

**Serendipitous *N,S*-Difunctionalization of Triazoles with Trifluoromethyl- β -diketones:
Access to Regioisomeric 1-Trifluoroacetyl-3-aryl-5-(2-oxo-2-arylethylthio)-1,2,4-
triazoles as DNA-Groove Binders**

Ranjana Aggarwal,^{a,b*} Prince Kumar,^a Mona Hooda,^c Suresh Kumar,^a

^aDepartment of Chemistry, Kurukshetra University, Kurukshetra-136119, Haryana, India

^bCouncil of Scientific and Industrial Research-National Institute of Science Communication and Policy Research, New Delhi 110012, India.

^cDepartment of Chemistry, Gurugram University, Gurugram-122003, Haryana, India.

*Corresponding author:

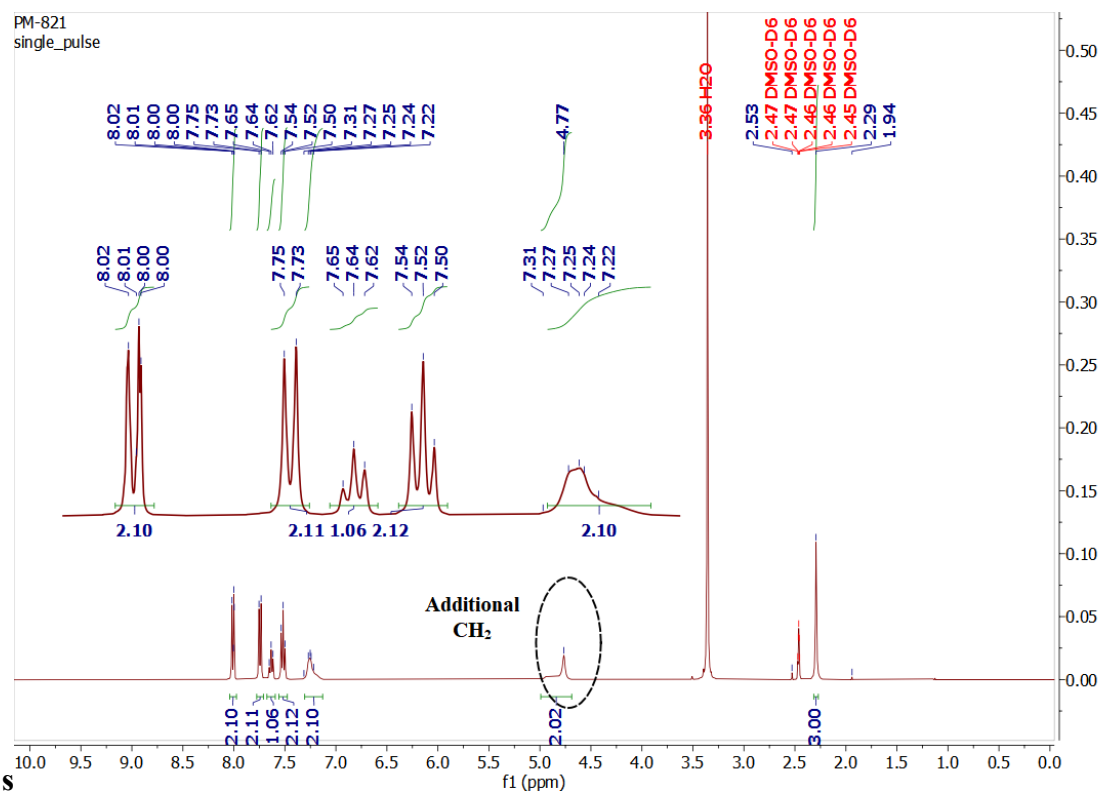
Prof. Ranjana Aggarwal, CSIR-National Institute of Science Communication and Policy
Research, New Delhi, India. Tel: +91-9896740740

