

CURRICULUM VITAE

MD SHOFIUR RAHMAN, Ph.D.

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RESEARCH INTEREST

- My research interests include supramolecular chemistry, host-guest interactions for molecular complexes, microelectromechanical systems (MEMS) sensors, chemical sensing, organic synthesis, computational chemistry, density functional theory (DFT), molecular docking, materials science, and environmental and oxidative-extractive desulfurization technology for producing greener fuels. I have published more than 90 papers with my colleagues in peer-reviewed international journals.

TEACHING AND RESEARCH EXPERIENCES

Assistant Professor

April 10, 2022 –Present

King Abdullah Institute for Nanotechnology, King Saud University, Saudi Arabia.

Research Associate

September 01, 2011 –March 31, 2022

Dept. of Chemistry, Memorial University of Newfoundland, St. John's, NL, Canada

Postdoctoral Fellow

March 03, 2009 –January 05, 2010

National Institute for Nanotechnology (NINT), University of Alberta, Edmonton

Postdoctoral Fellow

October 01, 2007–December 31, 2008

Department of Applied Chemistry, Saga University, Japan

Postdoctoral Fellow

April 01, 2008–February 27, 2009

Department of Applied Chemistry, Saga University, Japan

Assistant Professor of Chemistry

April 22, 2001 –September 27, 2004

Department of Chemistry, Khulna University of Engineering and Technology (KUET), Bangladesh.

RESEARCH ACCOMPLISHMENTS

H-Index factor: **17**

i10-index factor: **34**

Citations : **943**

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Scopus ID : **13807659300**

RESEARCH PROJECTS

- Since 2023 **Research Supporting Program**, King Saud University, Saudi Arabia, RSPD2023R1101; Role- PI
- Since 2023 **Institutional Funding Program for Research & Innovation**, "Ministry of Education" in Saudi Arabia, Project No. **IFKSUOR3-303**; **Role- PI (3rd phase)**, King Saud University
- Since 2022 **Institutional Funding Program for Research & Innovation**, Ministry of Education in Saudi Arabia, Project No. **IFKSURG-2-619**; **Role- PI (2nd phase)**, King Saud University.

EDUCATION

Ph. D. in Organic Chemistry

October 2004–September 2007

Department of Applied Chemistry, Saga University, Japan. Thesis: *Synthesis and Characterization of Artificial Allosteric Receptors Derived from Calix[n]arenes*.

Master of Philosophy (M. Phil.) in Organic Chemistry

December 1998–March 2001

Department of Chemistry, Bangladesh University of Engineering & Technology, Bangladesh. Thesis: *Synthesis and Pharmacological studies of Substituted 1,3,4-Thiadiazoline Derivatives*.

Master of Science (M. Sc) in Organic Chemistry

May 1995–March 1997

Department of Chemistry, University of Rajshahi, Bangladesh. Thesis: *Synthesis and Characterization of Certain Novel Sulphur and Nitrogen-Containing Macrocyclic Organic Compounds and Investigation of their Antibacterial Activities*.

Bachelor of Science (B. Sc) in Chemistry

September 1989–October 1994

Department of Chemistry, University of Rajshahi, Bangladesh

BOOK CHAPTERS

Book Title: **Modelling of Chemical Process Systems**

Chapter Contribution: **Rahman, S.**, Georghiou, P.E. and Alodhayb, A., Density functional theory (DFT) models for the desulfurization and extraction of sulfur compounds from fuel oils using ionic liquids. In *Modelling of Chemical Process Systems*, Ed. Imtaz, S.A. Elsevier, Radarweg 29, PO Box 211, 1000 AE Amsterdam, Netherlands, **2023**, 53-90. <https://doi.org/10.1016/C2020-0-01199-0>

