Curriculum Vitae

Brief Profile:

Dr. Velmurugan Gunasekaran is currently serving as an Assistant Professor in the Department of Chemistry at the National Institute of Technology Tiruchirappalli. He obtained his Ph.D. in Chemistry with a focus on computational modeling of optoelectronic materials, along with a detailed quantum chemical investigation of electronic structure, bonding, and reactivity in normal and abnormal N-heterocyclic carbene systems. He has more than 10 years of postdoctoral research experience at leading international institutions, including the Indian Institute of Technology Bombay, Southern Methodist University, USA, and Heidelberg University, Germany. During this period, he developed strong expertise in advanced computational chemistry, electronic structure theory, and interdisciplinary research involving both theoretical and experimental collaborations. His research focuses on computational inorganic and bioinorganic chemistry, particularly on understanding structure–property relationships in transition metal complexes. His work spans areas such as spin-state-dependent reactivity, molecular nanomagnets, bio-inspired catalysis, and sustainable chemical transformations, including CO_2 conversion. He has extensive experience in predicting spectroscopic parameters, including EPR, NMR, Mössbauer, IR, and Raman spectra, as well as analyzing spin Hamiltonian parameters using density functional theory and advanced *ab initio* methods. Dr. Velmurugan has published more than 70 research articles in peer-reviewed top international journals, including Angew. Chem., Int. Ed., J. Am. Chem. Soc., Chem. Eur. J., J. Comput. Chem., Dalton Trans., Eur. J. Inorg. Chem., New J. Chem., Chem. Commun., Org. Chem. Front., Appl. Organomet. Chem., Chem. Asian J., ChemistrySelect, RSC Adv., Phys. Chem. Chem. Phys, and Inorg. Chem., along with a book chapter. His publications have significantly advanced fundamental understanding in bioinorganic chemistry, catalysis, magnetism, and electronic structure theory. In addition to his research contributions, he is actively engaged in teaching and mentoring. He has substantial teaching experience and has supervised more than 30 undergraduate and postgraduate research students, guiding them in computational chemistry and interdisciplinary research. He is also actively involved in peer review for international journals, helping maintain high standards in scientific research. Dr. Velmurugan has received several recognitions and competitive fellowships, including the prestigious Ramanujan Fellowship from the Anusandhan National Research Foundation and the Young Scientist Scheme Research Grant from the Science and Engineering Research Board, as well as postdoctoral fellowships from reputed institutions in India, the USA, and Germany. With his strong academic background, international research experience, and commitment to excellence in teaching and research, he aims to build a vibrant research group and contribute significantly to the advancement of chemical sciences in India.

National Institute of Technology, Tiruchirappalli:
Performa for CV of Faculty/ Staff Members

1. Name: Dr. Velmurugan Gunasekaran
2. Designation: Assistant Professor
3. Office Address: Room No. CH319, OJAS Building, Department of Chemistry, NIT Tiruchirappalli – 620 015
4. Telephone (Direct) (Optional):

   Telephone : Extn (Optional):

   Mobile (Optional):
5. Email (Primary): velmurugan@nitt.edu Email (Secondary): veldft@gmail.com
6. Field(s) of Specialization: Bioinorganic Chemistry; Theoretical and Computational Chemistry; Molecular Modeling and Catalysis; Molecular Magnetism and Spin Hamiltonian Analysis; Quantum Chemical Studies of Reactivity and Electronic Structure; CO_2 Conversion and Sustainable Catalysis; Noncovalent Interactions and QTAIM; Optoelectronic Materials and Excited-State Chemistry.
7. Employment Profile

Job Title	Employer	From	To
Assistant Professor	NIT Tiruchirappalli, India	December 2025	Till Date
Post-Doctoral Research Associate	Institute of Inorganic Chemistry, Heidelberg University, Germany	February 2018	December 2025
Post-Doctoral Research Associate	Department of Chemistry, Southern Methodist University, Dallas, Texas, USA	April 2017	February 2018
Post-Doctoral Fellow	Department of Chemistry, Indian Institute of Technology Bombay, Mumbai, India	December 2014	December 2016

