PROFILE OF FINAL REPORT
FRGS/RAGS/ERGS/PRGS

Important Notes
- *Profile of Final Report is to be submitted to declare the project is completed.*
- *Full Report should be uploaded through IREP.*
- *All reports must be based on the actual findings of the reported project.*

Guidelines for writing the Profile of Final Report
- *Report should be written in 'Times New Roman 12' Font, with 1.5 line spacing*
- *Report should be 5 pages (excluding appendices/references)*
- *Report must be in English (Applicable for Research in Arabic as well)*

FRGS17-023-0589

Synthesis, Characterization And Biological Studies Of Substituted Thiadiazine Derivatives And Their Metal Complexes

Sponsored by MOHE

Fiona How Ni Foong

Department of Chemistry, Kulliyyah of Science

Research summary and findings: (3-4 pg)

A total of 16 substituted thiadiazine derivatives and 4 metal complexes were successfully synthesized and characterized. Melting point was determined for BBTHZ, B3THZ and 33THZ, while the other substituted thiadiazine derivatives were sticky and semi-solid. BBTHZ melted in the range of 142-144℃, while B3THZ melted in the range of 114℃-118℃. The melting point for 33THZ could not be determined because it stuck along the side of capillary tube. The CHNS for the BBTHZ, B3THZ and 33THZ and the metal complexes (Zn, Cu, Ni, Co) showed that they were in accordance with the expected structure. All the substituted thiadiazine derivatives were fully dissolved in the polar protic and except for water. They also easily dissolved in DMSO and DCM but required heating when dissolved in acetonitrile. It was observed that compounds B3THZ, 3BTHZ, 33THZ, 22THZ and 24THZ dissolved in acetonitrile without the need of heating. It is also observed that the similarity in these compounds is that they are yellow in colour except 24THZ which is brown. Derivatives that

are red and green in colour can only dissolved upon heating. As for the chloroform, most derivatives dissolved in it without the need of heating except for B2THZ. While compounds B4THZ, 4BTHZ, 42THZ, 43THZ and 44THZ were partially soluble in the solvent upon heating. This suggest that derivatives with 4-picolylamine dominantly influenced the solubility. Afterall, all derivatives did not dissolve in toluene.

The FTIR spectra were shown in Fig. 3 for derivatives 1-4 (BBTHZ, B2THZ, B3THZ, B4THZ), Fig. 4 for derivatives 5-8 (2BTHZ, 22THZ, 23THZ, 24THZ), Fig. 5 for derivatives 9-12 (3BTHZ, 32THZ, 33THZ, 34THZ) and Fig. 6 for derivatives 13-16 (4BTHZ, 42THZ, 43THZ, 44THZ). All the thiadiazine derivatives exhibited υ(C-N) in the region 1555 – 1632, the presence of sulfur was found from the υ(C=S) and υ(SCS), which occurred at 1416 -1532 and 683 -797 cm^{-1} respectively. The presence of the bands was in accordance to Kartiyar et al., 2003.