Selected List of Scientific Publications in Peer-reviewed Journals

1. Isalm, A.B.N.M.; Habib, M.A.; Hasan, M.M.; Hasan, M.R.; Karim, K.M.R.; Mahiuudin, M.; Yoshida, T.; Karim, M.R.; **Rahman, S.**; Albrithen, H.; Alodhayb, A.N.; Georghiou, P.E. Exploration of the synthesis, crystal structure, Hirshfeld surface analysis, binding properties, antibacterial activities, and molecular docking of a Schiff base nickel (II) Complex. *J. Mol. Struct.* **2025**, 1322, 140294, <https://doi.org/10.1016/j.molstruc.2024.140294>
2. Alanazi, R.; **Rahman, S.**; Al-Gawati, M.; Alarifi, N.; Alzahrani, K.E.; Alanazi, N.; Alodhayb, A.N. Investigating adsorption and removal of divalent Ca²⁺ and Pb²⁺ ions from aqueous solutions by gamma-irradiation using quartz tuning fork (QTF) sensor technique. *Journal of Saudi Chemical Society*, 2024, 101947, <https://doi.org/10.1016/j.jscs.2024.101947>
3. Islam, M.M.; Bigyan Sharma, B.; Wang, C.Z.; **Rahman, S.**; Alodhayb, A. N.; Georghiou, P.E.; Elsegood, M.R.J.; Yamato, T. Synthesis, Conformational Properties and DFT Computational Studies