8. Academic Qualifications

Examination	Board / University	Year	Division/ Grade	Subjects
Ph.D.	Bharathidasan University, Tiruchirappalli, India	2015	Thesis Highly Commended	Chemistry
M.Phil.	Presidency College (Autonomous), Chennai, India	2010	First Class with Distinction	Chemistry
M.Sc.	Presidency College (Autonomous), Chennai, India	2009	First Class with Distinction	Chemistry

B.Sc.	Thanthai Hans Roever College, Bharathidasan University, Perambalur, India	2007	First Class with Distinction	Chemistry

9. Academic/Administrative Responsibilities within the University

Position	Faculty/Department/Centre/Institution	From	To
Assistant Professor	Department of Chemistry, NIT Tiruchirappalli	December 2025	Till Date
B. Tech Lab Coordinator	Department of Chemistry, NIT Tiruchirappalli	April 2026	Till Date

10. Academic/Administrative Responsibilities outside the University

Position	Institution	From	To

11. Awards, Associateships etc.

Year of Award	Name of the Award	Awarding Organization
2025	Ramanujan Fellowship	Anusandhan National Research Foundation (ANRF), India
2019	ICBIC Travel Award	19th International Conference on Biological Inorganic Chemistry, Interlaken, Switzerland
2018	EuroBIC: SBIC Travel Award	14th European Biological Inorganic Chemistry Conference (EuroBIC 14), University of Birmingham, UK
2018	Post-Doctoral Fellowship	Institute of Inorganic Chemistry, Heidelberg University, Germany
2017	Post-Doctoral Fellowship	Southern Methodist University, Dallas, Texas, USA
2015	Young Scientist Scheme Research Grant	Science and Engineering Research Board (SERB), India
2015	Institute Post-Doctoral Fellowship	Indian Institute of Technology Bombay, India
2014	Best Paper Presentation Award (Poster)	International Symposium on Chemistry with Computers (CWC-2014), IICT and IIIT Hyderabad

12. Fellowships

Year of Award	Name of the Fellowship	Awarding Organization	From	To
2025	Ramanujan Fellowship	Anusandhan National Research Foundation, India	August 2025	August 2025

2018	Post-Doctoral Fellowship	Heidelberg University, Germany	February 2018	December 2025
2017	Post-Doctoral Fellowship	Southern Methodist University, USA	April 2017	February 2018
2015	Young Scientist Scheme Research Grant	Science and Engineering Research Board (SERB), India	November 2015	November 2015
2015	Institute Post-Doctoral Fellowship	Indian Institute of Technology, India	December 2014	December 2016

13. Details of Academic Work

(i) Curriculum Development.
(ii) Courses taught at Postgraduate and Undergraduate levels

CHIR11 Chemistry (B.Tech.)
CHIR12 Chemistry (B.Tech.)
CHPC21 Organic Chemistry: Fundamentals and Mechanism (B.Sc.B.Ed.)
CHAL41 Concepts in Chemistry (B.Sc.B.Ed.)

(iii) Projects guided at Postgraduate level

Ms. Yogita Shukla (2026-2027, Ongoing)
Title: Computational investigations into the decay pathways of high-valent iron bispidine complexes.

(iv) Other contribution(s)

14. Details of Major R&D Projects

Title of Project	Funding Agency	Duration		Status
		From	To	Ongoing/ Completed

15. Number of PhDs guided

Name of the PhD Scholar	Title of PhD Thesis	Role(Supervisor/ Co-Supervisor)	Year of Award

16. Participation in Workshops/ Symposia/ Conferences/ Colloquia /Seminars/ Schools etc.

Date (s)	Title of Activity	Level of Event	Role (Participant/	Event Organized by	Venue