E-mails: ranjana67in@yahoo.com, ranjanaaggarwal67@gmail.com

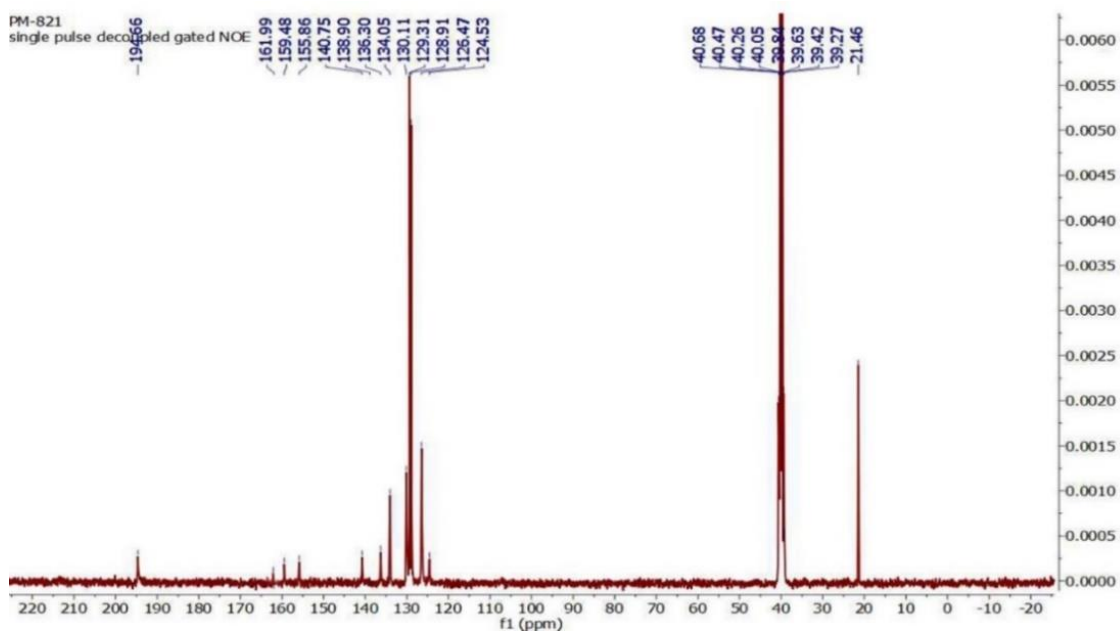
SUPPLEMENTARY DATA

1-Trifluoroacetyl-3-(4-tolyl)-5-((2-oxo-2-phenylethyl)thio)-1,2,4-triazole 14a

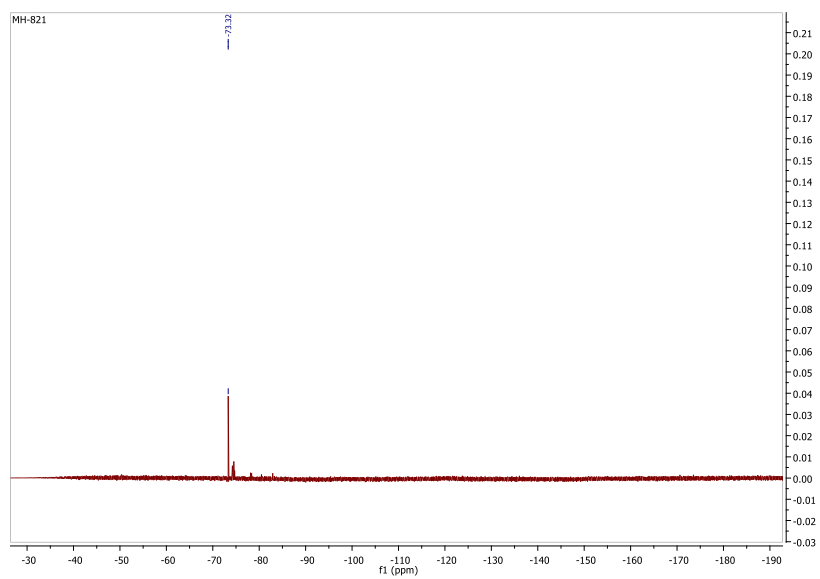
¹H of 14a



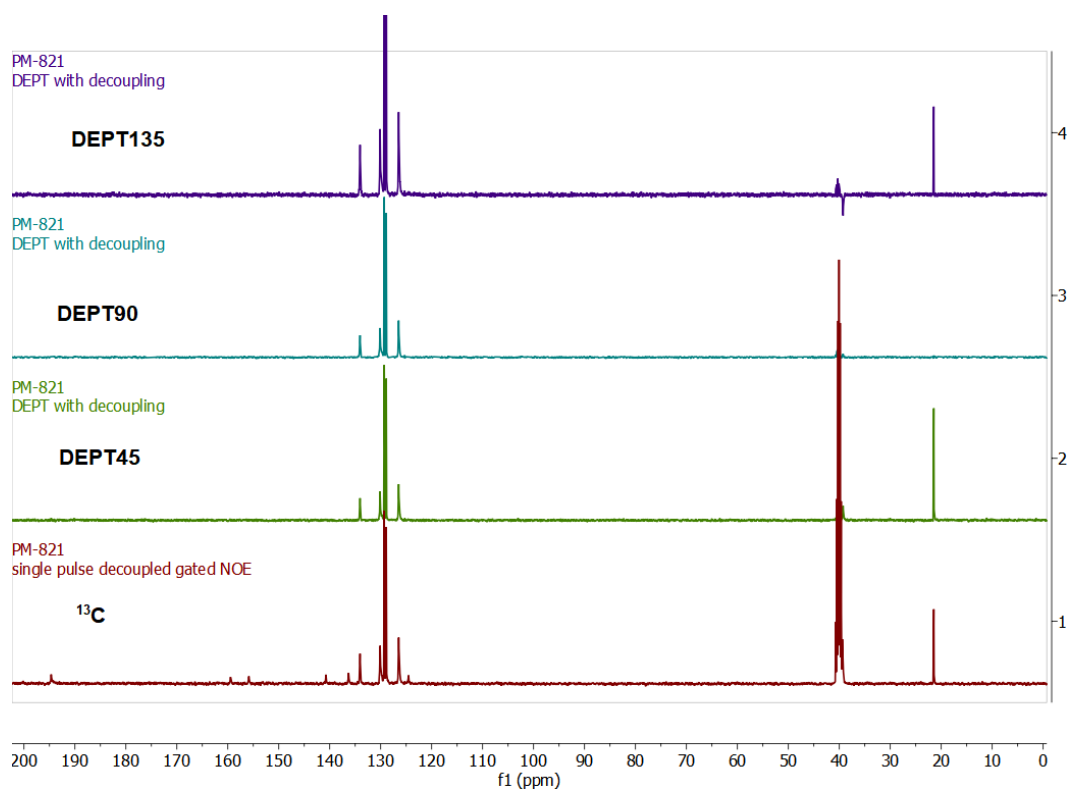
¹³C of 14a



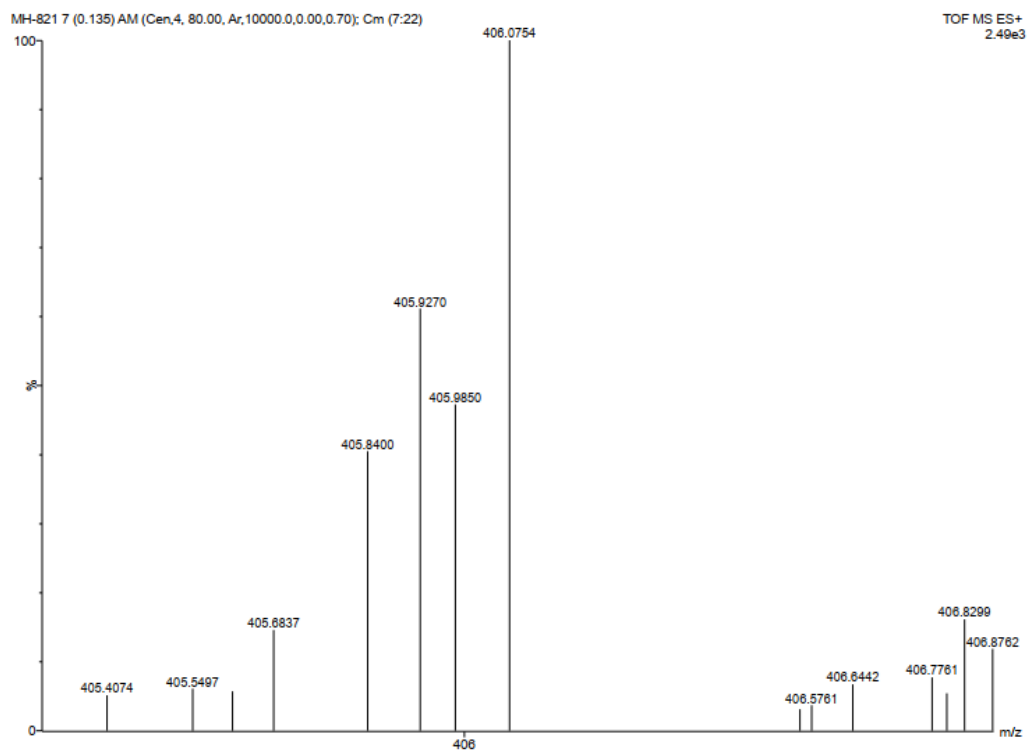
^{19}F of **14a**



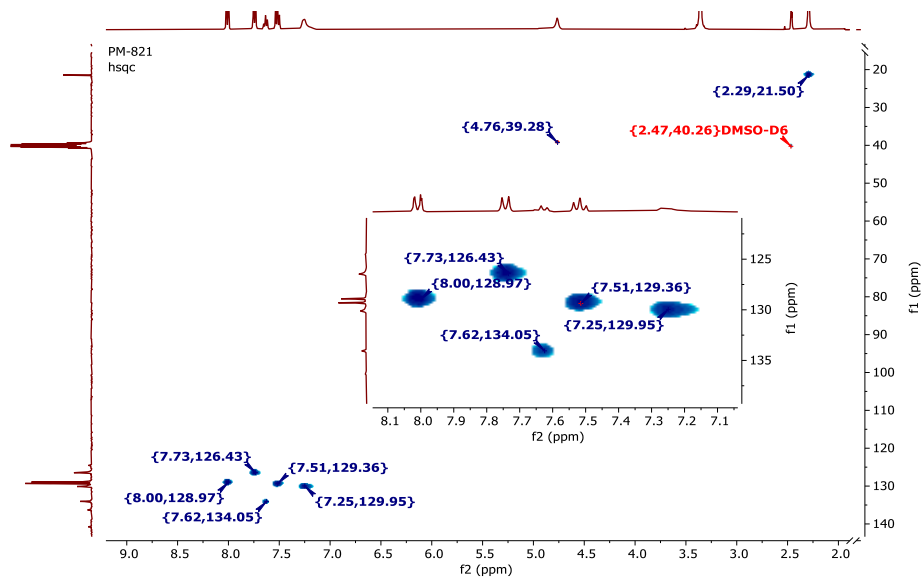
DEPT spectrum of **14a**