- of [3]Metacyclo[3](1,3)pyrenophanes, *ChemistrySelect*, **2024**, 9(32), e202401809, <https://doi.org/10.1002/slct.202401809>
4. Sager, A., **Rahman, S.**, Imtiaz, S.A., Zhang, Y., Alodhayb, A., Georghiou, P.E., M. Al-Gawati, Oxidative and Extractive Desulfurization of Fuel Oils Catalyzed by N-Carboxymethyl Pyridinium Acetate and N-Carboxyethyl Pyridinium Acetate Acidic Ionic Liquids: Experimental and Computational DFT Study, *ACS Omega* **2024**, 9(22), 23485-23498. <https://doi.org/10.1021/acsomega.3c09975>
 5. Saif, M.Z., Esha, N.J.I., Quayum, S.T., Rahman, S., Al-Gawati, M.A., Alsowaygh, G., Albrithen, H., Alodhayb, A.N., Poirier, R.A. and Uddin, K.M. Investigating the potential of 6-substituted 3-formyl chromone derivatives as anti-diabetic agents using in silico methods. *Scientific Reports*, **2024**, 14(1), p.13221. <https://doi.org/10.1038/s41598-024-63237-y>
 6. Labiba, A., Abbad, S.S.A., **Rahman, S.**, Alodhayb, A., Raymond A Poirier, R.A., Uddin, K.M. "Investigating Baxdrostat and Its Derivatives as Aldosterone Synthase Inhibitors for Resistant Hypertension: An *In Silico* Approach". *ChemistrySelect*, **2024**, 9(7), e202304929, <https://doi.org/10.1002/slct.202304929>
 7. Quayum, S.T., Esha, N.J.I., Siraji, S., Abbad, S.S.A., Alsunaidi, Z.H.A., Almatarneh, M.H., **Rahman, S.**, Alodhayb, A., Alibrahim, K.A., Kawsar, S.M.A., Uddin, K.M. "Exploring the effectiveness of flavone derivatives for treating liver diseases: Utilizing DFT, molecular docking, and molecular dynamics techniques" *MethodsX*, **2024**, 12, 102537, <https://doi.org/10.1016/j.mex.2023.102537>
 8. Uddin, K.M., Meem, M.H., Akter, M., **Rahman, S.**, Al-Gawati, M.A., Alarifi, N., Albrithen, H., Alodhayb, A., Poirier, R.A. and Bhuiyan, M.M.H. Design, synthesis, and bioevaluation of novel unsaturated cyanoacetamide derivatives: In vitro and in silico exploration. *MethodsX*, **2024**, 12, p.102691. <https://doi.org/10.1016/j.mex.2024.102691>
 9. Esha, N.J.I., Quayum, S.T., Saif, M.Z., Almatarneh, M.H., **Rahman, S.**, Alodhayb, A., Raymond A Poirier, R.A., Uddin, K.M. "Exploring the potential of fluoro-flavonoid derivatives as anti-lung cancer agents: DFT, molecular docking, and molecular dynamics techniques". *Int. J. Quant. Chem.*, **2024**, 124, e27274, <https://doi.org/10.1002/qua.27274>
