TH-NH MAPPING MODEL: A STARTER KIT FOR ¹H-NMR SPECTRAL INTERPRETATION

:: Abstract ::

Proton Nuclear Magnetic Resonance (¹H-NMR) interpretation plays an essential role in structural elucidations especially for unknown compound. Interpreting ¹H-NMR spectra may not be an easy task especially for the beginner (undergraduate students) since it is closely associated with the chemical shift (CS), integration (I) and multiplicity (M). Based on my observations, majority of chemistry students have been struggling to understand and associate all related information during the interpretation process. This personal observation is supported by findings reported in 2021, which claimed that the undergraduates took an uninformed bidirectional processing approach to understand basic principles of interpreting HNMR spectra¹. Thus, this starter kit maps the type of hydrogen (TH) and neighbouring hydrogen (NH) by featuring the three "CS-I-M" key-items, with an interactive color-coding. A survey on the effectiveness of this mapping model has revealed that student's level of confidence and performance have increased when practicing the ¹H-NMR interpretation. Students claimed that this model is easy-to-follow, interesting and can be converted into a Mobile App in the near future.

:: Objectives ::

The proposed mapping model is designed to emphasize two main objectives:

to improve student focus

:: Added Values ::

Users only need a **single source**, as this model COMPRISES:

- 1. Chemical shift (**CS**)
- Spin-spin splitting following the n+1 rule (M)
 Integration (I)



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to get students familiarized with the hydrogen signals and their respective neighbouring hydrogens

- 4. Type of protons (**TH**)
- 5. Adjacent atoms (NH)



	Step 1	Chemical Shift									
5	Step 2	Integration Number									
5	Step 3	Mu	Itiplicity								
5	Step 4	Type of I	hydrogen	(TH)							
Step 5		Neigbouring Hydrogen (NH)									

:: Commercialization Potential ::



MOBILE APP DEVELOPMENT (As per suggested by student)

User-friendly : able to be used anytime & anywhere

S Exciting and flounder-free

Designed and developed by:

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Q: What group are you pelong to?	 Undergraduate Students (USM - Full time) Undergraduate Students (Non-USM) Destaraduate Students (USM)
	50% Note: JIK 327 – Chemical Spectroscopy
Q: How useful is the TH- NH Mapping Model in ¹ H- NMR spectral nterpretation?	Q: Describe your level of confidence and performance when practicing the NMR interpretation using the TH- NH Mapping Model.
25% • Extremely • Very usefu • Moderately • Slightly us • Not at all	useful Juseful veful 1 y useful 75%

Reference: ¹Connor MC, Glass BH, Finkenstaedt-Quinn SA, and Shultz GV. (2021). Developing Expertise in 1H NMR Spectral Interpretation, The Journal of Organic Chemistry, 86 (2), 1385-1395.