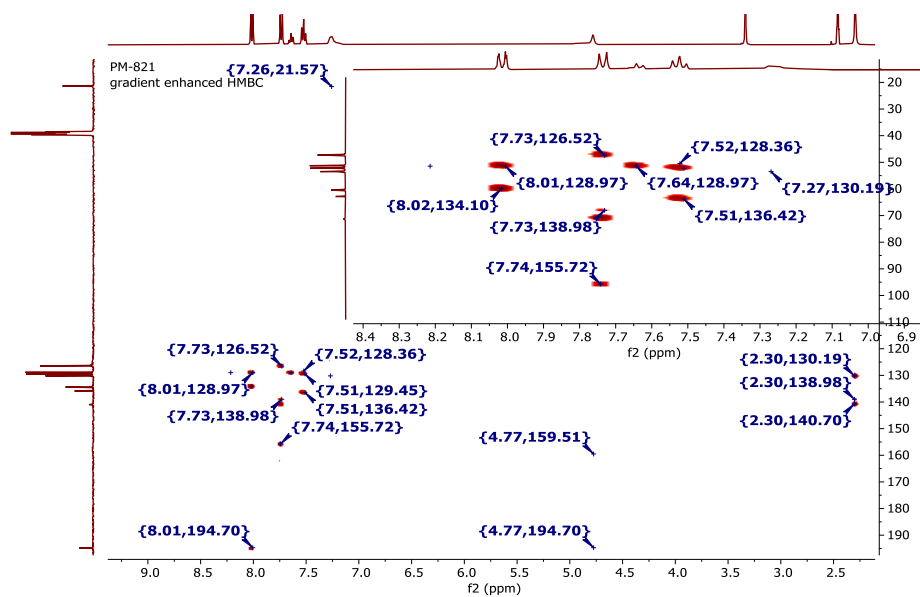
HRMS spectrum of compound 14a



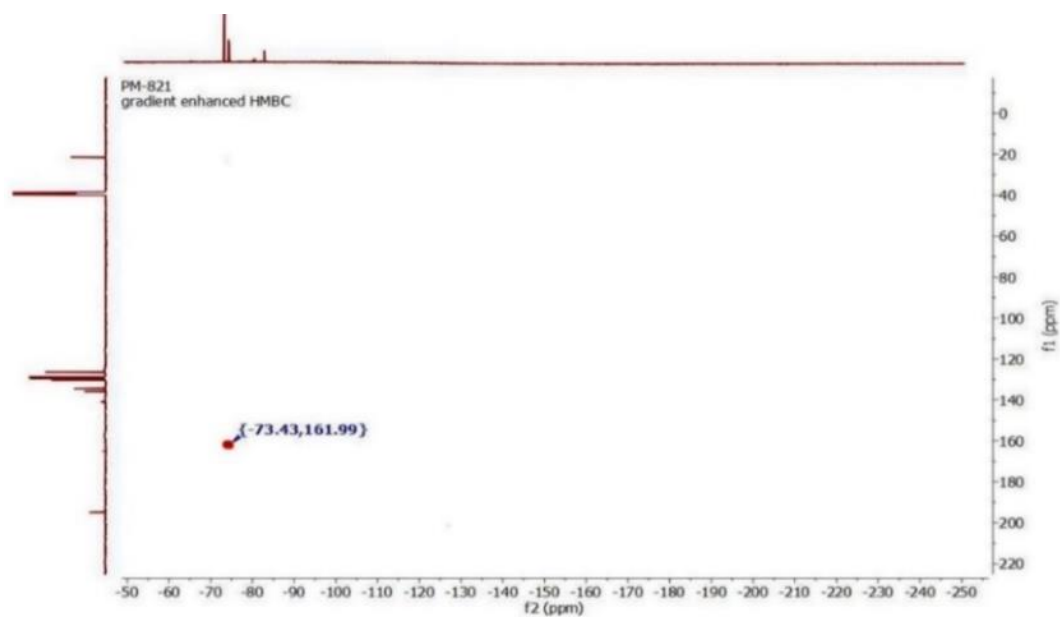
(¹H-¹³C) HSQC spectrum of compound 14a



$(^1\text{H}-^{13}\text{C})$ HMBC spectrum of compound **14a**

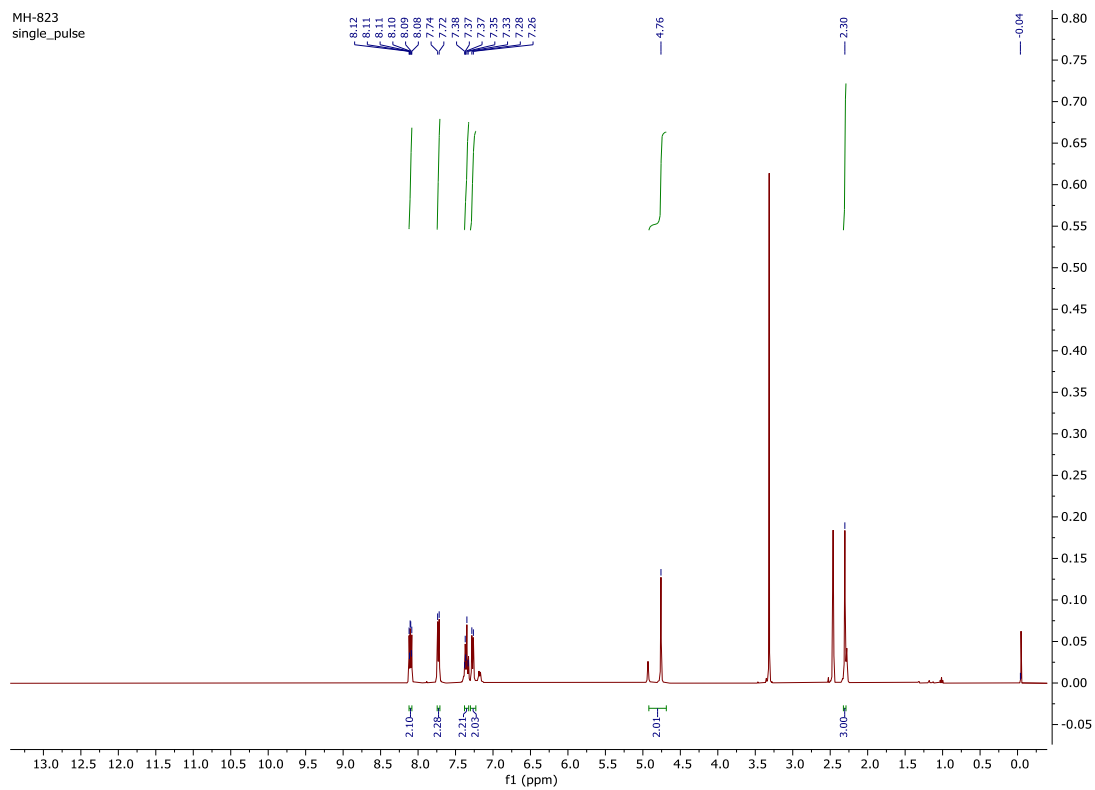


$(^{19}\text{F}-^{13}\text{C})$ HMBC spectrum of compound **14a**

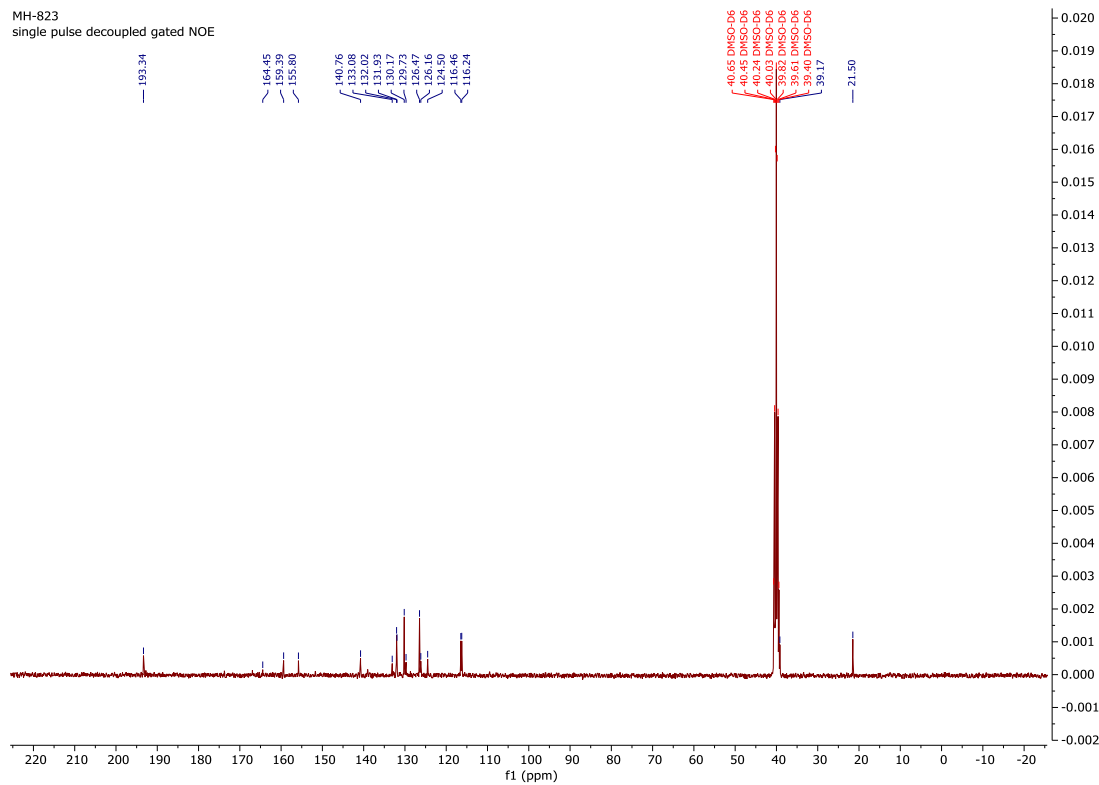


1-Trifluoroacetyl-3-(4-tolyl)-5-((2-oxo-2-(4-fluorophenyl)ethyl)thio)-1,2,4-triazole 14b