		(International / National/ Local)	Speaker/ Chairperson, Paper presenter, Any other)		
Mar. 5-7, 2025	DFG Research Unit FOR 5215 BioOxCat International Symposium	International	Poster Presenter	Bielefeld University, Germany	Bielefeld, Germany
Feb. 19-24, 2025	Winter School on Theoretical and Computational Chemistry	International	Participant	IIT Hyderabad, TIFR Hyderabad	Hyderabad, India
Feb. 26-28, 2024	Coordination Chemistry Meeting	International	Poster Presenter	Universitat Innsbruck, Austria	Innsbruck, Austria
Jan. 7-11, 2024	6th Symposium on Advanced Biological Inorganic Chemistry (SABIC-2024)	International	Poster Presenter	TIFR and IACS, Kolkata	Kolkata, India
Sep. 24-29, 2023	MPI Summer School on Spectroscopy and Electronic Structure of Transition Metal Complexes	International	Poster Presenter	Max Planck Institute for Chemical Energy Conversion, Wissenschafts park Gelsenkirchen	Gelsenkirchen, Germany
Aug. 28 – Sep 1, 2023	6th Quantum Bio-Inorganic Chemistry (QBIC-VI) Conference	International	Speaker	Institute of Physical Chemistry, Polish Academy of Sciences (IChF)	Warsaw, Poland
Feb. 19-24, 2023	15th CaRLa Winter School	International	Poster Presenter	Heidelberg University, Germany	Heidelberg, Germany
Sep. 18-22, 2022	58th Symposium on Theoretical Chemistry (STC 2022)	International	Poster Presenter	Heidelberg University, Germany	Heidelberg, Germany
Aug. 28	44th International	International	Poster	ICCOM-	Rimini,

– Sep. 2, 2022	Conference on Coordination Chemistry (ICCC 2022)		Presenter	CNR, Italy	Italy
Aug. 11-16, 2019	19th International Conference on Biological Inorganic Chemistry (ICBIC-19)	International	Poster Presenter	University of Zurich	Interlaken, Switzerland
July 21-25, 2019	20th IUPAC International Symposium on Organometallic Catalysis Directed Towards Organic Synthesis (OMCOS)	International	Poster Presenter	Heidelberg University, Germany	Heidelberg, Germany
Mar. 3-5, 2019	Coordination Chemistry Meeting	International	Speaker	Ludwig-Maximilians-University Munich, Germany	Munich, Germany
Feb. 17-22, 2019	12th CaRLa Winter School	International	Poster Presenter	Heidelberg University, Germany	Heidelberg, Germany
Dec. 13-14, 2018	New Frontiers in Chemical Science (NFCS)	International	Poster Presenter	IIT Bombay, India	Maharashtra, India
Oct. 10-11, 2018	ACS Publications FORUM, Scientific Diversity in Inorganic/Organic Chemistry in Europe	International	Poster Presenter	Heidelberg University, Germany	Heidelberg, Germany
Aug. 26-30, 2018	14th European Biological Inorganic Chemistry Conference (EuroBIC 14)	International	Poster Presenter	University of Birmingham	Birmingham, UK
Jun. 26 – Jul. 1, 2016	8th Molecular Quantum Mechanics (MQM 2016)	International	Poster Presenter	Uppsala University, Sweden	Uppsala, Sweden
May	Modern Trends in	International	Poster	IIT Bombay,	Mumbai,

