Org. Chem.</i> 31(2), e3758	2018

To this end, under my own responsibility, pursuant to art. 46 and art. 47 of Presidential Decree 445/2000 and subsequent amendments, and aware of the legal sanctions under article 76 of the same Presidential Decree in case of false declarations, I hereby

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