¹H of 14b

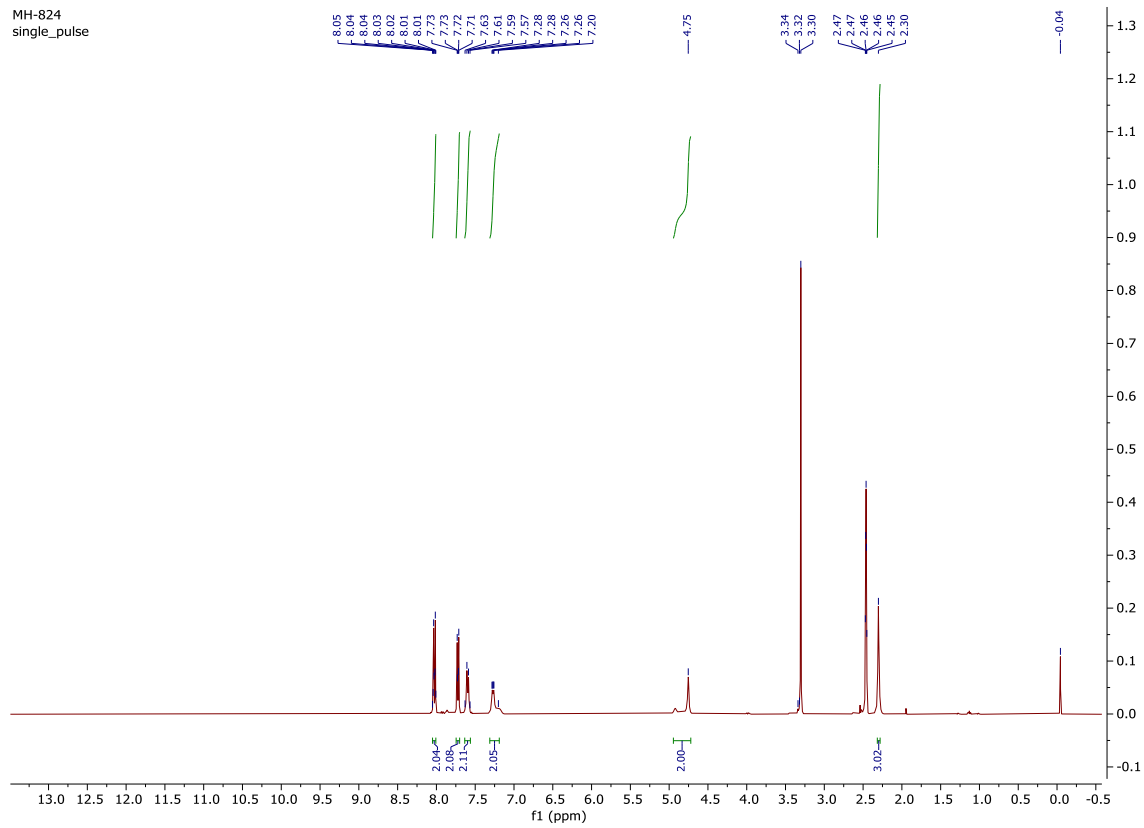


¹³C of 14b

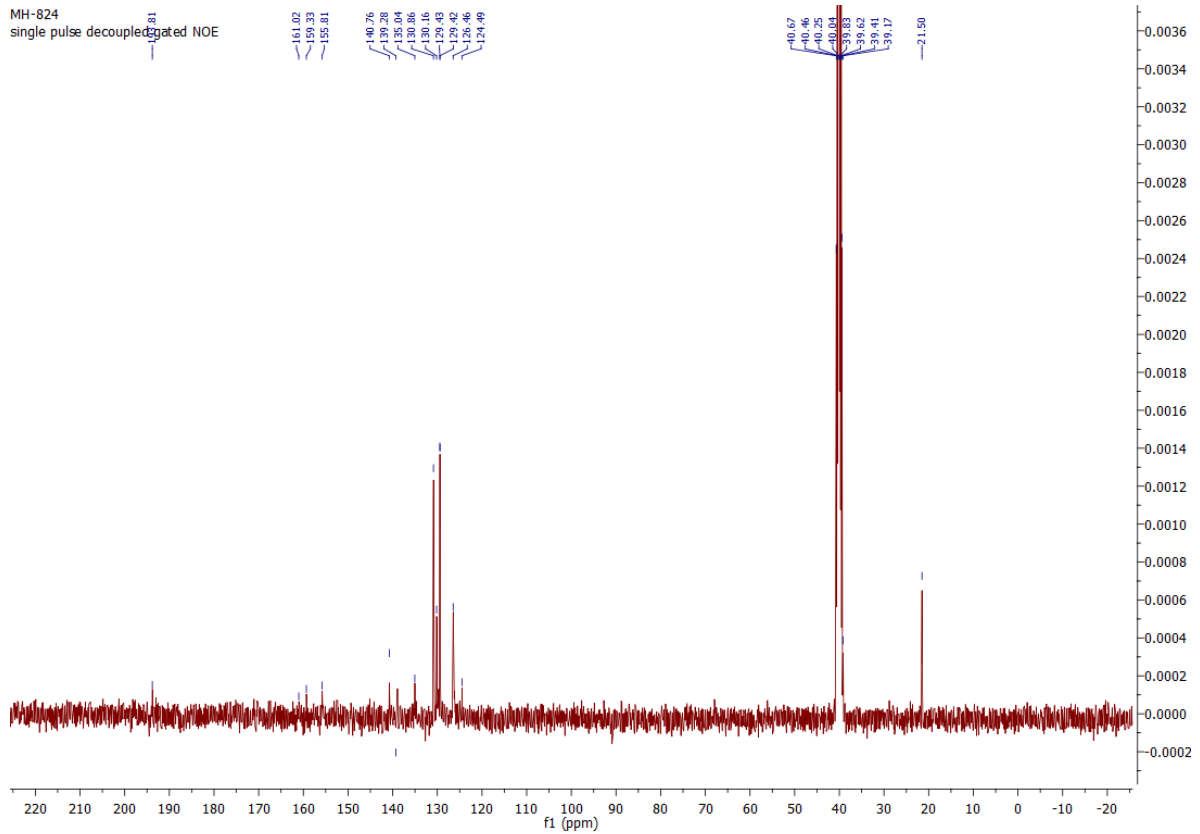


1-Trifluoroacetyl-3-(4-tolyl)-5-((2-oxo-2-(4-chlorophenyl)ethyl)thio)-1,2,4-triazole 14c

