

Electronic Supplementary Information

For

Utilizing perhalopyridine-based alkynes as suitable precursors for the synthesis of novel poly(1,2,3-triazolyl)-substituted perhalopyridines

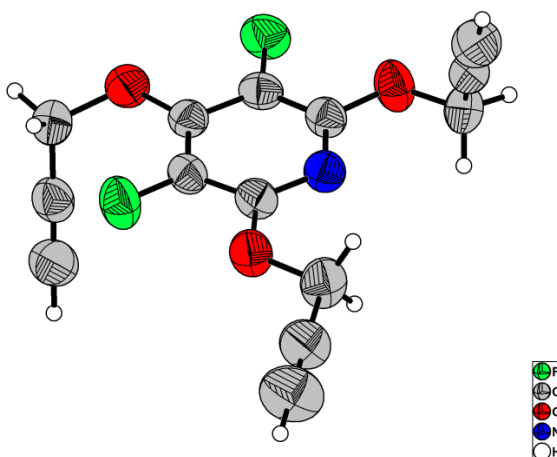
Fereshteh Khorasani^a, Reza Ranjbar-Karimi^{*a} and Kazem Mohammadiannejad^b

^aDepartment of Chemistry, Vali-e-Asr University of Rafsanjan, Rafsanjan 77176, Islamic Republic of Iran.

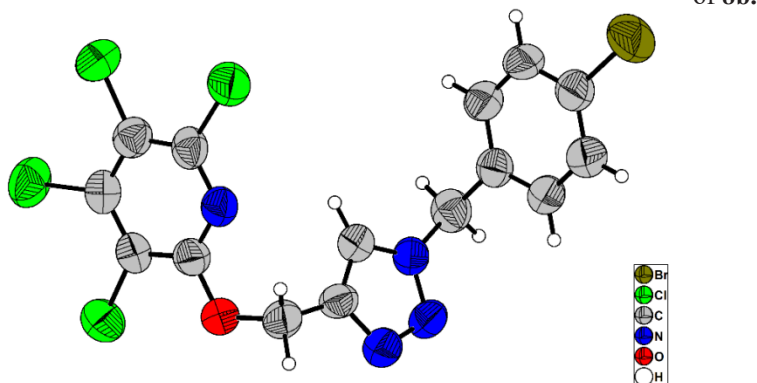
^bNMR Laboratory, Faculty of Science, Vali-e-Asr University of Rafsanjan, Rafsanjan 77176, Islamic Republic of Iran.

*Corresponding author, Fax: +98-343-131-2429; Tel: +98-343-131-2429, E-mail: r.ranjbarkarimi@vru.ac.ir (R. Rnjbar-Karimi).

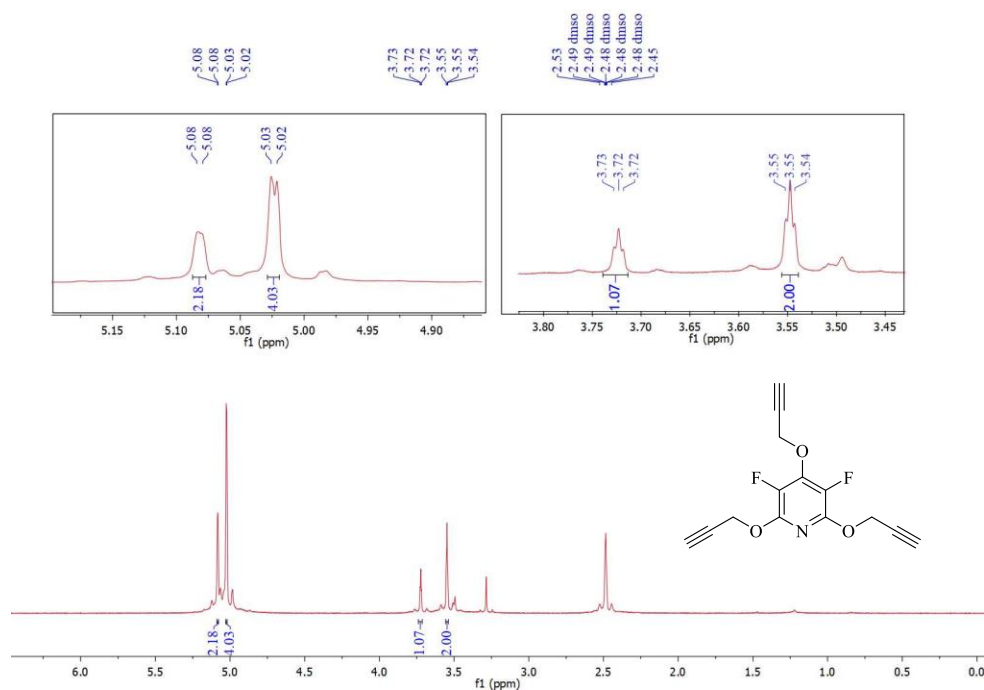
1. Crystal structure of **3a**.



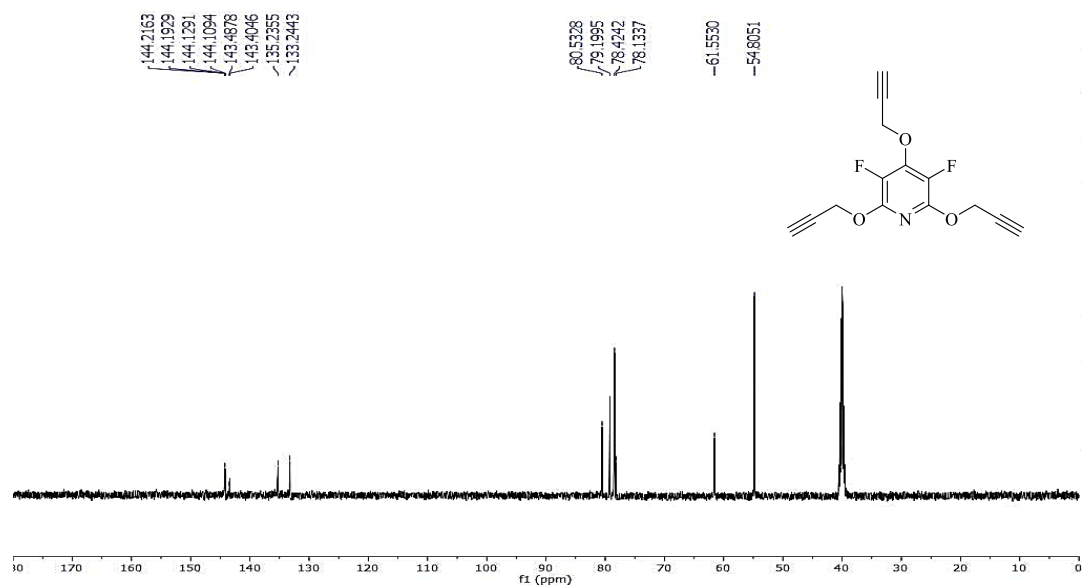
2. Crystal structure



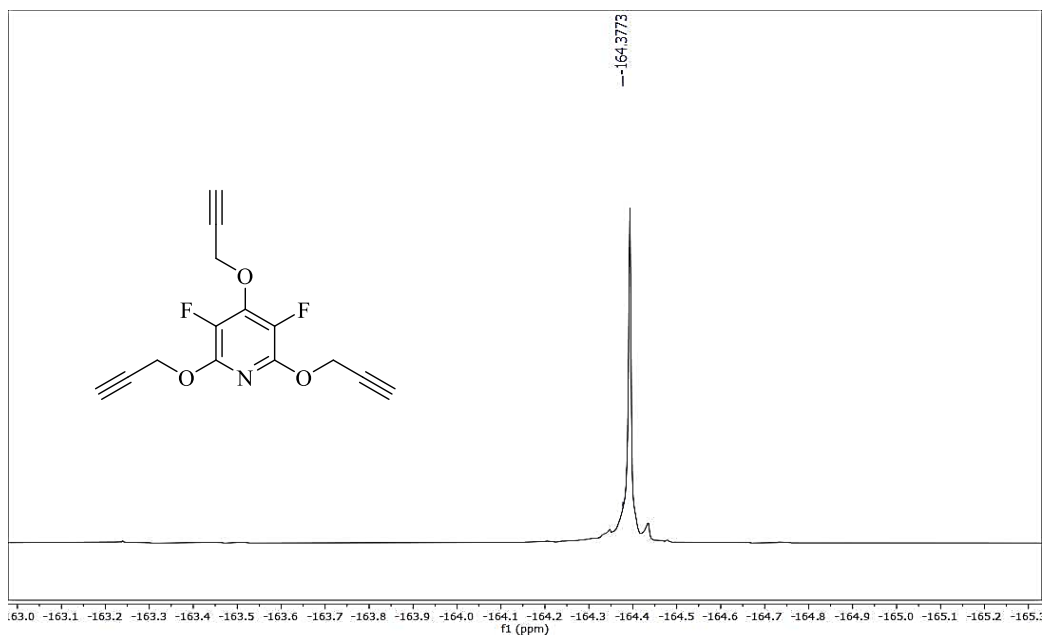
3. NMR spectra of the synthesized compounds **3a-c**