19-21, 2016	Molecular Magnets (MTMM)		Presenter	India	India
May 16-18, 2016	Workshop on Electronic Structure of Coordination Complexes (WESCC)	International	Participant	IIT Bombay, India	Mumbai, India
Dec. 18-21, 2014	Theoretical Chemistry Symposium (TCS 2014)	International	Poster Presenter	NCL and IISER Pune	Pune, India
Jan. 18-19, 2014	International Symposium on Chemistry with Computers (CWC-2014)	International	Poster Presenter (Best Poster Award)	IICT and IIIT Hyderabad	Hyderabad, India
Jan. 2-22, 2014	DST-SERB Winter School on Modeling Chemical and Biological (Re)Activity	International	Participant	IICT and IIIT, Hyderabad, India	Hyderabad, India
June 14-15, 2013	Symposium on Theoretical & Computational Chemistry: Frontiers and Challenges (STCC-FC)	International	Poster Presenter	Bharathidasan University, Tamil Nadu, India	Tiruchirappalli, India
March 3-4, 2013	International Conference on New Emerging Trends in Chemistry, A Satellite Conference of MCBR-3	International	Presenter	IIS University, Jaipur, India	Jaipur, India
Feb. 26 – Mar. 1, 2013	The 3rd Indo-German Conference on Modeling Chemical and Biological (Re)activity (MCBR-3)	International	Poster Presenter	NIPER and IISER, Mohali, India	Mohali, India
Dec. 19-22, 2012	Theoretical Chemistry Symposium (TCS 2012)	International	Poster Presenter	IIT Guwahati, India	Guwahati, India

July 23-27, 2012	Short term course on "Computational Methods in Chemistry	National	Speaker	NIT Tiruchirappalli, India	Tiruchirappalli, India
Jan. 2-6, 2012	Workshop on Introduction to Gaussian: Theory and Practice	International	Poster Presenter	CLRI and IIT Madras, Chennai, India	Chennai, India
Aug. 29, 2011	Seminar on Recent Developments in Chemistry	National	Participant	Bharathidasan University and RJSF, Tiruchirappalli, India	Tiruchirappalli, India
Apr. 6-16, 2011	Workshop on Introduction to ab initio Calculations	National	Participant	University of Hyderabad, India	Hyderabad, India
Dec. 8-12, 2010	Theoretical Chemistry Symposium (TCS 2010)	International	Poster Presenter	IIT Kanpur	Kanpur, India
Nov. 3-13, 2010	School on Understanding Molecular Simulations (UMS 2010)	National	Participant	IIT Kanpur India	Kanpur, India

17. Workshops/ Symposia/ Conferences/ Colloquia/Seminars Organized (as Chairman/ Organizing Secretary/ Convenor / Co-Convenor)

Title of Activity	Level of Event (International/ National/ Local)	Date (s)	Role	Venue

18. Invited Talks delivered

Topic	Date	Inviting Organization
The biological function of the patellamides in the ascidian – prochloron symbiosis	Jan. 7-8, 2025	Presidency College (Autonomous), Chennai, India
A dicopper(II)-based carbonic anhydrase model – quantum-chemical evaluation of the mechanistic pathway	Aug. 28 – Sep 1, 2023	Polish Academy of Sciences (IChF), Warsaw, Poland
Optoelectronic applications: computational landscape – fiction and science	Mar. 23-24, 2022	Selvamm Arts and Science College (Autonomous), Namakkal, India

Theoretical study on ruthenium-catalyzed transformation of carbon dioxide: an alternative approach towards methanol	Mar. 3-5, 2019	Ludwig-Maximilians-University Munich, Germany
Introduction to theoretical and computational chemistry	July 23-27, 2012	NIT Tiruchirappalli, India

19. Membership of Learned Societies

Type of Membership (Ordinary Member/ Honorary Member / Life Member)	Organization	Membership No. with date

20. Academic Foreign Visits

Country	Duration of Visit	Programme

21. Publications

(A) Refereed Research Journals:

Author(s)	Title of Paper	Journal	Volume (No.)	Page numbers	Year	Impact Factor of the Journal
Velmurugan. G.; Comba. P.	The reactivity of bispidine ligand based iron(IV) and iron(V) oxido species for the demethylation of acetic acid.	J. Comput. Chem.	2026	DOI: 10.1002/jcc.70369	2026	4.8
Nagaraj. K.; Velmurugan. G.; Paramasivam. S.; Hessini. K.; Shah. M.	Modulating outer-sphere electron transfer in cobalt(III) metallo-surfactants using ionic liquids and lipid vesicles	Int. J. Chem. Kinet.	2026	DOI:10.1002/kin.700391	2026	2.0
Bhandary, D.; Sahoo, L.;	Bioinspired Cu(II) complexes with	Dalton Trans.	55	2297-2311	2026	3.8