¹H of 14c



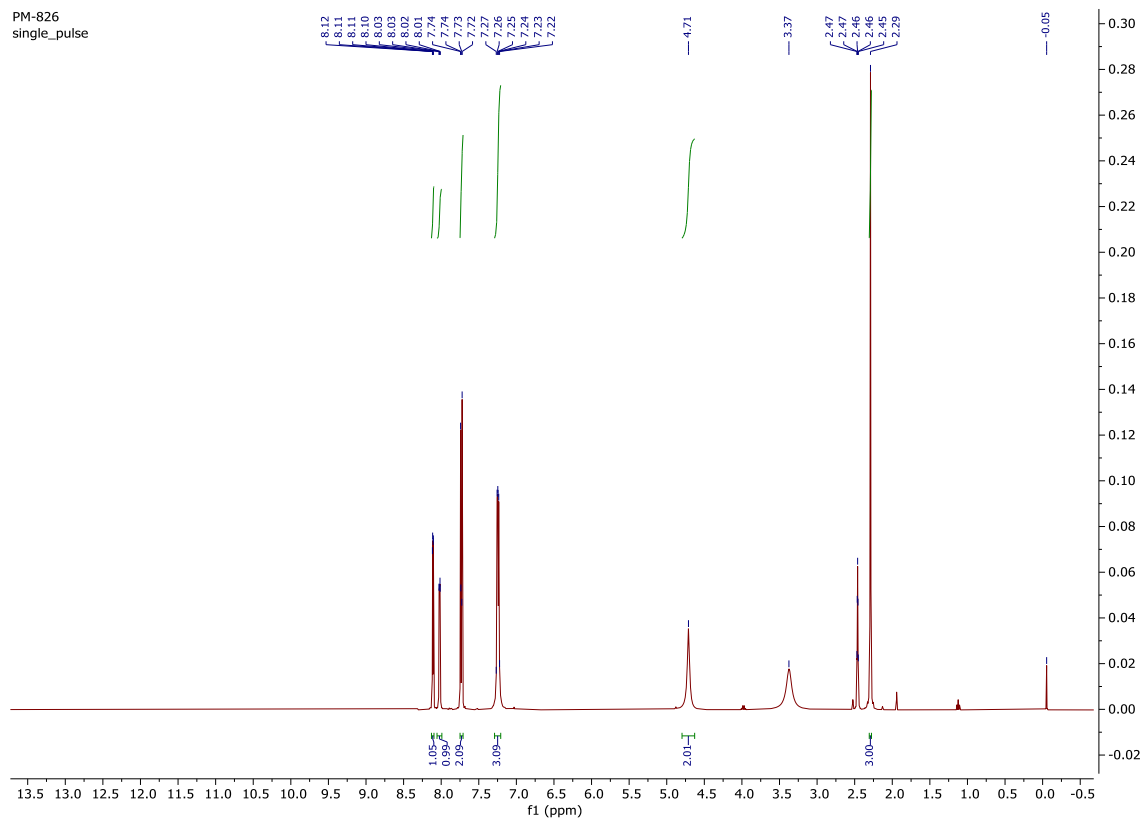
¹³C of 14c



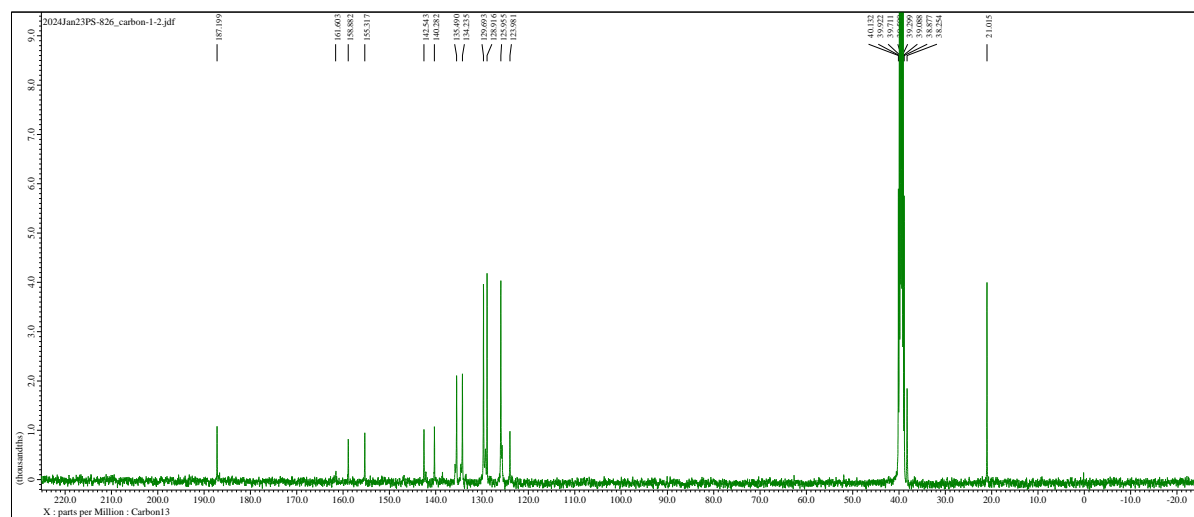
1-Trifluoroacetyl-3-(4-tolyl)-5-((2-oxo-2-(thienyl)ethyl)thio)-1,2,4-triazole 14d

¹H of 14d

PM-826
single_pulse

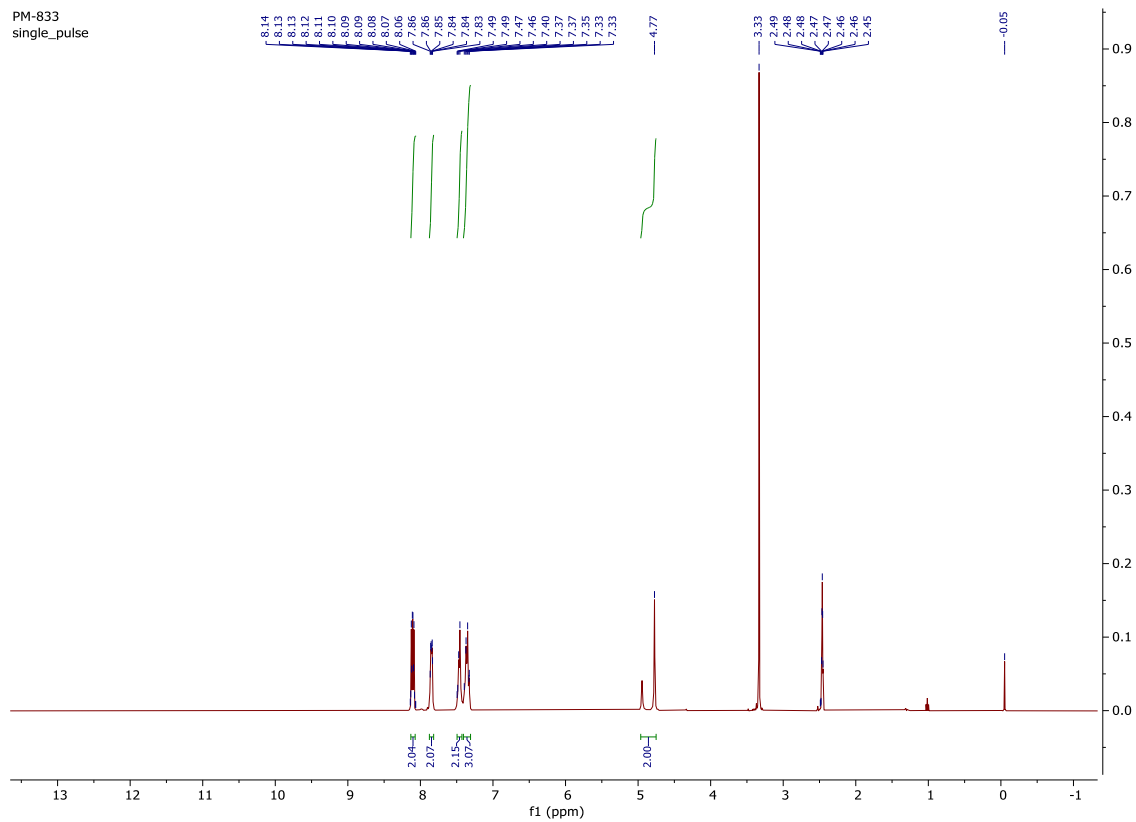


¹³C of 14d

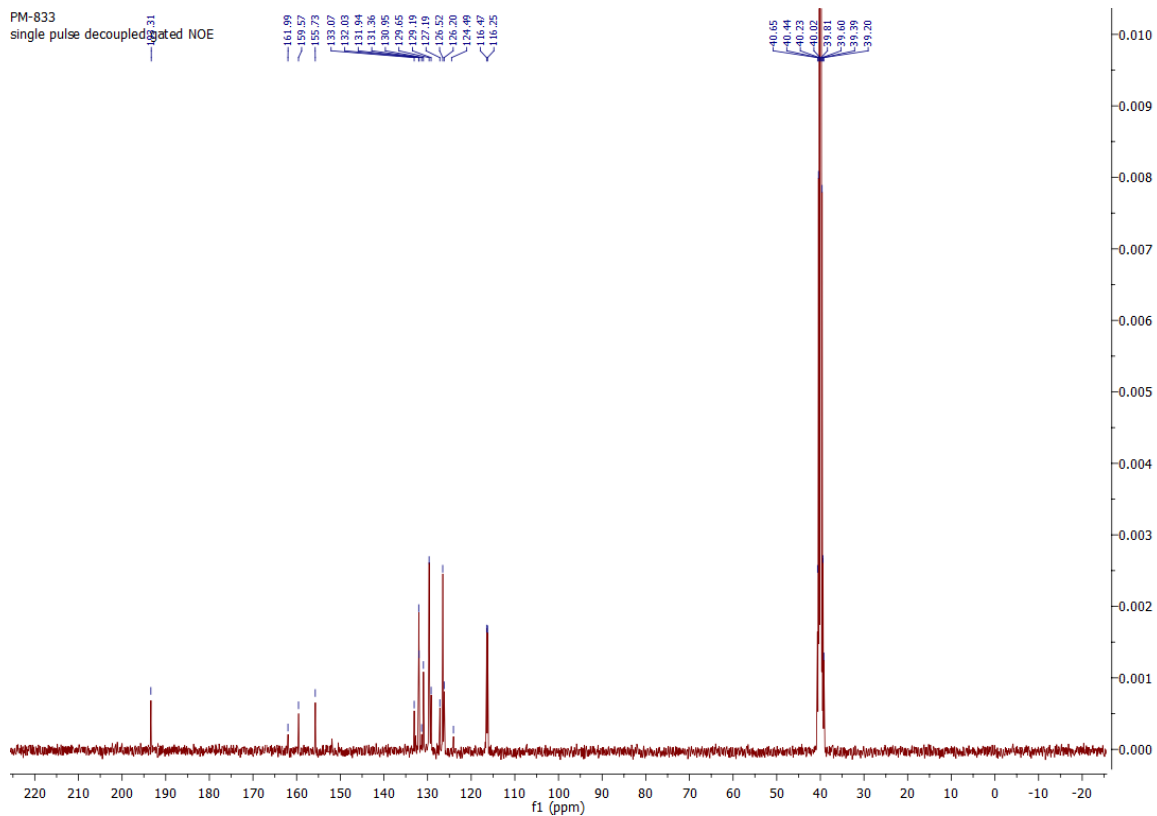


1-Trifluoroacetyl-3-phenyl)-5-((2-oxo-2-(4-fluorophenyl)ethyl)thio)-1,2,4-triazole 14e