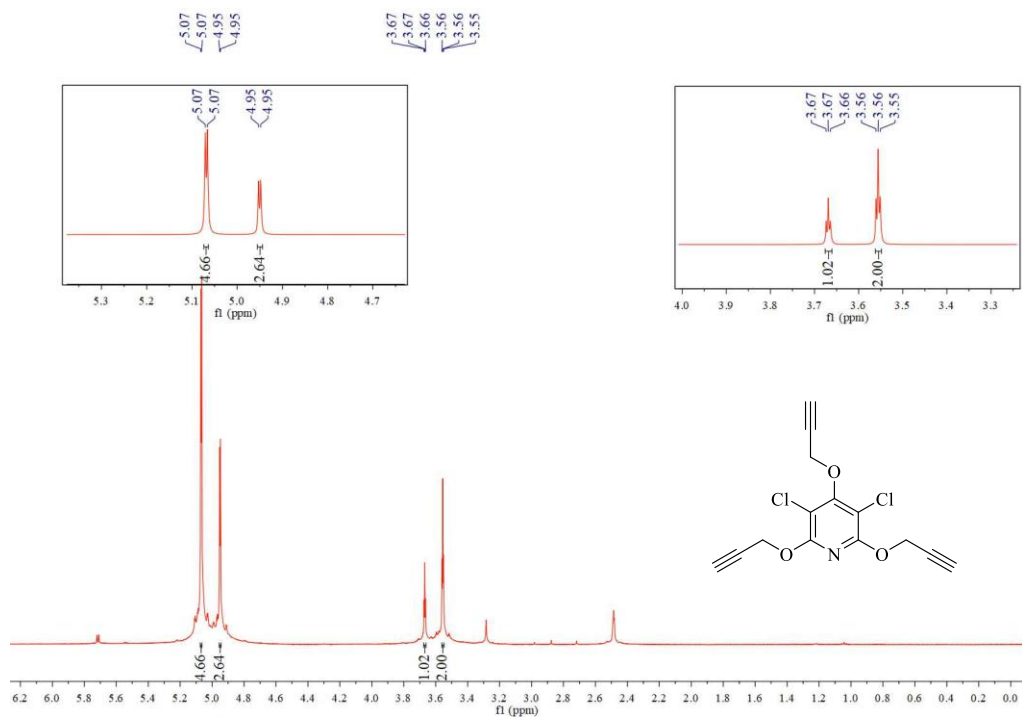
^1H NMR spectrum of 3,5-difluoro-2,4,6-tris(prop-2-yn-1-yloxy)pyridine **3a**



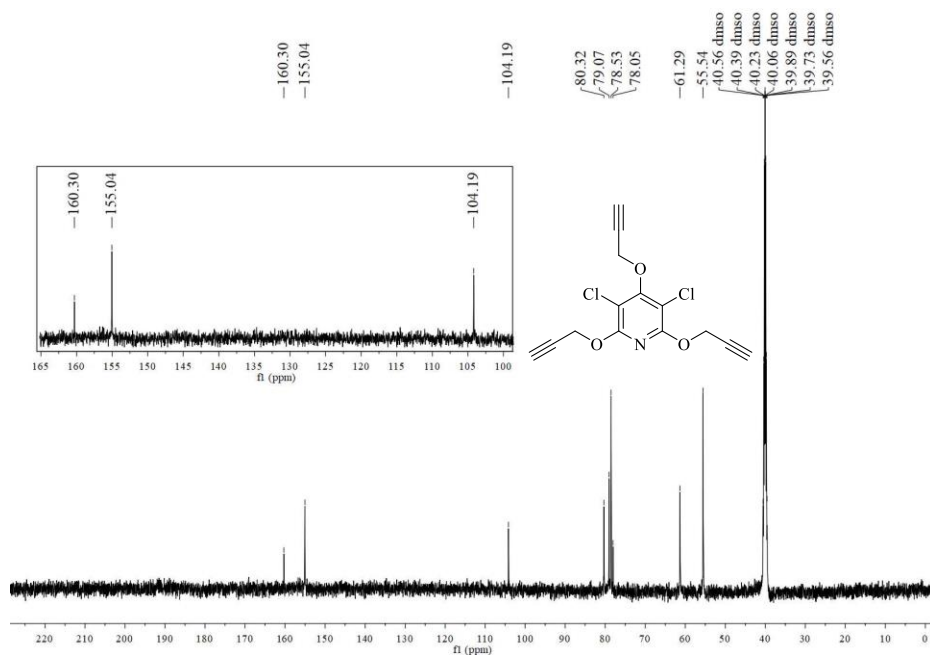
^{13}C NMR spectrum of 3,5-difluoro-2,4,6-tris(prop-2-yn-1-yloxy)pyridine **3a**



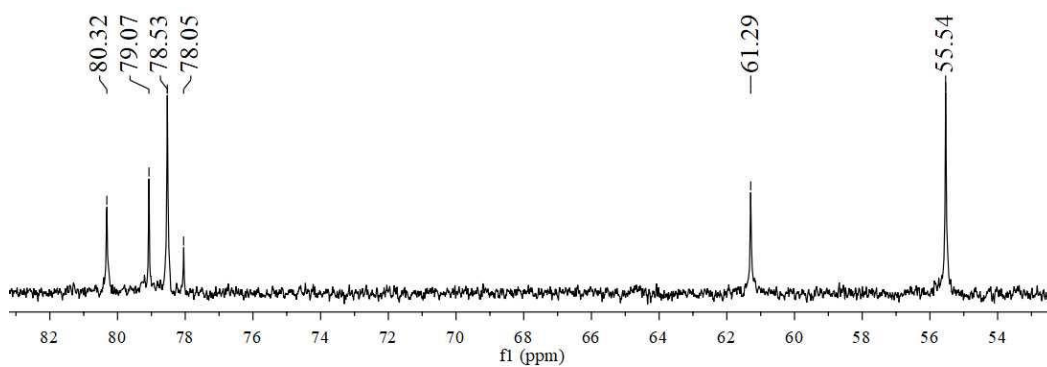
^{19}F NMR spectrum of 3,5-difluoro-2,4,6-tris(prop-2-yn-1-yloxy)pyridine **3a**



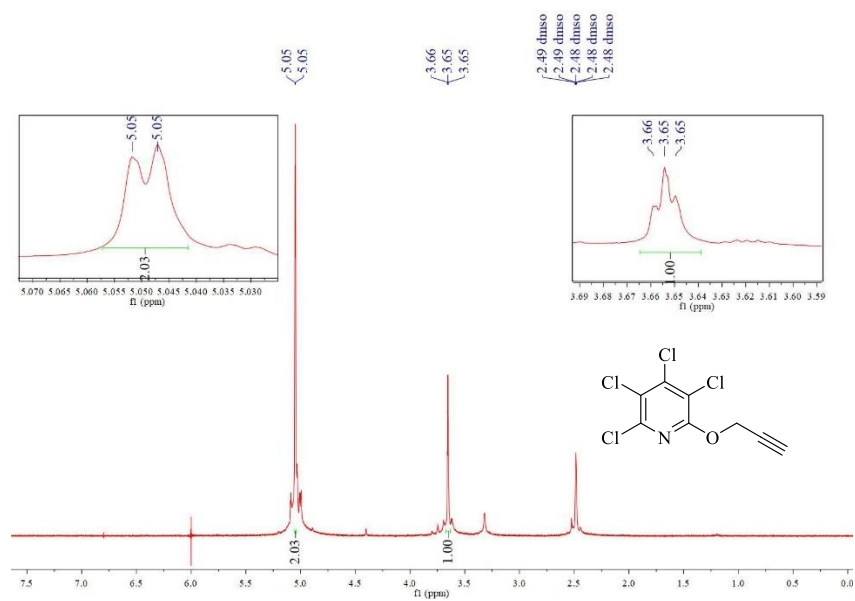
^1H NMR spectrum of 3,5-dichloro-2,4,6-tris(prop-2-yn-1-yloxy)pyridine **3b**