 10. Suha, H.N., Hossain, M.S., **Rahman, S.**, Alodhayb, A., Hossain, M.M., Kawsar, S.M., Poirier, R. and Uddin, K.M. In Silico Discovery and Predictive Modeling of Novel Acetylcholinesterase (AChE) Inhibitors for Alzheimer's Treatment. *Medicinal Chemistry*, **2024**. <https://doi.org/10.2174/0115734064304100240511112619>
 11. Upoma, N.J., Akter, N., Ferdousi, F.K., Sultan, M.Z., **Rahman, S.**, Alodhayb, A., Alibrahim, K.A. and Habib, A.. Interactions of Co (II)-and Zn (II) porphyrin of 5, 10, 15, 20-tetrakis (1-methyl-4-pyridinio) porphyrin with DNA in Aqueous Solution and Their Antimicrobial Activities. *ACS omega*, **2024**, 9(20), pp.22325-22335. <https://doi.org/10.1021/acsomega.4c01708>
 12. Hossain, M.S., Al Abbad, S.S., Alsunaidi, Z.H., **Rahman, S.**, Alodhayb, A.N., Hossain, M.M., Poirier, R.A. and Uddin, K.M. Evaluation of novel pyridoxal isonicotinoyl hydrazone (PIH) derivatives as potential anti-tuberculosis agents: An in-silico investigation. *International Journal of Quantum Chemistry*, **2024**, 124(9), p.e27381. <https://doi.org/10.1002/qua.27381>
 13. Ananth, V., Ashok, V., Mathi, S., Pandiaraj, S., **Rahman, S.**, Alarifi, N., Alodhayb, A.N. and Shetti, N.P., 2024. Synthesis of bimetal-decorated N-doped carbon nanoparticles for enhanced oxygen evolution reaction. *FlatChem*, **2024**, 45, p.100648. <https://doi.org/10.1016/j.flatc.2024.100648>
 14. Islam, M.W., Akter, R., Islam, M.M., Islam, R., Jamal, A.S.I.M., Chowdhury, A., Zohora, F.T., **Rahman, S.**, Alodhayb, A., Rony, S.R. and Limon, T.R. Synthesis, Antibacterial, Antioxidant and DFT Computational Studies of Acetophenone-Based Chalcone Derivatives. *Chemistry Africa*, 7(4), **2024**, 1803-1816. <https://doi.org/10.1007/s42250-024-00891-9>
 15. Al-Ghamdi, A.R., **Rahman, S.**, Al-Wabli, R.I., Al-Mutairi, M.S. and Rahman, A.M. Synthesis, Cytotoxicity, and Photophysical Investigations of 2-Amino-4, 6-diphenylnicotinonitriles: An

Experimental and Theoretical Study. *Molecules*, **2024**, 29(8), 1808.
<https://doi.org/10.3390/molecules29081808>