Velmurugan, G.; Mukherjee, G.	tunable axial donors: Unravelling structure-function correlations in phenoxazinone synthase mimics.					
Velmurugan. G.; Narayanan, R.; Hada, M.; Venuvanalingam, P.	Unraveling the enhanced reactivity of abnormal N-heterocyclic carbene palladium complexes over their normal analogues: Insights from DFT studies.	Eur. J. Inorg. Chem.	29	e202500520	2026	2.4
Massoud, S.S.; Louka, F.R.; Guizouarn, T.; Fischer, R.C.; et al.; Velmurugan, G.; Comba, P.; Pointillart, F.	Structural and magnetic properties of lanthanide-tetraphenol-cyclen complexes: Slow magnetic relaxation of the Nd(III) complex.	New J. Chem.	50	307-316	2026	3.3
Poongodi. R.; Vijayalakshmi. K.; Manjula. R.; et al.; Velmurugan. G.; Nagaraj. K.	Facile biofabrication and characterization of silver, iron, and bimetallic nanoparticles using Belou marmelos leaf extract.	Surf. Interfaces	78	108147	2025	6.2
Velmurugan, G.; Mukherjee, G.; Bagha,	Computational and experimental insights into a	Z. Anorg. Allg. Chem. (ZAAC)	651	e202500189	2025	1.5

U.K.; Sastri, C.V.; Comba, P.	ferric cumylperoxido species stabilized in a bispidine scaffold.					
Panua, A.; Velmurugan, G.; Comba, P.; Rath, H.	Targeted synthesis of a positional isomer of aromatic N-methyl N-confused corrole and its organo-copper(III) complex.	Chem. Commun.	61	17436-17439	2025	4.9
Jana, M.; Velmurugan, G.; Sahoo, S.; Comba, P.; Rath, H.	Core modified N-confused pentaphyrin variants with adaptive (anti)aromaticity	Org. Chem. Front.	12	6885-6893	2025	4.9
Weisser, K.; Weber, E.T.; Velmurugan, G.; Cula, B.; et al.; Comba, P.; de Visser, S.P.; Limberg, C.	Promiscuity in molecular mimics of the cysteine dioxygenase: effects of selenium in the substrate and cobalt as the central metal ion.	Angew. Chem. Int. Ed.	137	e202507578	2025	16.6
Velmurugan, G.; Comba, P.	Theoretical insights into the oxidation of substrates by high-spin iron(III)-acylperoxido complexes.	Eur. J. Inorg. Chem.	28	e20240083	2025	2.4
Panua, A.; Velmurugan, G.; Comba, P.; Rath, H.	Copper(III) organometallic complexes of non-(anti)aromatic	Dalton Trans.	54	4267-4275	2025	3.8

	and aromatic doubly N-confused porphyrinoids.					
Massoud, S.S.; Mautner, F.A.; et al.; Velmurugan, G.; Comba, P.; Pointillart, F.	SMM behavior in distorted trigonal bipyramid and tetrahedral cobalt(II) complexes based on tripodal tetradentate phenolic amines.	Eur. J. Inorg. Chem.	28	e202400777	2025	2.4
Nagaraj, K.; Gurupriya, R.; Shah, M.; Hessini, K.; Velmurugan, G.; Raja, K.; Badgujar, N.P.	Pharmaceutical evaluation of cis-[Co(trien)(4-CNP)($C_{12}H_{25}NH_2$)]$^{3+}$: A metallosurfactant with DNA/tRNA affinity and broad-spectrum bioactivity.	J. Mol. Liq.	435	128173	2025	5.8
Uthra, C.; Nagaraj, K.; Muralitharan, G.; Al-Ansari, M.M.; Velmurugan, G.	Synthesis, characterization and apoptosis induction by cyanobacteria-derived neurotoxins.	Chem. Pap.	79	8971-8986	2025	3.0
Nagaraj, K.; Raja, K.; Al-Otibi, F.O.; et al.; Velmurugan. G.; Shah, F.	Structural variability and antimicrobial efficacy of barium oxide-doped copper oxide (BaO@CuO) nanocomposites via co-precipitation.	Chem. Afr.	8	2035-2044	2025	2.5