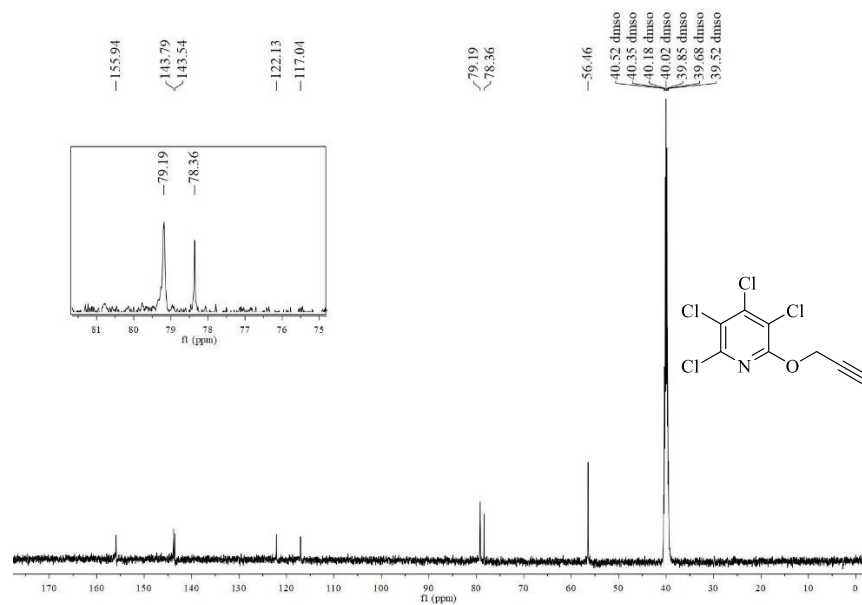
13C NMR spectrum of 3,5-dichloro-2,4,6-tris(prop-2-yn-1-yloxy)pyridine **3b**



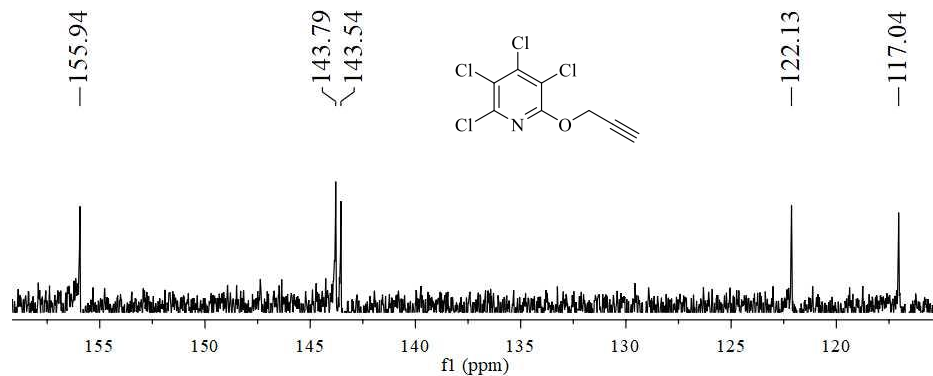
Expanded 13C NMR spectrum of 3,5-dichloro-2,4,6-tris(prop-2-yn-1-yloxy)pyridine **3b**



¹H NMR spectrum of 2,3,4,5-tetrachloro-6-(prop-2-yn-1-yloxy)pyridine **3c**

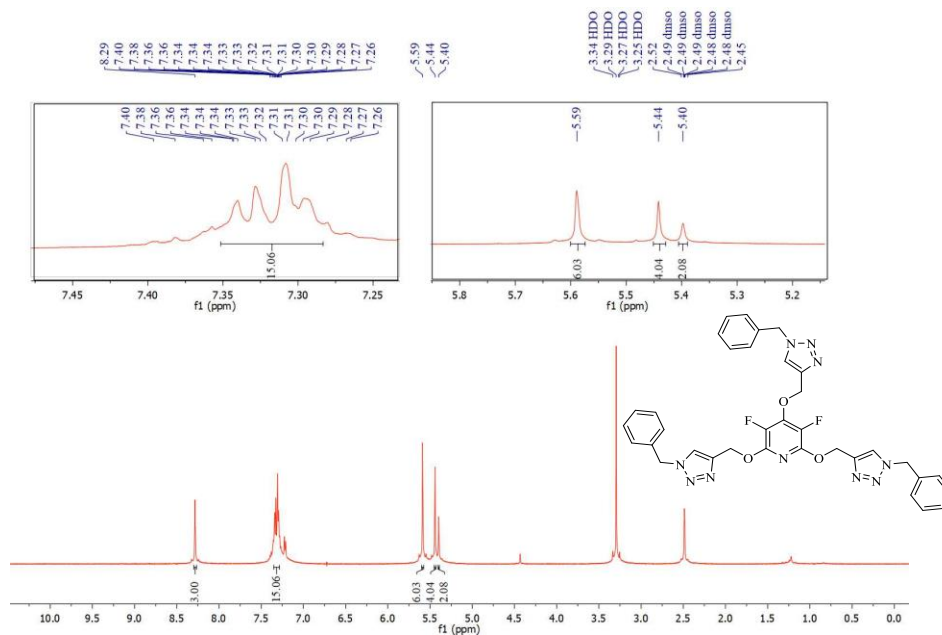


¹³C NMR spectrum of 2,3,4,5-tetrachloro-6-(prop-2-yn-1-yloxy)pyridine **3c**

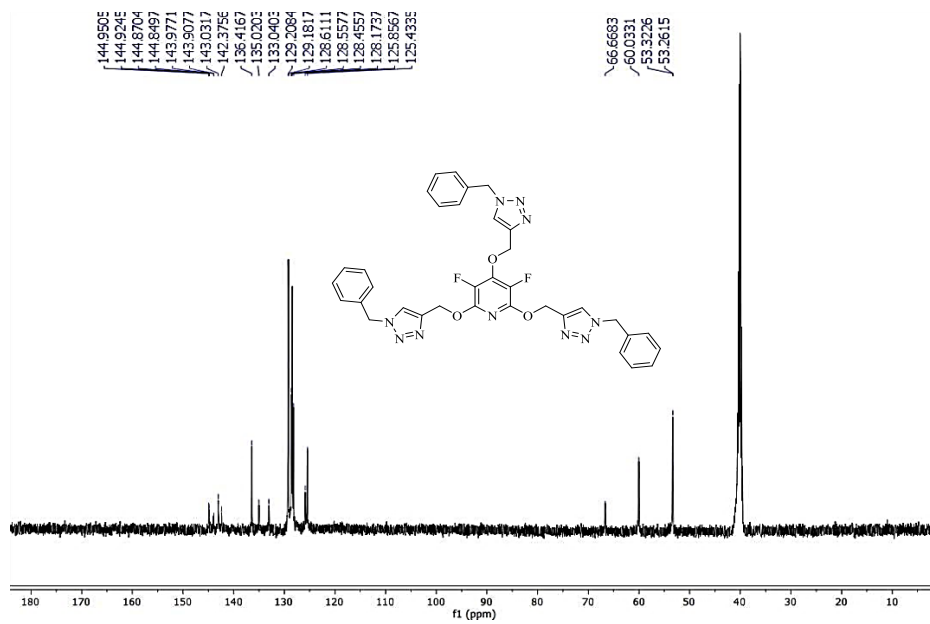


Expanded ¹³C NMR spectrum of 2,3,4,5-tetrachloro-6-(prop-2-yn-1-yloxy)pyridine **3c**

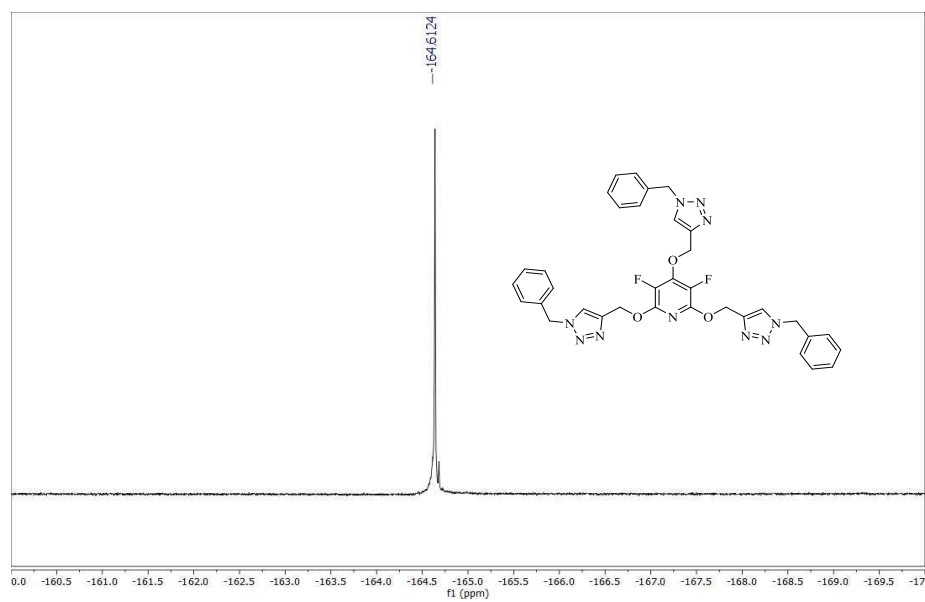
6. NMR spectra of synthesized tris(1,2,3-triazoles) **5a-f** and **7a-d**