16. Mohanty, S.S., Dutta, P., Das, J.K., Mohapatra, S.K., **Rahman, S.**, Alanazi, R., Alanazi, N. and Alodhayb, A.N. Analog performance and linearity analysis of a p-type group IV-IV SiGe TFET. *Journal of Computational Electronics*, 23(2), **2024**, 244-256. <https://doi.org/10.1007/s10825-024-02141-0>
17. Alrashed, H., Obeid, A., Albrithen, H., Muthuramamoorthy, M., **Rahman, S.**, Al-Gawati, M.A. and Alodhayb, A.N. Modeling the mechanical response of microelectromechanical system (MEMS)-based sensors to volatile alcohol vapors: A finite element analysis. *AIP Advances*, **2024**, 14(3), <https://doi.org/10.1063/5.0195105>
18. Aqueel Ahmed, A.T., Nurhidayati, N., Hidayah Rayanisaputri, F.R., Alibrahim, K.A., Khadtare, S.S., **Rahman, S.**, Alodhayb, A.N., Rochman, N.T. and Ansari, A.S. Thermal atomic layer deposition of aluminum oxide, nitride, and oxynitride: A mechanistic investigation. *AIP Advances*, **2024**, 14(3). <https://doi.org/10.1063/5.0190183>
19. Meem, M.H., Yusuf, S.B., Al Abbad, S.S., **Rahman, S.**, Al-Gawati, M., Albrithen, H., Alodhayb, A.N. and Uddin, K.M., 2024. Exploring the anticancer and antibacterial potential of naphthoquinone derivatives: a comprehensive computational investigation. *Frontiers in Chemistry*, **2024**, 12, 1351669. <https://doi.org/10.3389/fchem.2024.1351669>
20. Labiba, A., Al Abbad, S.S., **Rahman, S.**, Alodhayb, A., Poirier, R.A. and Uddin, K.M., 2024. Investigating Baxdrostat and Its Derivatives as Aldosterone Synthase Inhibitors for Resistant Hypertension: An In Silico Approach. *ChemistrySelect*, 9(7), p.e202304929. <https://doi.org/10.1002/slct.202304929>
21. Liu, Y.L., Wu, L.F., Wu, C., **Rahman, S.**, Alodhayb, A., Redshaw, C., Georghiou, P.E. and Yamato, T., 2024. A facile and sensitive hexahomotrioxacalix [3] arene-based fluorescent sensor for the detection of trace amounts of 2, 4, 6-trinitrophenol. *Sci. Total Environ.*, **2024**, 908, 168209. <https://doi.org/10.1016/j.scitotenv.2023.168209>
22. **Rahman, S.**, Al-Gawati, M.A., Alfaifi, F.S., Alenazi, W. F., Alarifi, N., Albrithen, H., Alodhayb, A.N. and Georghiou, P.E. Detection of Aromatic Hydrocarbons in Aqueous Solutions Using Quartz Tuning Fork Sensors Modified with Calix[4]arene Methoxy Ester Self-Assembled Monolayers: Experimental and Density Functional Theory Study, *Molecules* **2023**, 28(19), 6808.
23. **Rahman, S.**, Al-Gawati, M.A., Alfaifi, F.S., Muthuramamoorthy, M., Alanazi, A.F., Albrithen, H., Alzahrani, K.E., Assaifan, A.K., Alodhayb, A.N. and Georghiou, P.E. The Effect of Counterions on the Detection of Cu²⁺ Ions in Aqueous Solutions Using Quartz Tuning Fork (QTF) Sensors Modified with L-Cysteine Self-Assembled Monolayers: Experimental and Quantum Chemical DFT Study. *Chemosensors*, **2023**, 11(2), 88.
24. **Rahman, S.**, Georghiou, P.E. and Alodhayb, A., 2023. Density functional theory (DFT) models for the desulfurization and extraction of sulfur compounds from fuel oils using ionic liquids. In *Modelling of Chemical Process Systems*, Ed. Imtaz, S.A. Elsevier, Radarweg 29, PO Box 211, 1000 AE Amsterdam, Netherlands, **2023**, 53-90.
25. Uddin, K.M., Sakib, M., Siraji, S., Uddin, R., **Rahman, S.**, Alodhayb, A., Alibrahim, K.A., Kumer, A., Matin, M.M. and Bhuiyan, M.M.H. Synthesis of New Derivatives of Benzylidinemalononitrile and Ethyl 2-Cyano-3-phenylacrylate: In Silico Anticancer Evaluation. *ACS omega*, **2023**, 8(29), 25817-25831.
26. Wu, C., **Rahman, S.**, Jiang, X.K., Wang, C.Z., Alodhayb, A., Alibrahim, K.A., Georghiou, P.E. and Yamato, T. A fluorescent receptor for alkylammonium ions based on an anthryl-linked triazole-modified hexahomotrioxacalix [3] arene. *Journal of Molecular Structure*, **2023**, 1286, p.135615.
27. Assaifan, A.K., Al-Gawati, M.A., Alzahrani, K.E., Alqahtani, S.F., Aldakhil, S.M., Alodhayb, A.N., **Rahman, S.** and Albrithen, H., 2023. Quartz Tuning Fork-Based Biosensor for the Direct Detection of Human Cytomegalovirus. *Journal of King Saud University-Science*, **2023**, 102703.