¹H of 14e



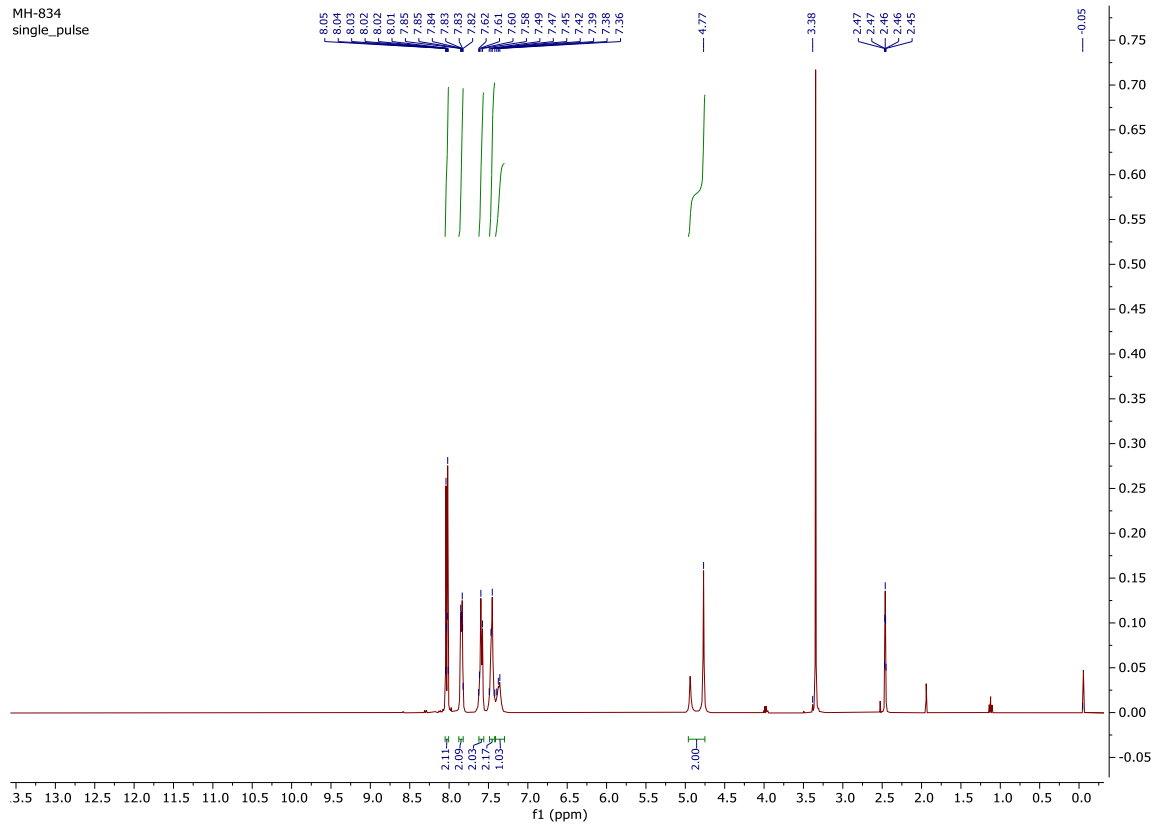
¹³C of 14e



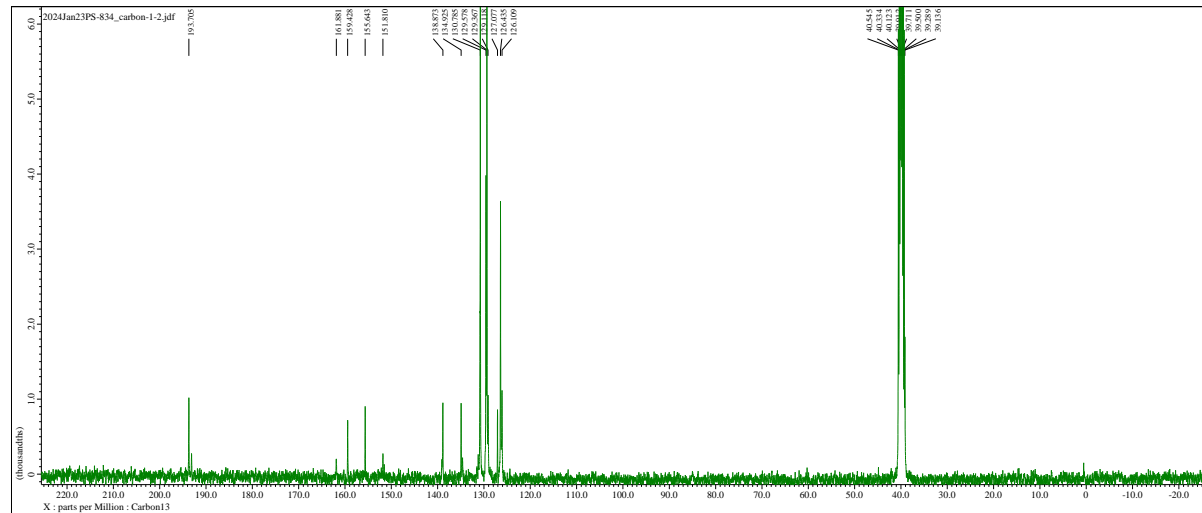
1-Trifluoroacetyl-3-phenyl-5-((2-oxo-2-(4-chlorophenyl)ethyl)thio)-1,2,4-triazole 14f

¹H of 14f

MH-834
single_pulse

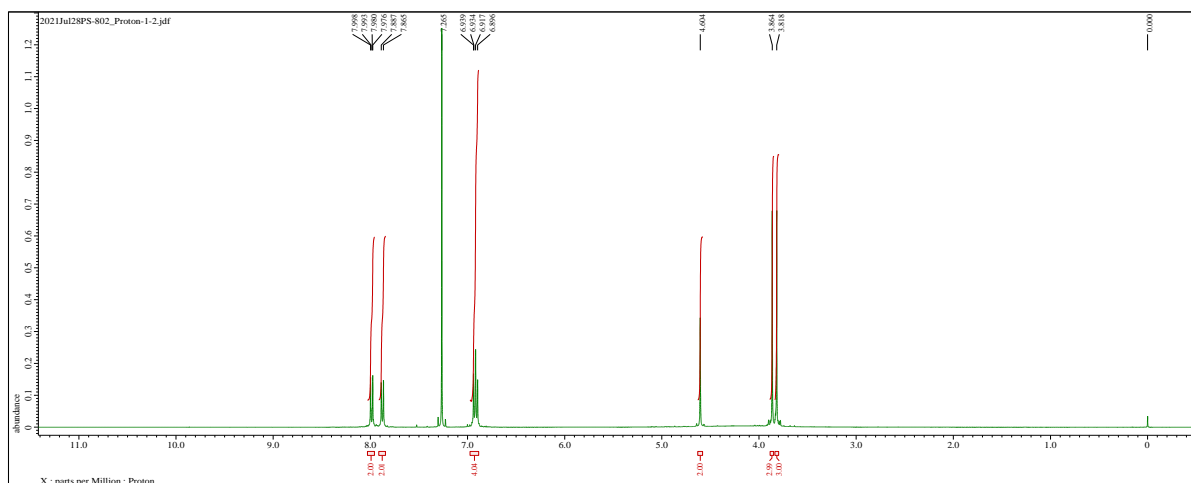


¹³C of 14f

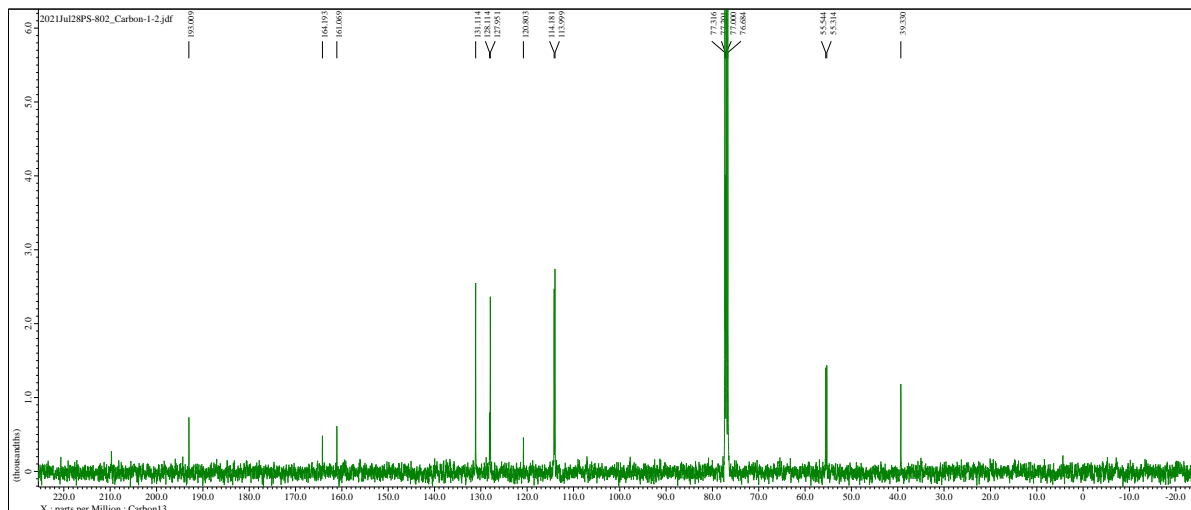


1-Trifluoroacetyl-3-(4-methoxyphenyl)-5-((2-oxo-2-(4-methoxyphenyl)ethyl)thio)-1,2,4-triazole 14k