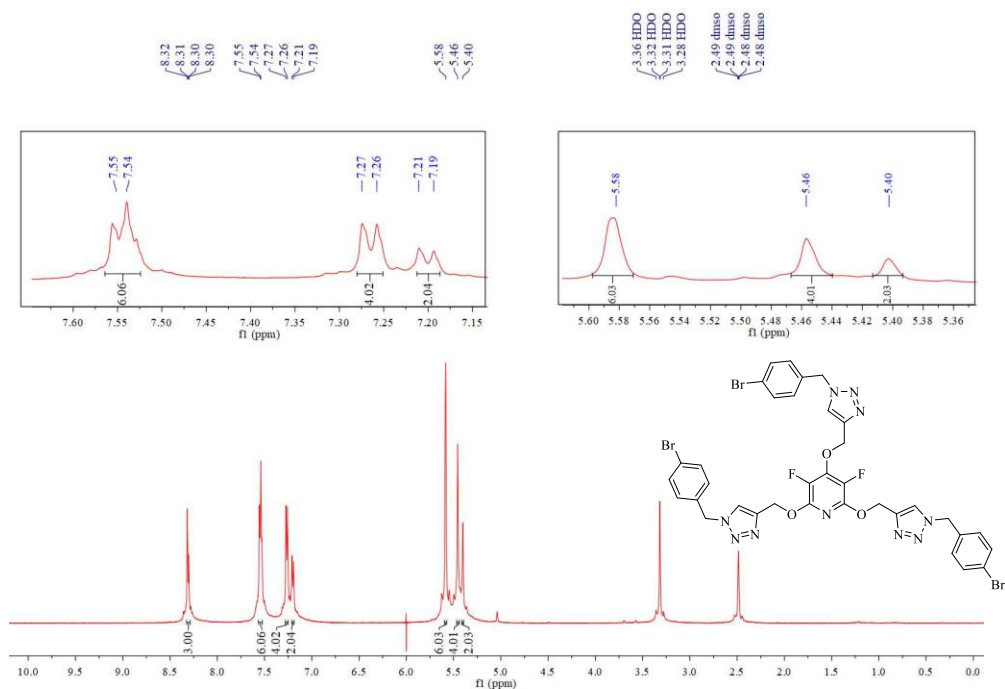
¹H NMR spectrum of 2,4,6-tris((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **5a**



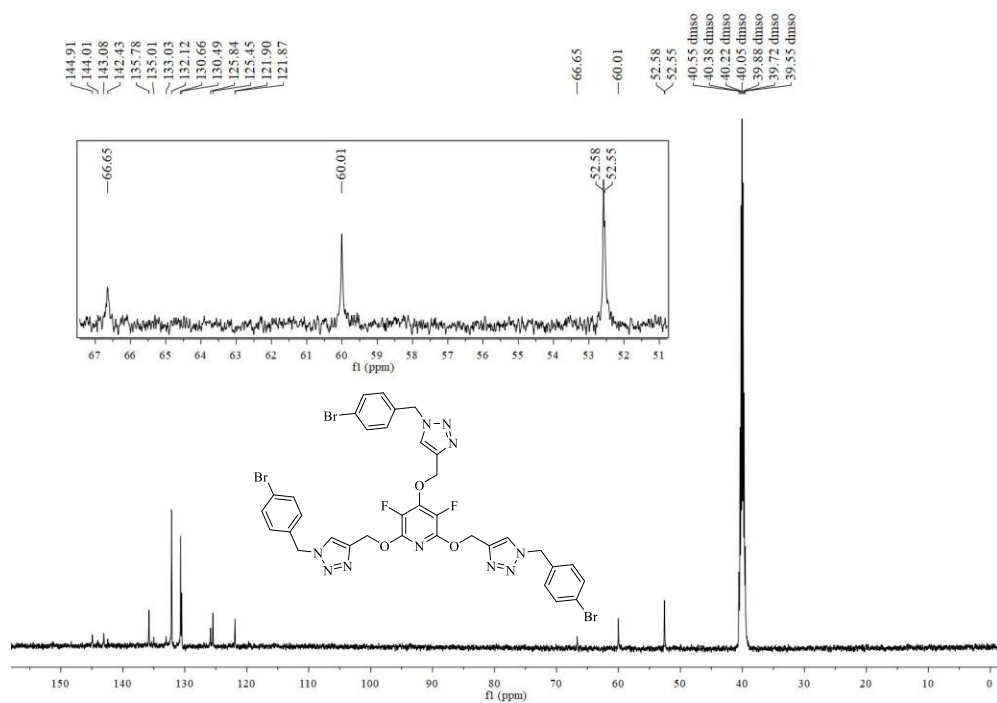
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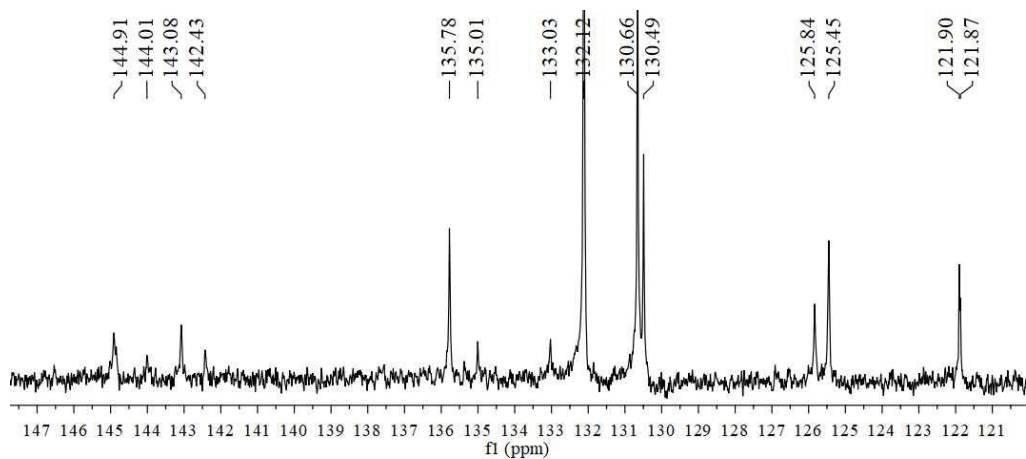
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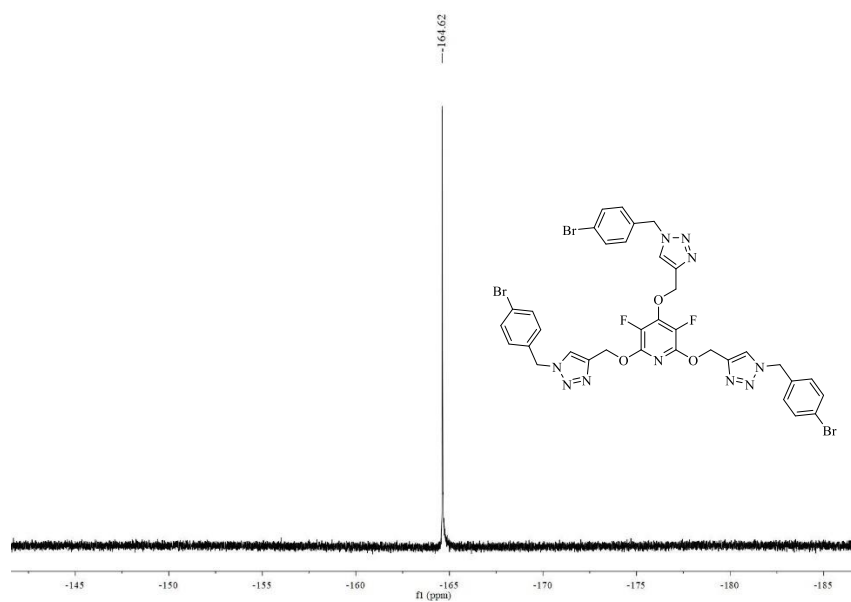
¹H NMR spectrum of 2,4,6-tris((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **5b**