Uthra, C.; Shunmugam, S.; Nagaraj, K.; Muralitharan, G.; Albeshr, M.F.; Velmurugan, G.	Ultra-fast liquid chromatography detection of beta-N-methylamine-l-alanine and its isomers in cycad seeds.	Food Chem. Toxicol.	202	115503	2025	6.5
Vijayalakshmi, K.; Vidhyulatha, N.; et al.; Velmurugan, G.; Nagaraj, K.	Computational and experimental investigation of biogenic zinc oxide nanoparticles synthesized from Clausena dentata leaf extract.	Food Biosci.	68	106371	2025	5.2
Nagaraj, K.; Uthra, C.; Albeshr, M.F.; Raja, K.; Velmurugan, G.	A comparative study of methanol and aqueous extracts of Cucumis trigonus: phytochemical composition, antioxidant, antimicrobial, and cytotoxic activities.	Chem. Pap.	79	2287-2298	2025	3.0
Nagaraj, K.; Karthikeyan, A.; Velmurugan, G.; et al.	Synthesis, crystal structure, and computational investigation of zinc-cytosine coordination complex.	Appl. Organomet. Chem.	39	e70215	2025	3.3
Kaliyaperumal, R.; Nagaraj, K.; Sakthikumar, K.;	Green synthesis and characterization of ZnO/alpha-Fe_2O_3	Appl. Organomet. Chem.	39	e70121	2025	3.3

Albeshr, M.F.; Velmurugan, G.	nanocomposites using Hydrocotyle umbellata leaf extract.					
Nagaraj, K.; Thangamuniyandi, P.; Velmurugan, G.; Alotaibi, K.M.; Raja, K.; Sharma, B.K.	Green synthesis of eosin-Y coated silver nanoparticles for sensitive and selective fluorometric detection of L-Dopa.	J. Fluoresc.	35	7893-7904	2025	2.5
Panua, A.; Velmurugan, G.; Comba, P.; Rath, H.	Syntheses of variants of pi(sigma) aromatic modified N-methyl N-confused porphyrinoids with adaptive properties.	Chem. Asian J.	2024	e202401196	2024	3.4
Nagaraj, K.; Velmurugan, G.; et al.	Metallo-surfactant complex-assisted biomimetic synthesis of silver nanoparticles: Exploring relativistic effects in catalytic and sensing applications.	Chemistry Select	9	e202403711	2024	2.1
Jana, M.; Velmurugan, G.; Comba, P.; Rath, H.	X-ray characterization of core-modified N-confused fused porphyrinogen and genesis of pi(sigma)	Org. Chem. Front.	11	5077-5085	2024	4.9

	(anti)aromatic N-confused fused porphyrinoids.					
Shabulal, N.S.; Perumal, T.; et al.; Nagaraj, K.; Velmurugan, G.; et al.	Green synthesis of silver nanoparticles: Understanding biological activities - anticancer, antimicrobial, and plasmid DNA cleavage.	New J. Chem.	48	13764-13775	2024	3.3
Thangamuniyandi, P.; Nagaraj, K.; Velmurugan, G.; et al.	Green synthesis of starch-capped CdS nanoparticles doped with Copper(II) and Manganese(II): Structural, optical, and photocatalytic properties.	Eur. J. Inorg. Chem.	2024	e202400291	2024	2.4
Velmurugan, G.; Baur, P.; Comba, P.	A dicopper(II)-based carbonic anhydrase model - quantum-chemical evaluation of the mechanistic pathway.	Angew. Chem. Int. Ed.	2024	e202319530	2024	16.6
Mukherjee, G.; Velmurugan, G.; Kerscher, M.; Satpathy, J.K.; Sastri, C.V.; Comba, P.	Mechanistic insights into amphoteric reactivity of an iron-bispidine complex.	Chem. Eur. J.	2024	e202303127	2024	3.9
Hadeler, J.; Velmurugan	Natural abiotic iron-oxido-	J. Am. Chem.	145	24590-24602	2023	16.4