¹H of 14k

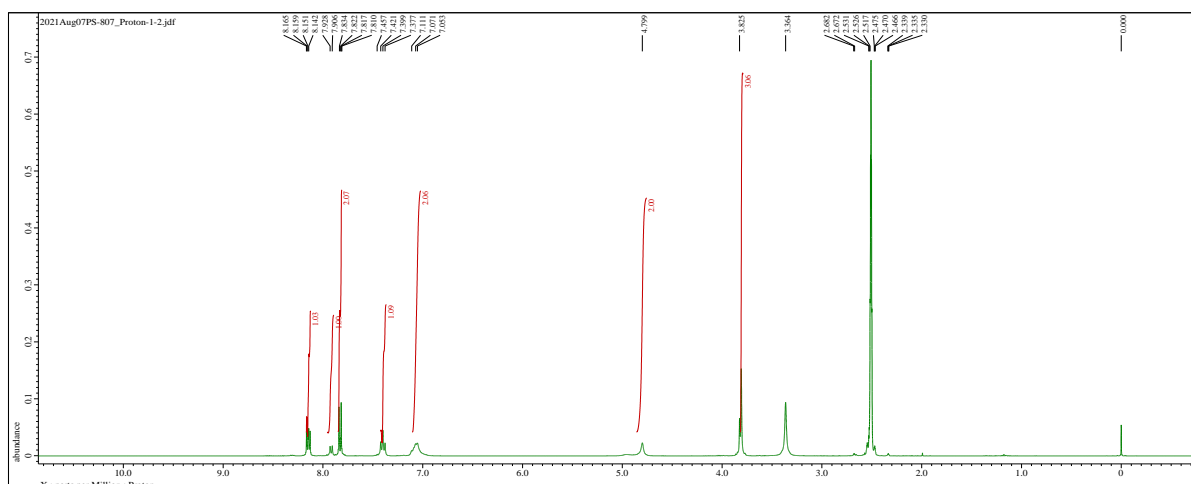


¹³C of 14k

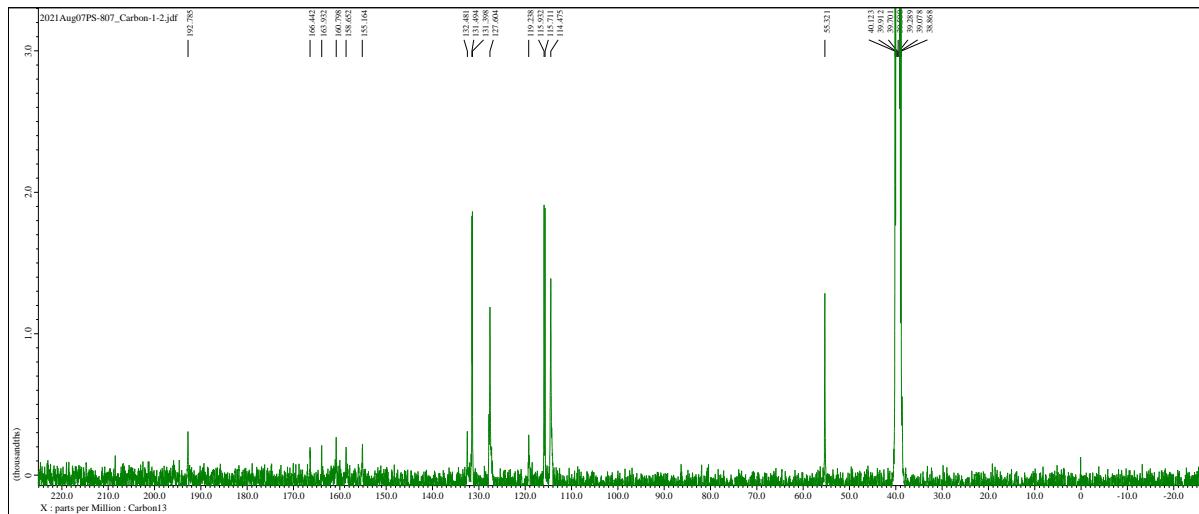


1-Trifluoroacetyl-3-(4-methoxyphenyl)-5-((2-oxo-2-thienylethyl)thio)-1,2,4-triazole 14l

¹H of 14l



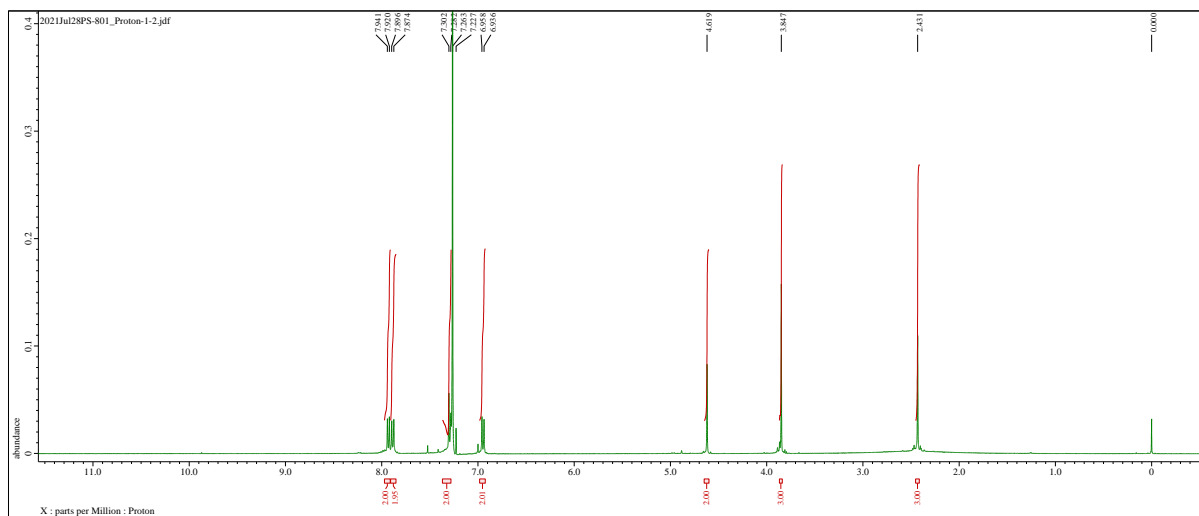
¹³C of 14l



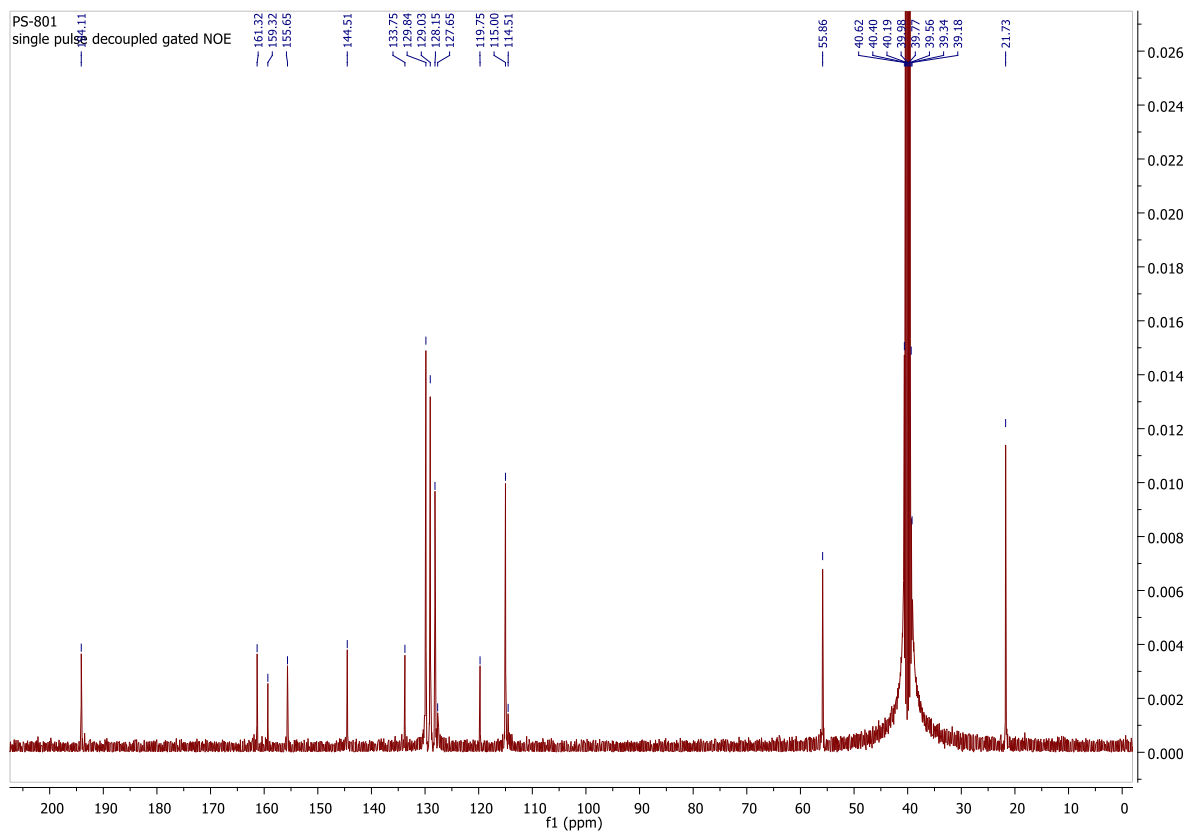
1-Trifluoroacetyl-3-(4-methoxyphenyl)-5-((2-oxo-2-(4-tolyl)ethyl)thio)-1,2,4-triazole