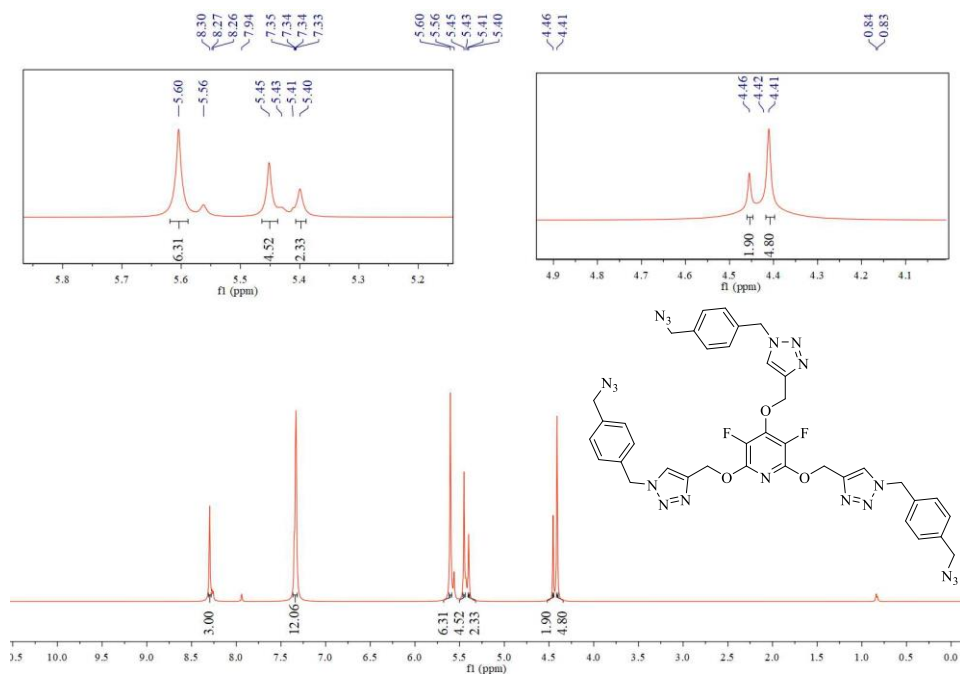
¹³C NMR spectrum of 2,4,6-tris((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **5b**



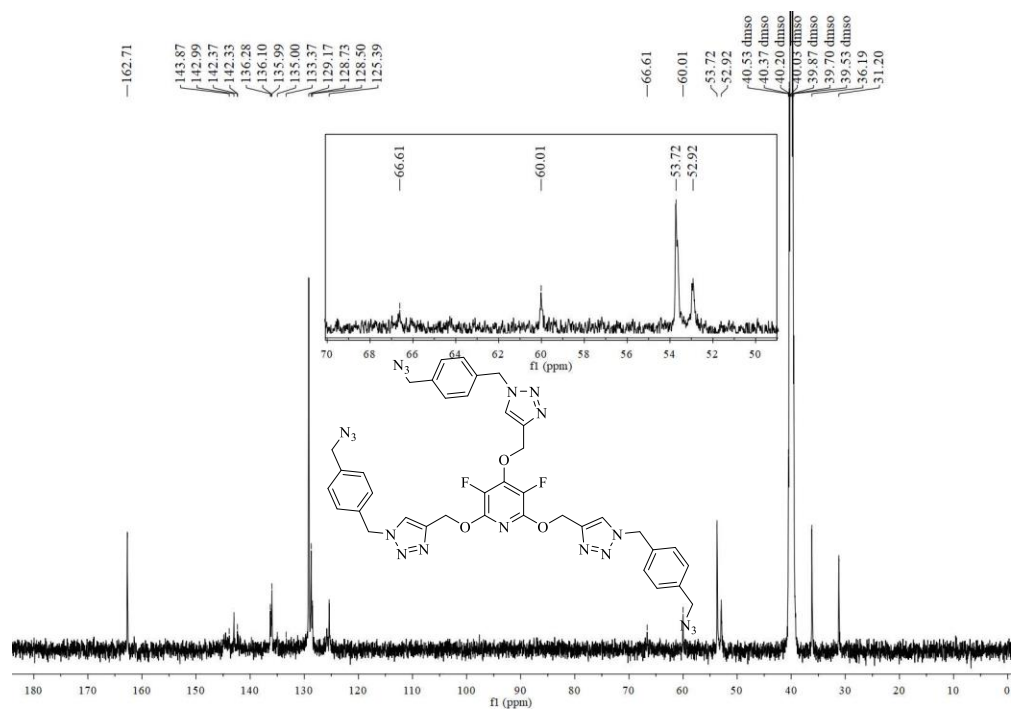
Expanded ^{13}C NMR spectrum of 2,4,6-tris((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **5b**



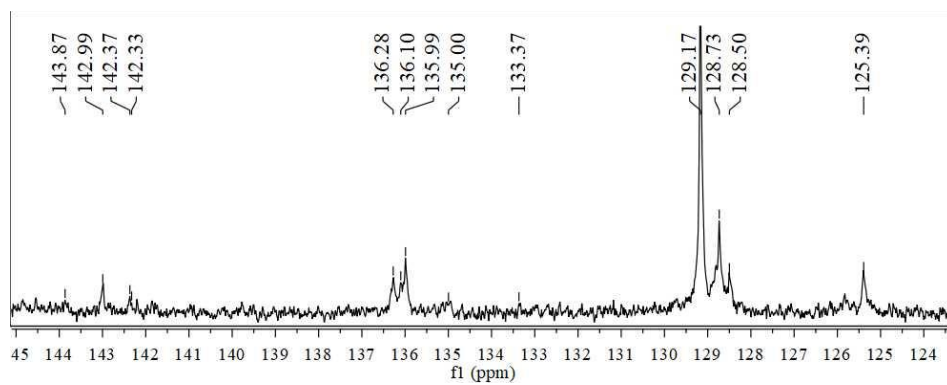
^{19}F NMR spectrum of 2,4,6-tris((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **5b**



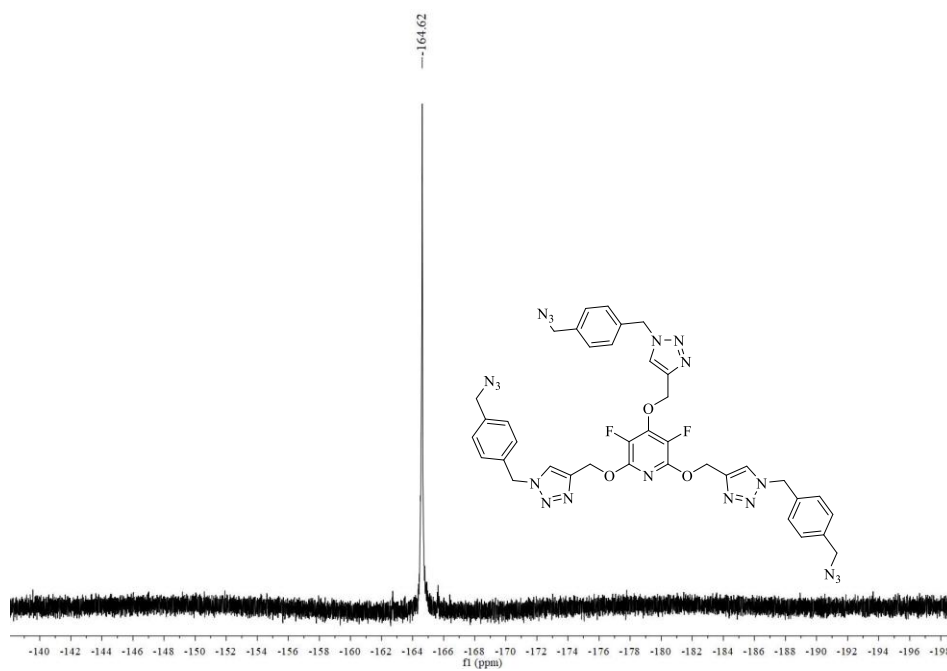
¹H NMR spectrum of 2,4,6-tris((1-(4-(azidomethyl)benzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **5c**



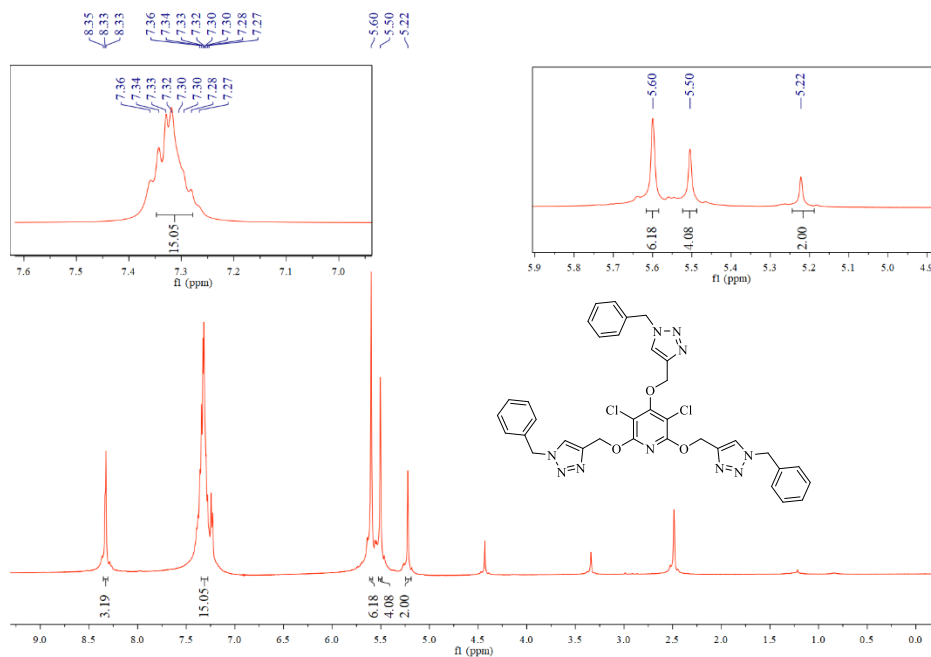
¹³C NMR spectrum of 2,4,6-tris((1-(4-(azidomethyl)benzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **5c**