28. Rahman AF, Bakheit AH, **Rahman S**, Mostafa GA, Alrabiah H. Procainamide Charge Transfer Complexes with Chloranilic Acid and 2, 3-Dichloro-5, 6-dicyano-1, 4-benzoquinone: Experimental and Theoretical Study. *Processes*, **2023**, 11(3):711.
29. Islam MM, Islam R, Hassan SM, Karim MR, Rahman MM, **Rahman S**, Hossain MN, Islam D, Shaikh MA, Georghiou PE. Carboxymethyl chitin and chitosan derivatives: synthesis, characterization and antibacterial activity. *Carbohydrate Polymer Technologies and Applications*. **2023**, 10:100283.
30. Begum, M.S.; Das, D.; Zangrando, E.; **Rahman, S.**, Alodhayb, A.; Begum, M.K.; Sheikh, C.M.; Miyatake, R.; Howlader, M.B.H.; Karim, M.R.; Chowdhury, M.B. A dithiocarbazate N, S Schiff base ligand with a long alkyl chain: Synthesis, characterization, DFT study and antimicrobial activity of its Ni (II) complex. *J. Mol. Struct.* **2023**, 1277, 134808, <https://doi.org/10.1016/j.molstruc.2022.134808>.
31. Alsaigh, R.A., **Rahman, S.**, Alfaifi, F.S., Al-Gawati, M.A., Shalla, R., Alzaid, F., Alanazi, A.F., Albrithen, H., Alzahrani, K.E., Assaifan, A.K. and Alodhayb, A.N. Detection of Volatile Alcohol Vapors Using PMMA-Coated Micromechanical Sensors: Experimental and Quantum Chemical DFT Analysis, *Chemosensors* **2022**, 10(11), 452
32. Alshammri, A., Alsaigh, R., Alzahrani, K.E., Assaifan, A.K., Albrithen, H., Braim, M., Pandiaraj, S., Alsaigh, R.A., **Rahman, S.**, Alfaifi, F.S., Al-Gawati, M.A., Shalla, R., Alzaid, F., Alanazi, A.F., Albrithen, H., Alzahrani, K.E., Assaifan, A.K. and Alodhayb, A.N. Detection of Volatile Alcohol Vapors Using PMMA-Coated Micromechanical Sensors: Experimental and Quantum Chemical DFT Analysis, *Chemosensors* **2022**, 10(11), 452
33. Alshammri, A., Alsaigh, R., Alzahrani, K.E., Assaifan, A.K., Albrithen, H., Braim, M., Pandiaraj, S., Juliet, A.V., Sanchana, G., Alkallas, F.H., Trabelsi, A.B.G., Tahani A A., Nadiyah, A., Muthumareeswaran M. Rahman, S., Alodhayb, A. Quality Factor of a Microchannel Microresonator as a Function of Viscosity and its Vibrational Mode: An Experimental and Computational Analysis. *IEEE Sensors Journal*. **2022**.
34. Georghiou, P.E.; **Rahman, S.**; Assiri, Y.; Valluru, G.K.; Menelaou, M.; Alodhayb, A.; Braim, M.; Beaulieu, L.; Development of calix [4] arenes modified at their narrow-and wider-rims as potential metal ions sensor layers for microcantilever sensors: further studies, *Can. J. Chem.* **2022**. 133523.
35. Yu, Z.D., Dong, X.X., Cao, J.Y., Zhao, W.X., Bi, G.H., Wang, C.Z., Zhang, T., **Rahman, S.**, Georghiou, P.E., Lin, J.B. and Yamato, T. Substituent effects on the intermolecular interactions and emission behaviors in pyrene-based mechanochromic luminogens, *J. Mater. Chem. C*, **2022**, 10, 9310–9318
36. Nath B.D.; Islam, M.M.; Karim, M.R.; **Rahman, S.**; Shaikh, M.A.A.; Georghiou, P.E.; Menelaou, M. Recent Progress in Metal-Incorporated Acyclic Schiff-Base Derivatives: Biological Aspects, *ChemistrySelect*, **2022**, 7, e20210429.
37. Islam, M.M.; Wang, C.-Z.; Sharma, B.; **Rahman, S.**; Georghiou, P.E.; Alodhayb, A.; Matsumoto, T.; Tanaka, J.; Yamato, T. Synthesis and DFT conformational analysis of trimethylfunctionalized [2.2]metacyclophanes and their Lewis-acid assisted reactions, *J. Mol. Struct.* **2022**, 1266, 133523.
38. **Rahman, S.**; Tomiyasu, H.; Wang, C.-Z.; Georghiou, P.E.; Alodhayb, A.; Carpenter-Warren, C.L.; Elsegood, M.R.J.; Teat, S.; Redshaw, C.; Yamato, T. Allosteric binding properties of a 1, 3-alternate thiocalix [4] arene-based receptor having phenylthiourea and 2-pyridylmethyl moieties on opposite faces, *New J. Chem.*, **2021**, 45, 19235-19243
39. Yan, X.; **Rahman, S.**; Rostami, M.; Tabasi, Z.A.; Khan, F.; Alodhayb, A.; Zhang, Y. "Carbon Quantum Dot-Incorporated Chitosan Hydrogel for Selective Sensing of Hg²⁺ Ions: Synthesis, Characterization, and Density Functional Theory Calculation". *ACS Omega*, **2021**, 6(36), 23504–23514.