14m

¹H of 14m

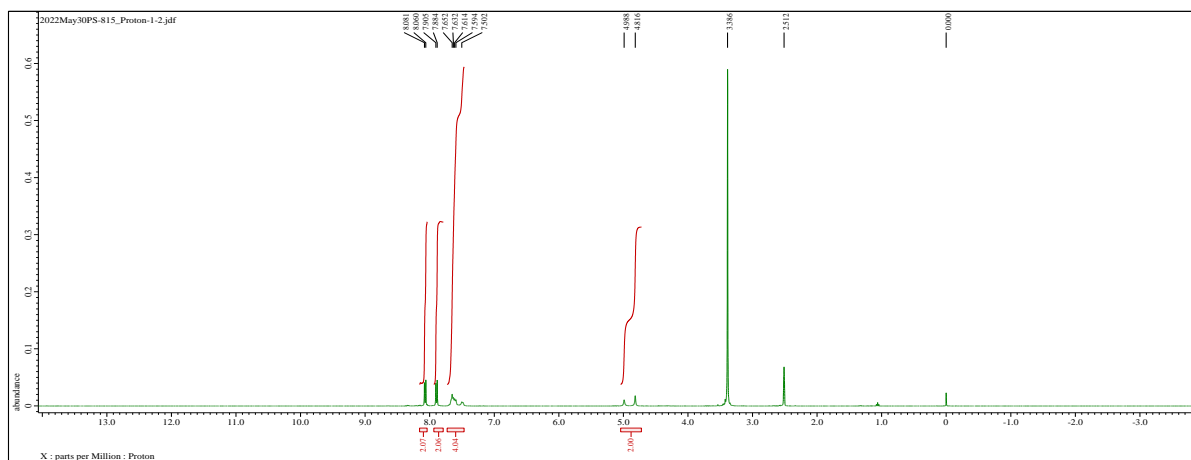


¹³C of 14m

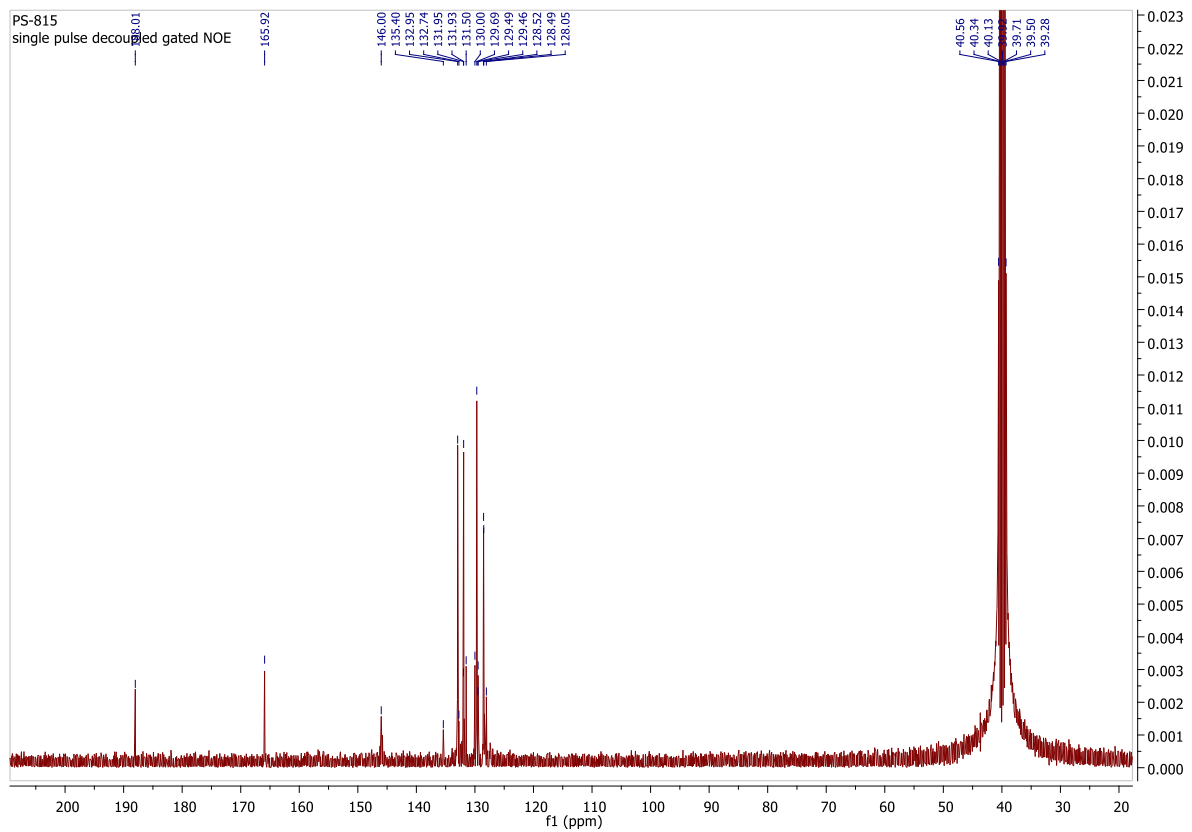


1-Trifluoroacetyl-3-(4-chlorophenyl)-5-((2-oxo-2-(4-bromophenyl)ethyl)thio)-1,2,4-triazole 14n

¹H of 14n

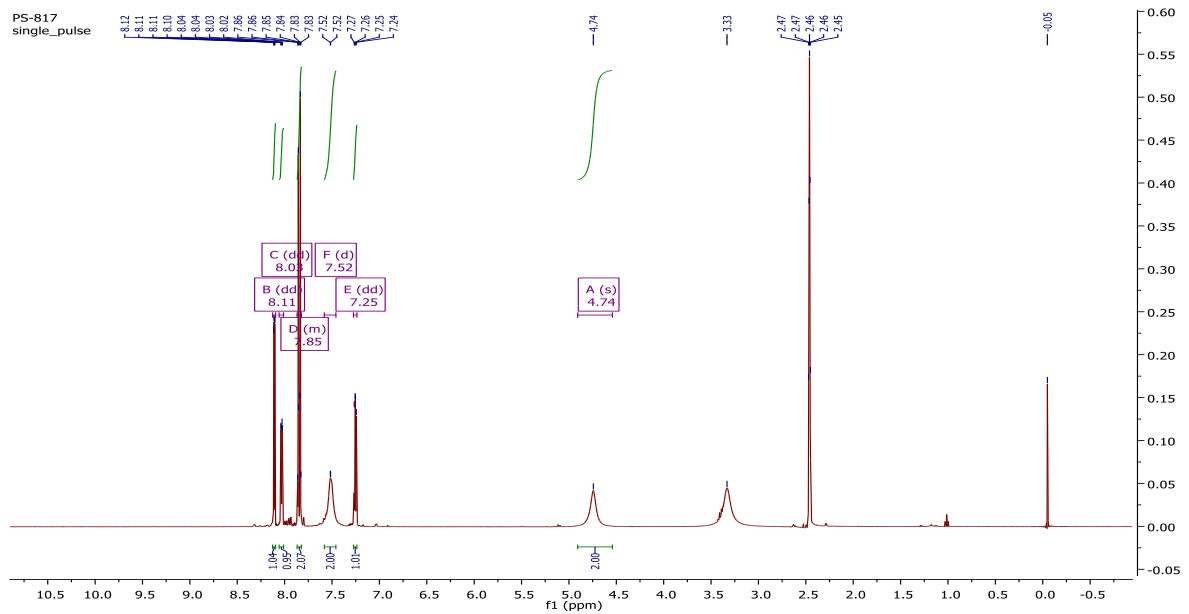


¹³C of 14n



1-Trifluoroacetyl-3-(4-chlorophenyl)-5-((2-oxo-2-thienylethyl)thio)-1,2,4-triazole 14o

¹H of 14o



^{13}C of 14o