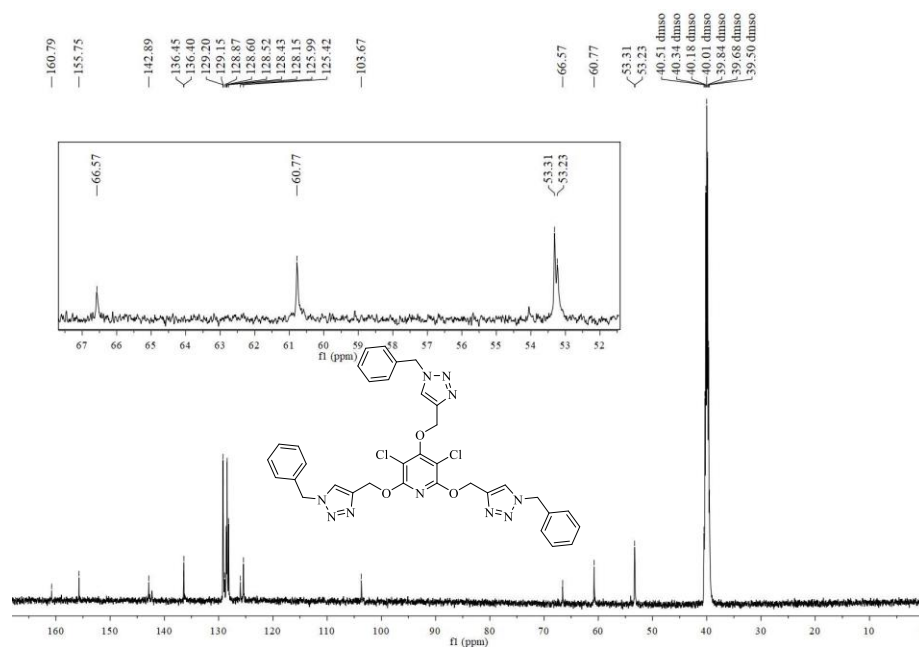
Expanded ^{13}C NMR spectrum of 2,4,6-tris((1-(4-(azidomethyl)benzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **5c**



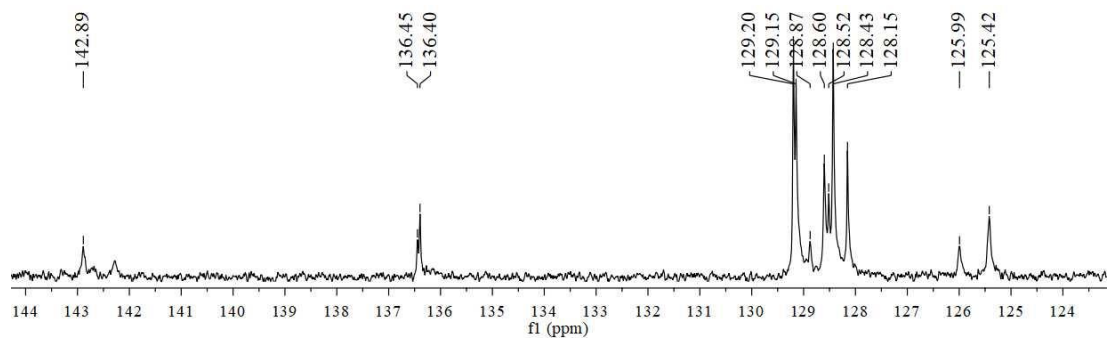
^{19}F NMR spectrum of 2,4,6-tris((1-(4-(azidomethyl)benzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **5c**



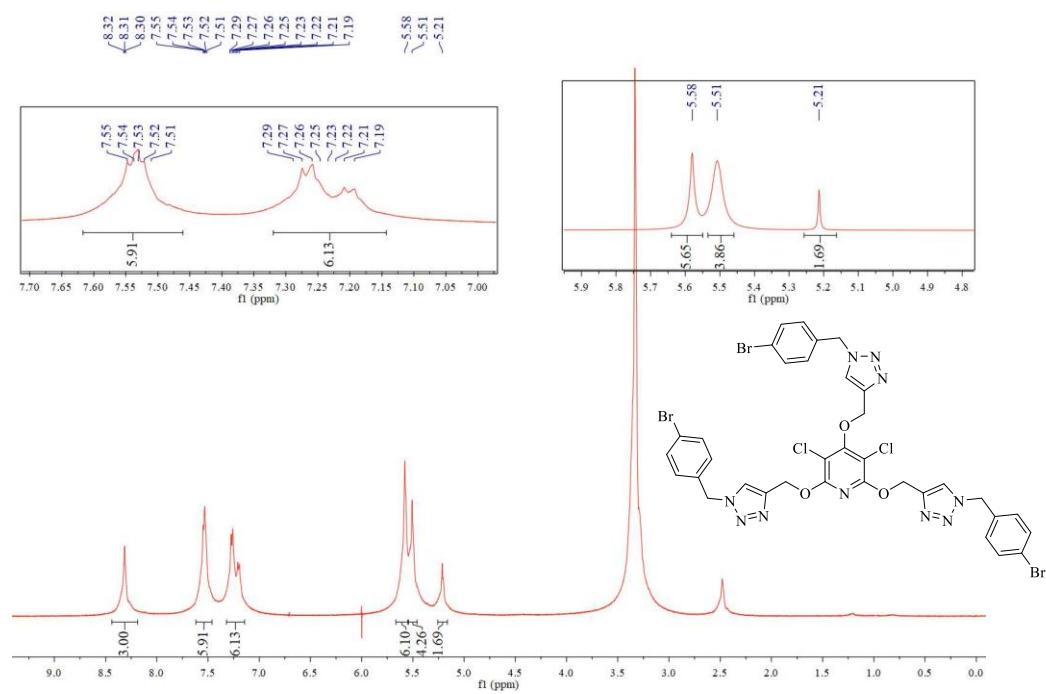
¹H NMR spectrum of 2,4,6-tris((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)-3,5-dichloropyridine **5d**



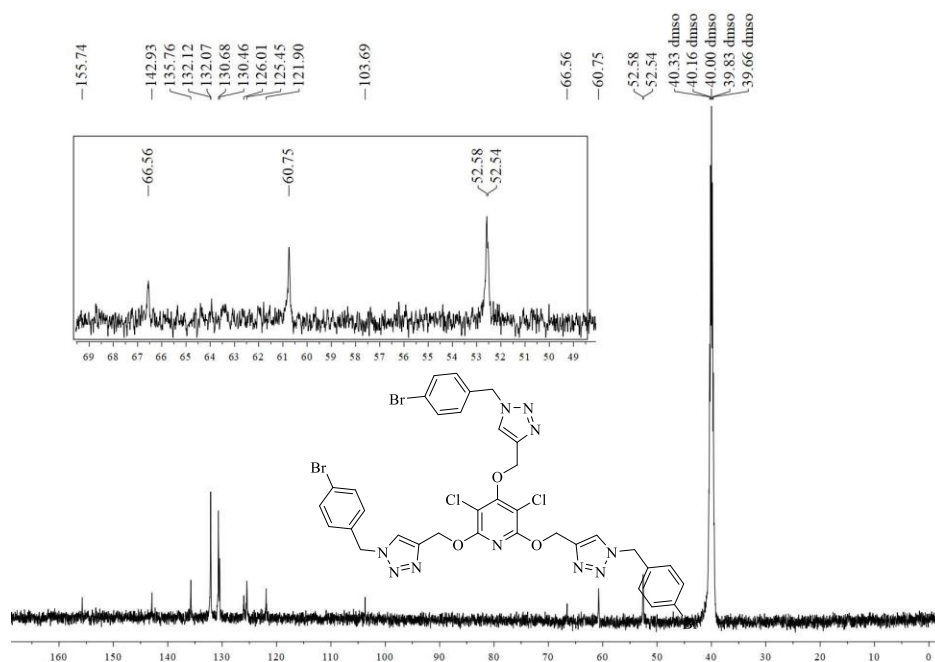
¹³C NMR spectrum of 2,4,6-tris((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)-3,5-dichloropyridine **5d**