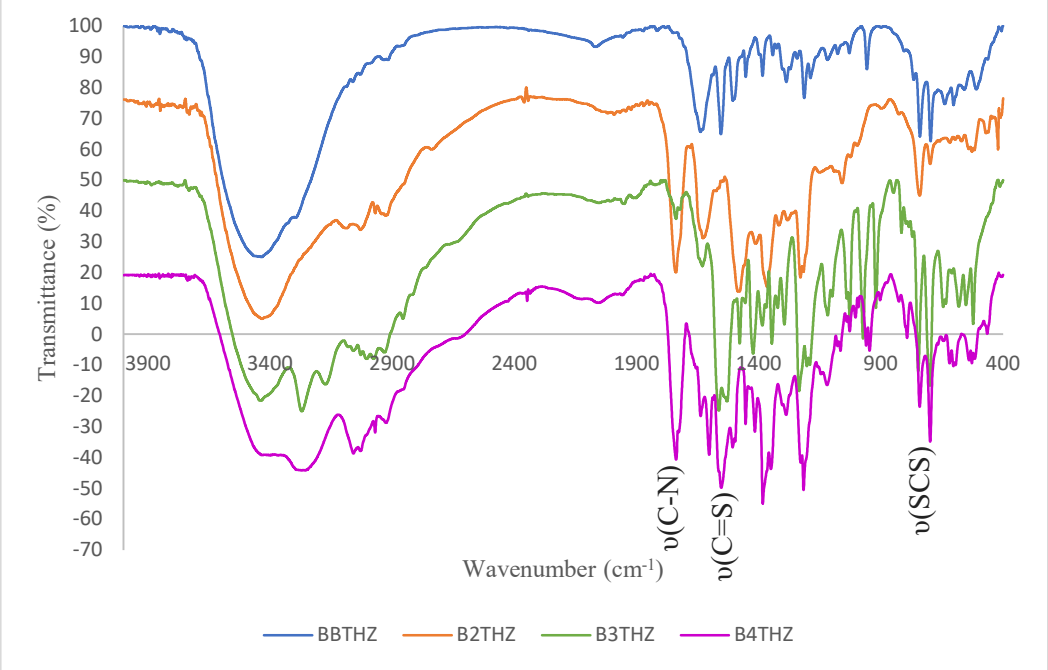

Figure 3 FTIR spectra of thiadiazine derivatives BBTHZ, B2THZ, B3THZ and B4THZ

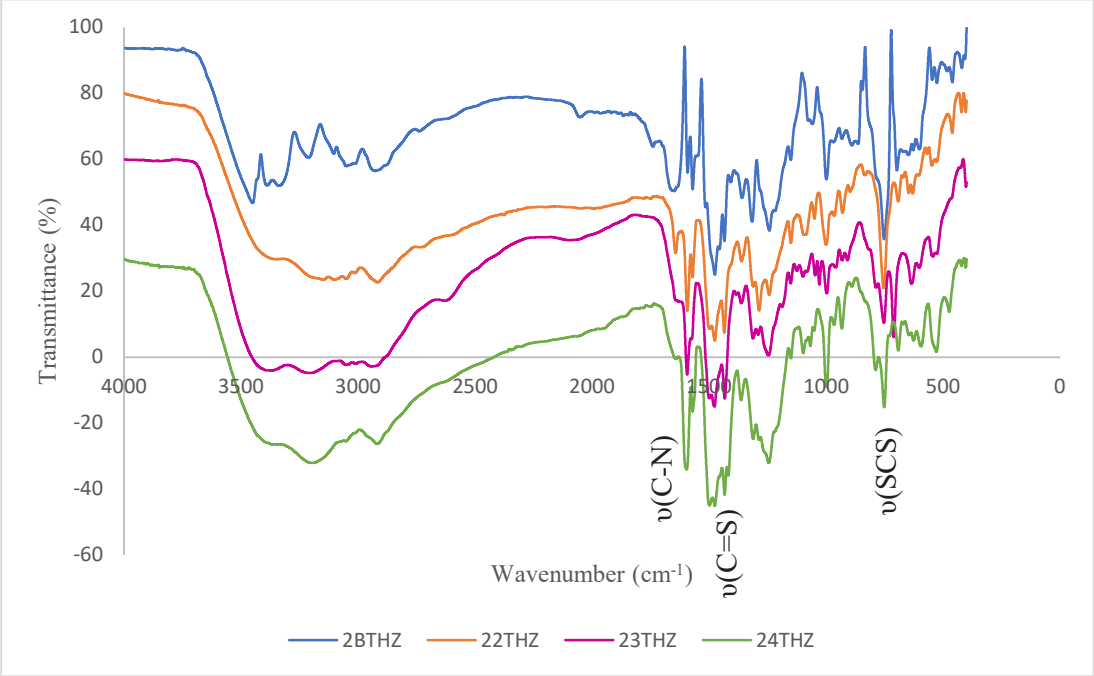

Figure 4 FTIR spectra of thiadiazine derivatives 2BTHZ, 22THZ, 23THZ and 24THZ

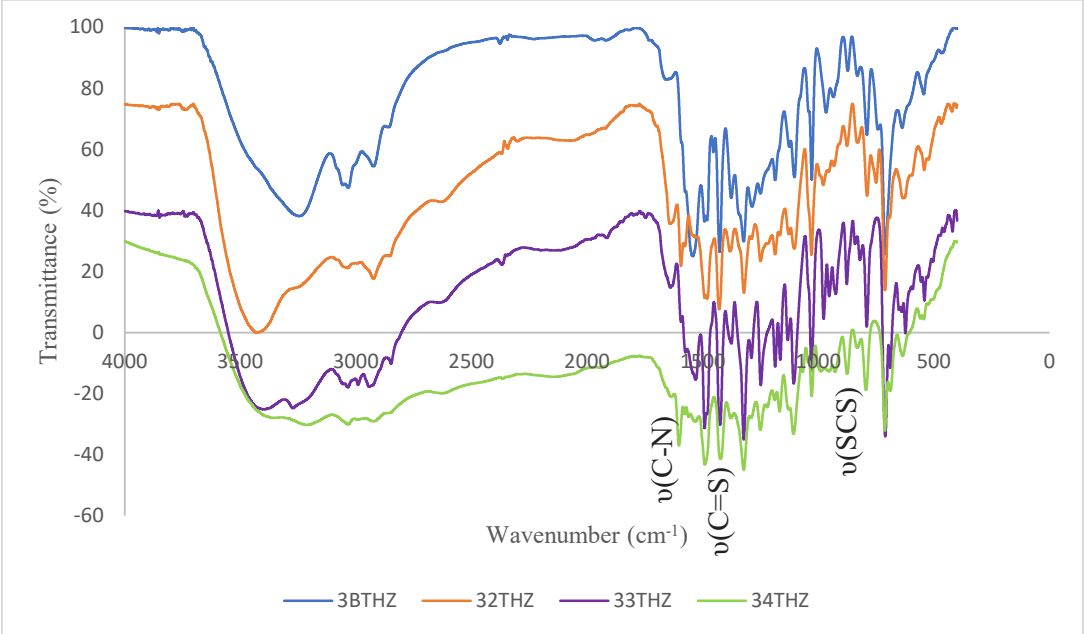

Figure 5 FTIR spectra of thiadiazine derivatives 3BTHZ, 32THZ, 33THZ and 34THZ

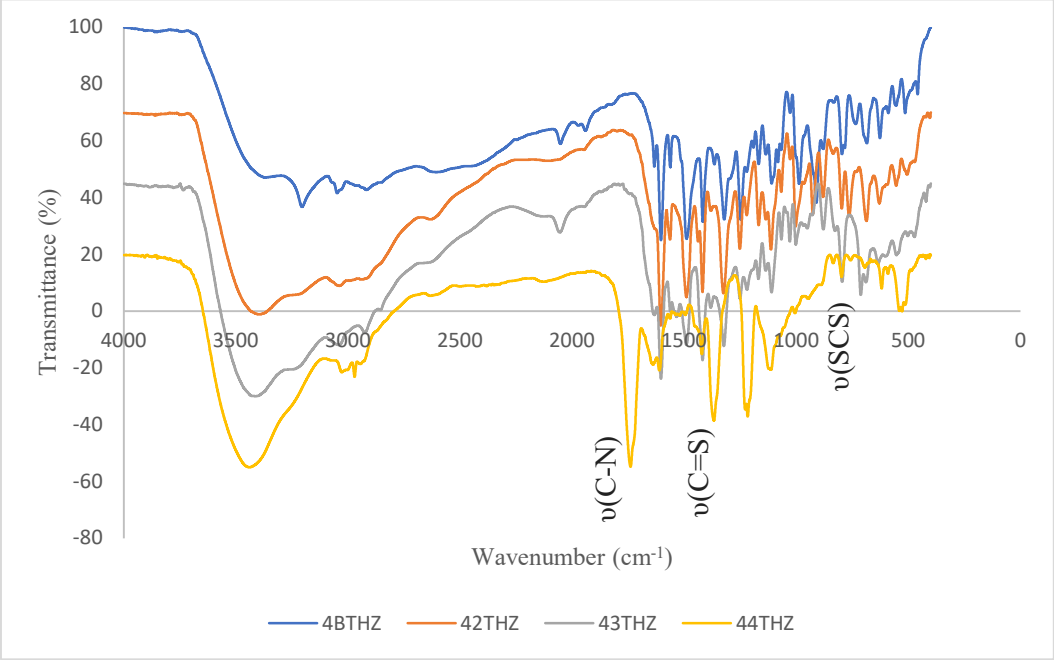

Figure 6 FTIR spectra of thiadiazine derivatives 4BTHZ, 42THZ, 43THZ and 44THZ

As for the NMR, the peaks obtained were similar as the predicted one with little difference in the chemical shift (ppm). One proton in 3P pyridine ring is located at the most left of the spectrum, indicating it to be the most de-shielded proton due its location which is the nearest to =S. This observation applies to all ligands 32THZ, 33THZ and 34THZ. Consequently, ^{13}C NMR spectrum showed C=S group to be at the most left in the spectrum with predicted value of 191.2 ppm. Ligand 32THZ showed presence of this C at 182.52 ppm, ligand 33THZ at 192.87 ppm and ligand 34THZ at 195.9 ppm.

Cytotoxic assays were conducted using BBTHZ (L1), B2THZ (L2), B3THZ (L3), B4THZ (L4), 2BTHZ (L5), 22THZ (L6) and 23THZ (L7). All these seven ligands are assayed using human colorectal adenocarcinoma cell line, HT29 treated within 24 hours. Vinblastine is used as positive control in this experiment and all ligands are soluble in DMSO.