, G.; Lauer, R.; Radhamani, R.; Keppler, F.; Comba, P.	mediated formation of C1 and C2 compounds from environmentally important methyl-substituted substrates.	Soc.				
Kopp, I.; Cieslik, P.; et al.; Velmurugan, G.; et al.; Comba, P.	Bispidine chelators for radiopharmaceutical applications with lanthanide, actinide, and main group metal ions.	Inorg. Chem.	62	20754-20768	2023	4.3
Sahoo, S.; Velmurugan, G.; Comba, P.; Rath, H.	meso-meso 1,3-Bis(E-vinyl)azulene bridged tetrathiaoctaphyrins: Synthesis and spectroscopic and theoretical characterization.	Org. Chem. Front.	10	5601-5609	2023	4.9
Comba, P.; Rajaraman, G.; Sarkar, A.; Velmurugan, G.	What controls the magnetic anisotropy in heptacoordinate high-spin cobalt(II) complexes? A theoretical perspective.	Dalton Trans.	51	5175-5183	2022	3.8
Panneerselvam, M.; Kathiravan, A.; et al.; Velmurugan, G.; Jaccob, M.	Delineating the effect of substituent and pi-bridge flip on the photophysical properties of pyrene derivatives.	J. Mater. Sci.	57	10724-10735	2022	4.0

Baur, P.; Comba, P.; Velmurugan, G.	Efficient synthesis for a wide variety of patellamide derivatives and phosphatase activity of copper-patellamide complexes.	Chem. Eur. J.	2022	e202200249	2022	3.9
Azam, M.; Velmurugan, G.; Trzesowska-Kruszynska, A.; Al-Resayes, S.I.; Kruszynski, R.; Venuvanalingam, P.	A bowl-shaped phenoxido-bridged binuclear zinc complex: Experimental and theoretical studies.	Inorg. Chim. Acta	534	120807	2022	2.5
Cieslik, P.; Comba, P.; et al.; Velmurugan, G.; Wadepohl, H.	Exceptional Manganese(II) stability and Manganese(II)/ Zinc(II) selectivity with rigid polydentate ligands.	Angew. Chem. Int. Ed.	134	e2021155	2022	16.6
Bleher, K.; Comba, P.; et al.; Velmurugan, G.; Yang, S.	Non-heme-iron-mediated selective halogenation of unactivated carbon-hydrogen bonds.	Chem. Eur. J.	28	e2021034	2022	3.9
Sahoo, S.; Velmurugan, G.; Chakraborty, B.; Comba, P.; Rath, H.	NIR absorbing aromatic (antiaromatic) vinylogous carbasapphyrins with built-in fused dipolar aromatic	Org. Chem. Front.	8	6909-6915	2021	4.9