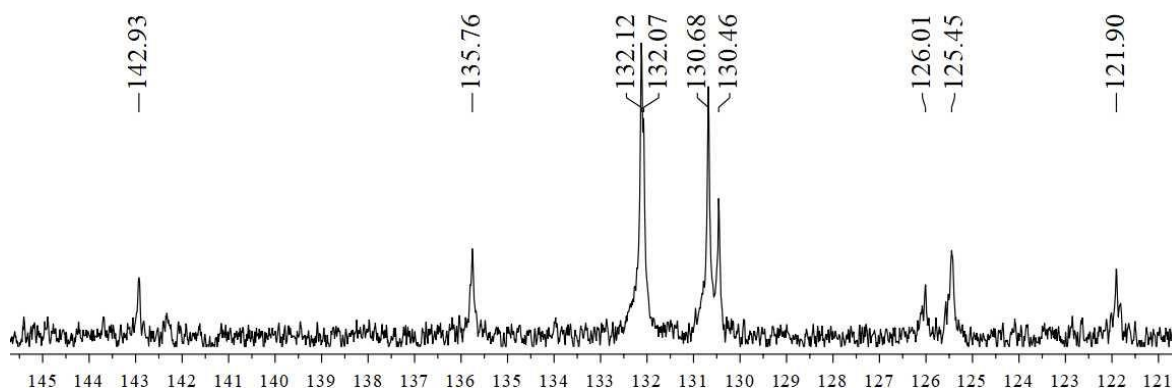
Expanded ^{13}C NMR spectrum of 2,4,6-tris((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)-3,5-dichloropyridine **5d**



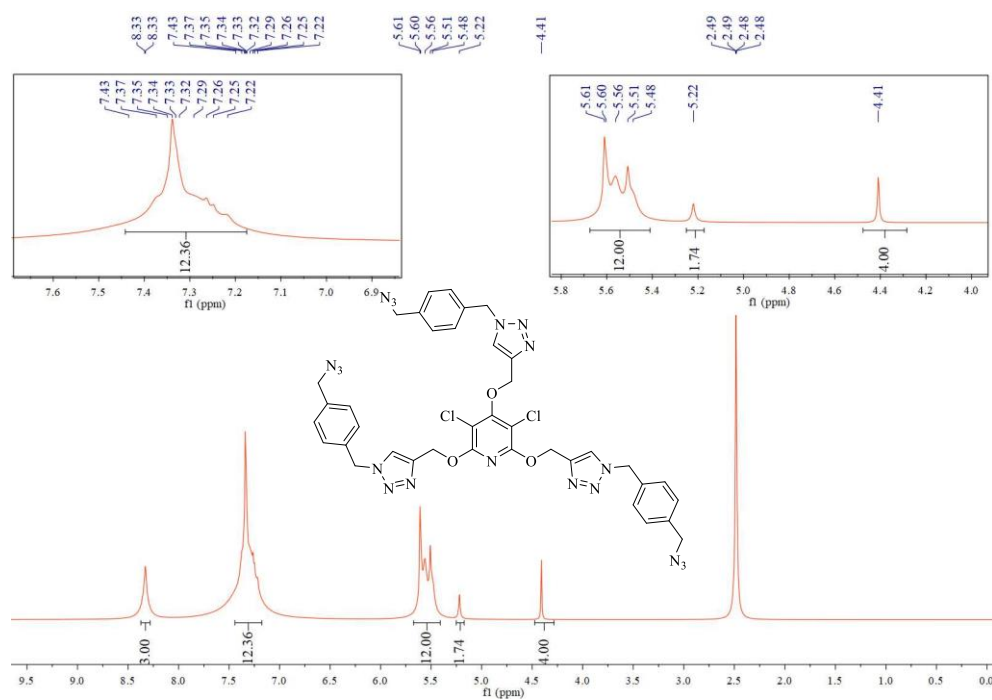
^1H NMR spectrum of 2,4,6-tris((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-dichloropyridine **5e**



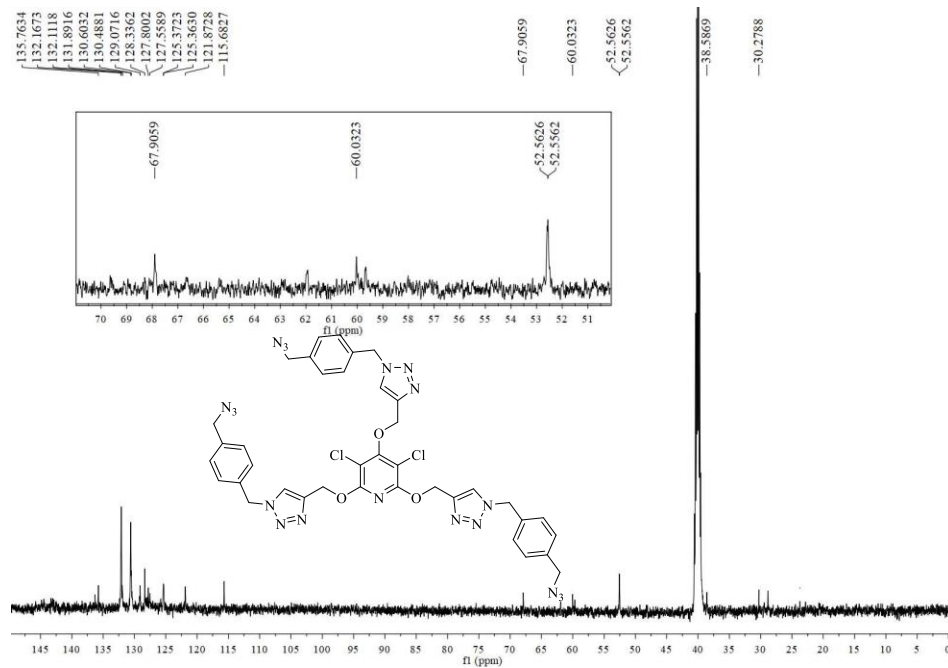
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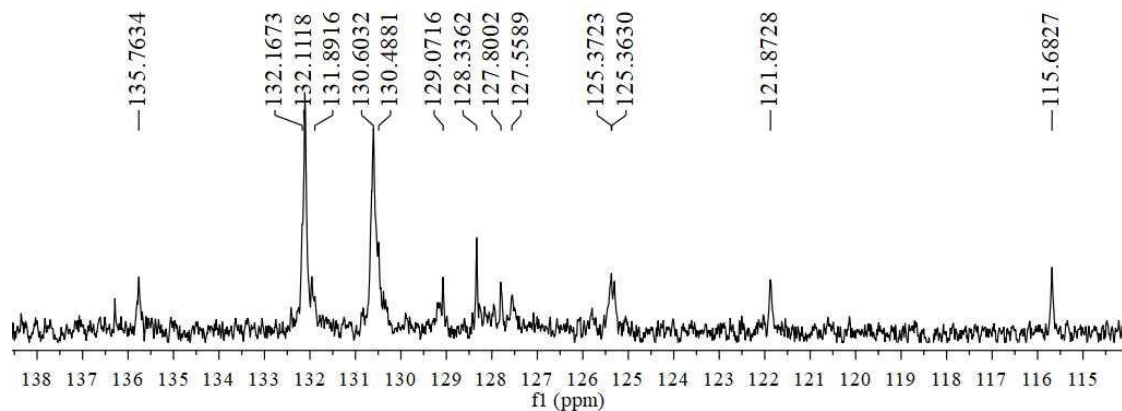
Expanded ¹³C NMR spectrum of 2,4,6-tris((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-dichloropyridine **5e**



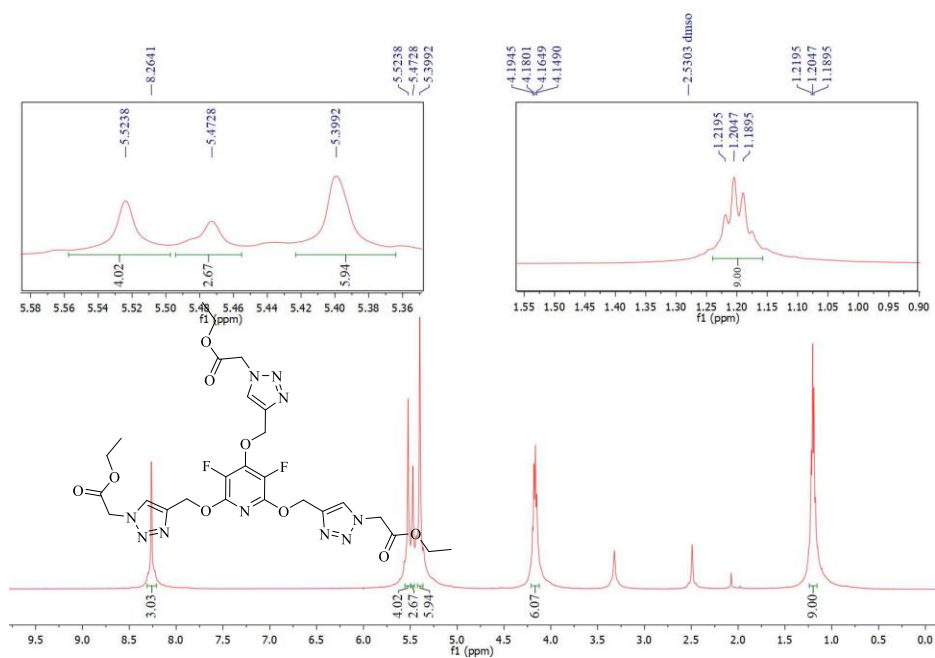
¹H NMR spectrum of 2,4,6-tris((1-(4-(azidomethyl)benzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-dichloropyridine **5f**