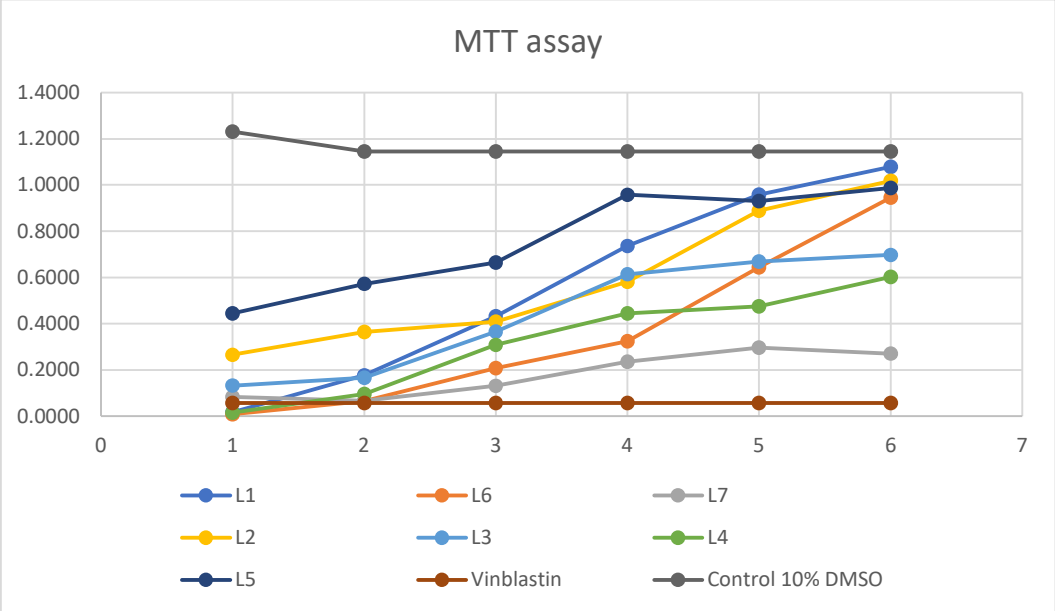

Figure 7: MTT assay result against HT29 (24 hour)

The graph's concentration value is formatted in reverse order, from the most concentrated to least concentrated. All compounds portrayed anticancer property against HT29 as the cell viability decreases as concentration increases. L1, L2, L6 and its crystal and ligand 2 showed uniform decrement of cell viability when the concentration increases. At 1 mg/ml, vinblastine has cell viability percentage of 0.056 but most treatments showed higher value except L1, L4 and L7 with value of 0.0167, 0.0160 and 0081. Nonetheless, values observed from the other treatments are not much different therefore all ligands are justified to have cytotoxic activity against this cancer cell line.

Financial Report and Asset Report:

Date Printed: 18-01-2021 10:17:22

FINANCIAL SUMMARY DETAILS

Project ID	FRGS17-023-0589
Title	Synthesis, Characterization And Biological Studies Of Substituted Thiadiazine Derivatives And Their Metal Complexes
Kulliyyah	Kulliyyah of Science
Duration	39

Researchers	
ASSOC. PROF. DR. Fiona How Ni Foong (6467)	Principal
ASSOC. PROF. DR. Solachuddin Jauhari Arief (5731)	Co-Researcher

Fund Summary

Vote Code	Description	Initial Allocation (RM)	Current Allocation (RM)	Disburse (RM)	Committed (RM)	Balance (RM)
V11000	Research Assistant (RA)	0.00	24,000.00	24,000.00	0.00	0.00
V21000	Travelling Expenses And Subsistence	0.00	0.00	0.00	0.00	0.00
V23000	Communication and Utilities	0.00	0.00	0.00	0.00	0.00
V24000	Rental	0.00	0.00	0.00	0.00	0.00
V27000	Research Materials & Supplies	0.00	29,000.00	28,996.83	0.00	3.17
V28000	Maintenance services	0.00	0.00	0.00	0.00	0.00
V29000	Professional Services & Other Services including Printing & Hospitality, Honorarium for subjects	0.00	17,200.00	17,194.02	0.00	5.98
V35000	Equipment	0.00	0.00	0.00	0.00	0.00
V36000	Miscellaneous Research Advancement	0.00	0.00	0.00	0.00	0.00
Total		**0.00**	**70,200.00**	**70,190.85**	**0.00**	**9.15**

Fund Received Detail

Receive Date	Description	Receipt No	Total	Vote Code
No records				

Outputs (For FRGS/RAGS/ERGS):

a) Human Capital Development

Details of student

Student full name : Dayang Fatin Nadhirah Binti Abang Sapani

IC/ Passport No. : 931026-13-6578

Student ID : G1711142

Citizenship : Malaysian

Year of Graduation : On-going

Thesis Title :

b) Publication

None

c) Intellectual Property

None

d) Additional Outputs

None

References:

Katiyar, D., Tiwari, V. K., Tripathi, R. P., Srivastava, A., Chaturvedi, V., Srivastava, R., & Srivastava, B. S. (2003). Synthesis and antimycobacterial activity of 3,5-disubstituted thiadiazine thiones. Bioorganic & Medicinal Chemistry, 11(20), 4369–4375. https://doi.org/10.1016/S0968-0896(03)00480-2