	hydrocarbon.					
Cieslik, P.; Comba, P.; et al.; Velmurugan, G.	Molecular magnetic properties of a Dysprosium(III) complex coordinated to a nonadentate bispidine ligand.	Z. Anorg. Allg. Chem. (ZAAC)	647	843-849	2021	1.5
Craig, G.; Velmurugan, G.; Wilson, C.; Valiente, R.; Rajaraman, G.; Murrie, M.	Magnetic properties of a family of $[Mn^{III}_4Ln^{III}_4]$ wheel complexes: An experimental and theoretical study.	Inorg. Chem.	58	13815-13825	2019	4.3
Shimizu, I.; Morimoto, Y.; Velmurugan, G.; Gupta, T.; et al.; Comba, P.	Characterization and reactivity of a tetrahedral copper(II) alkylperoxido complex.	Chem. Eur. J.	25	11157-11165	2019	3.9
Dey, S.; Velmurugan, G.; Rajaraman, G.	How important is the coordinating atom in controlling magnetic anisotropy in Uranium(III) single-ion magnets? A theoretical perspective.	Dalton Trans.	48	8976-8988	2019	3.8
Muruganantham, S.; Velmurugan, G.; et al.; Venuvanalingam, P.; Renganathan, R.	Impact of tunable 2-(1H-indol-3-yl)acetonitrile based fluorophores towards optical, thermal and electroluminesc	RSC Adv.	9	14544-14557	2019	3.9

	ence properties.					
Parveen, S.; Velmurugan, G.; Venuvanalingam, P.; Sinn, E.; Govindarajan, S.	Water-soluble Cobalt(II) and Cobalt(III) complexes supported by new triazine Schiff base ligands: Synthesis, structure and biological evaluation.	J. Photochem. Photobiol. B	189	152-164	2018	4.3
Sarkar, A.; Velmurugan, G.; Rajeshkumar, T.; Rajaraman, G.	Deciphering the origin of invariance in magnetic anisotropy in $\{Fe^{II}S_4\}$ complexes: A theoretical perspective.	Dalton Trans.	47	9980-9984	2018	3.8
Cecily Mary Glory, D.; et al.; Velmurugan, G.; et al.	Optical, Fluorescence with quantum analysis of hydrazine (1,3-dinitro phenyl) by DFT and Ab initio approach.	J. Mol. Struct.	1163	480-495	2018	3.4
Hanninen, M.; Mota, A.; et al.; Velmurugan, G.; Rajaraman, G.; Colacio, E.	Magneto-structural properties and theoretical studies of a family of simple heterodinuclear phenoxide/alkoxide bridged $Mn^{III}Ln^{III}$ complexes.	Inorg. Chem.	57	3683-3698	2018	4.3
Fraser, H.W.L.; Nichol, G.S.; Velmurugan	Magneto-structural correlations in a family of di-alkoxo bridged	Dalton Trans.	46	7159-7168	2017	3.8

, G.; Rajaraman, G.; Brechin, E.K.	chromium dimers.					
Sabina, X.J.; Karthikeyan, J.; Velmurugan, G.; Tamizh, M.M.; Shetty, A.N.	Design and in vitro biological evaluation of substituted chalcones synthesized from nitrogen mustards as potent microtubule targeted anticancer agents.	New J. Chem.	41	4096-4109	2017	3.3
Singh, S.K.; Pandey, B.; Velmurugan, G.; Rajaraman, G.	Key role of higher order symmetry and electrostatic ligand field design in the magnetic relaxation of low-coordinate Er(III) complexes.	Dalton Trans.	46	11913-11924	2017	3.8
Muruganantham, S.; et al.; Velmurugan, G.; et al.; Venuvanalingam, P.; Renganathan, R.	Green light-emitting 2-(1H-indol-3-yl)acetonitrile-based D-A fluorophores - a combined theoretical and experimental study.	Mater. Chem. Front.	1	1373-1383	2017	6.0
Mukherjee, S.; Velmurugan, G.; et al.; Rajaraman, G.; Tang, J.; Ghosh, S.K.	Influence of tuned linker functionality on modulation of magnetic properties and relaxation dynamics in a	Inorg. Chem.	55	11283-11298	2016	4.3

	family of six isostructural Ln2 complexes.					
Azam, M.; Velmurugan, G.; et al.; Venuvanalingam, P.	Structural elucidation and physicochemical properties of mononuclear Uranyl(VI) complexes incorporating dianionic units.	Sci. Rep.	6	32898	2016	4.0
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(B) Conferences/Workshops/Symposia Proceedings

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(C) Books & Monographs

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