40. Islam, M.M.; Sharma, B.; **Rahman, S.**; Alodhayb, A.; Georghiou, P.E.; Yamato, T. Synthesis, structures and DFT calculations of 9-Methoxy [3.3] metaparacyclophanes and their Lewis acid-catalyzed reactivity, *J. Mol. Struct.* **2021**, 1236, 130334.
41. Georghiou, P.E., **Rahman, S.**, Alrawashdeh, A., Alodhayb, A., Valluru, G., Unikela, K.S. and Bodwell, G.J., Synthesis, supramolecular complexation and DFT studies of a bis (pyrene)-appended 'capped' triazole-linked calix [4] arene as Zn²⁺ and Cd²⁺ fluorescent chemosensors. *Supramolecular Chemistry*, **2020**, 1–9.
42. Islam, M.M., Georghiou, P.E., **Rahman, S.** Yamato, T. Calix[3]arene-Analogous Metacyclophanes: Synthesis, Structures and Properties with Infinite Potential, *Molecules*, **2020**, 25(18), 4202.
43. Akther, T., Islam, M.M., Kowser, Z., Matsumoto, T., Tanaka, J., **Rahman, S.**, Alodhayb, A., Georghiou, P.E., Redshaw, C. Yamato, T. Synthesis and Structures of [2. n] Metacyclophan-1-enes and their Conversion to Highly Strained [2. n] Metacyclophane-1-yne. *Eur. J. Org. Chem.* **2020**, 4167–4175.
44. Mohamed, H., **Rahman, S.**, Imtiaz, S.A. and Zhang, Y. Oxidative-Extractive Desulfurization of Model Fuels Using a Pyridinium Ionic Liquid. *ACS omega*, **2020**, 5(14), 8023–8031.
45. Islam, M.M.; Feng, Z.; **Rahman, S.**; Georghiou, P. E.; Matsumoto, T.; Tanaka, J.; Alodhayb, A.; Redshaw C.; Yamato, T. Studies on Lewis-Acid Induced Reactions of 8-Methoxy[2.2]-metacyclophanes: a New Synthetic Route to Alkylated Pyrenes, *ChemistrySelect*, **2020**, 5, 1269–1274.
46. Rajeev, N.; Swaroop, T. R.; Alrawashdeh, A. I.; **Rahman, S.**; Alodhayb, A.; Anil, S. M.; Kiran, K. R.; Chandru, C.; Georghiou, P. E.; Rangappa, K. S.; Sadashiva, M. P. Reaction of Arylmethyl Isocyanides and Arylmethylamines with Xanthate Esters: A Facile and Unexpected Synthesis of Carbamothioates, *Beilstein J. Org. Chem.* **2020**, 16, 159–167.
47. Islam, M.M.; Feng, Z.; **Rahman, S.**; Georghiou, P. E.; Matsumoto, T.; Tanaka, J.; Alodhayb, A.; Redshaw C.; Yamato, T. Synthesis, Structures and Lewis-Acid-Induced Isomerization of 8-Methoxy[2.2]metaparacyclophanes and a DFT Study, *ChemistrySelect*, **2019**, 4, 3630–3635.
48. Rahman, S.; Helleur, R.; MacQuarrie, S.; Papari, S.; Hawboldt, K. Upgrading and isolation of low molecular weight compounds from bark and softwood bio-oil through molecular distillation, *Sep. Purif. Technol.* **2018**, 194, 123–129.
49. Paris E. Georghiou, P. E.; Rahman, S.; Alodhayb, A.; Nishimura, H.; Lee, J.; Wakamiya, A.; Scott, L. T. Calixazulenes: azulene-based calixarene analogues – an overview and recent supramolecular complexation studies, *Beilstein J. Org. Chem.* **2018**, 14, 2488–2494.
50. Islam, M.M.; Wang, C.-Z.; Feng, Z.; Rahman, S.; Georghiou, P. E.; Alodhayb, A.; Yamato, T. Synthesis, Structures and DFT Computational Studies of [3.1.1]Metacyclophanes Containing Benzofuran Rings, *ChemistrySelect*, **2018**, 3(48), 13542-13547,
51. Jiang, X.-K.; Ikejiri, Y.; Wu, C.; Rahman, S.; Georghiou, P.E.; Zeng, X.; Elsegood, M.R.J.; Redshaw, C.; Teat, S.J.; Yamato, T. A Hexahomotrioxacalix[3]arene-Based Ditopic Receptor for Alkylammonium Ions Controlled by Ag⁺ Ions. *Molecules*, **2018**, 23, 467.
52. Mahmood, A.D.; Rahman, S.; Georghiou, P.E. Synthesis, Complexation and DFT Computational Studies of Bis(naphthyl)methane-"capped" triazole-Linked calix[4]arenes as Fe³⁺ fluorescent chemosensors, *ChemistrySelect*, **2017**, 2(3), 1214-1218.
53. Kowser, Z.; Rayhan, U.; Rahman, S.; Georghiou, P. E. A fluorescence "turn-on" sensor for multiple analytes: OAc⁻ and F⁻ triggered fluorogenic detection of Zn²⁺ in a cooperative fashion, *Tetrahedron*, **2017**, 73, 5418-5424