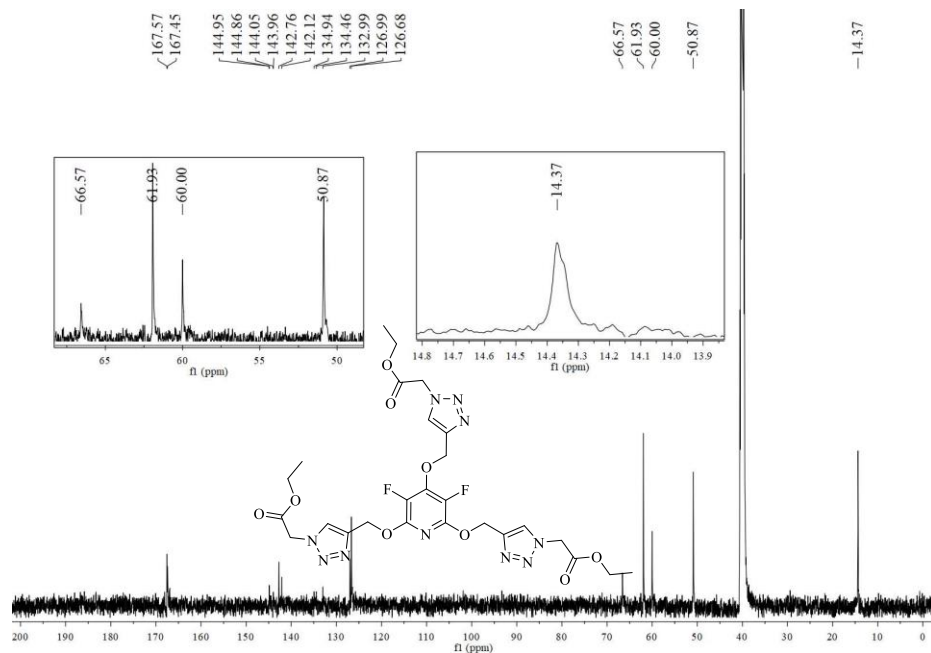
¹³C NMR spectrum of 2,4,6-tris((1-(4-(azidomethyl)benzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-dichloropyridine **5f**



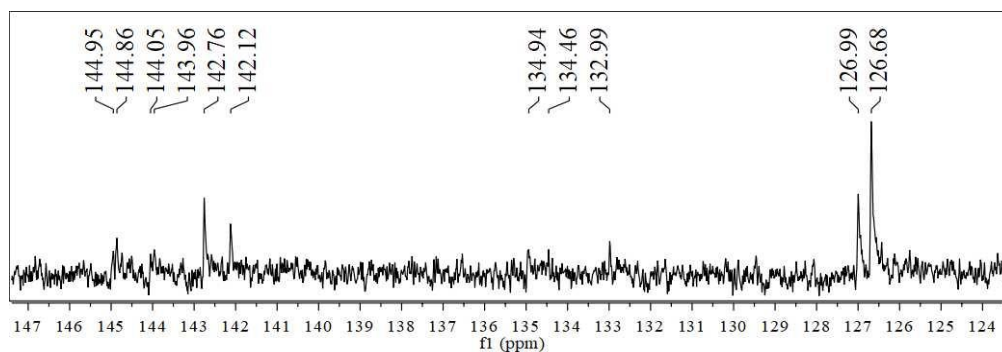
Expanded ^{13}C NMR spectrum of 2,4,6-tris((1-(4-(azidomethyl)benzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-dichloropyridine **5f**



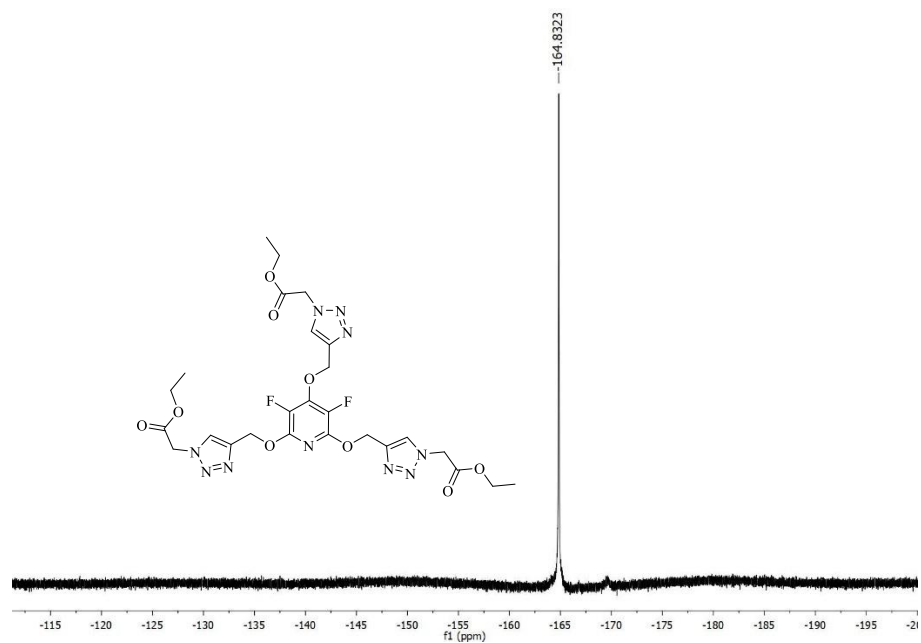
^1H NMR spectrum of triethyl 2,2',2''-(((3,5-difluoropyridine-2,4,6-triyl)tris(oxy))tris(methylene))tris(1H-1,2,3-triazole-4,1-diyl))triacetate **7a**



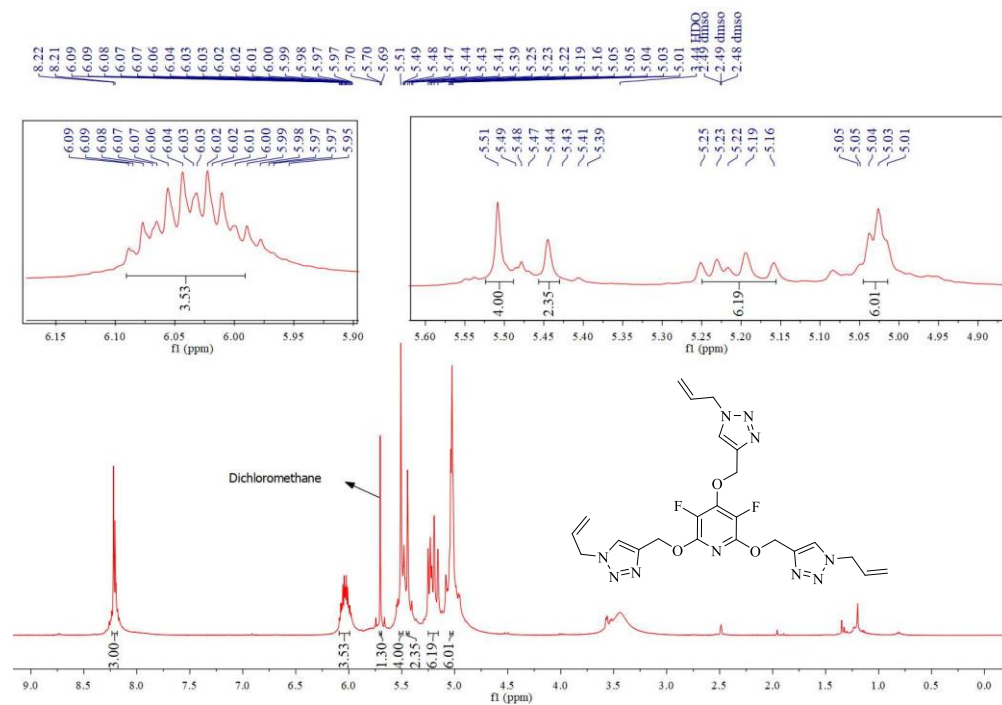
¹³C NMR spectrum of triethyl 2,2',2''-(((3,5-difluoropyridine-2,4,6-triyl)tris(oxy))tris(methylene))tris(1H-1,2,3-triazole-4,1-diyl))triacetate **7a**



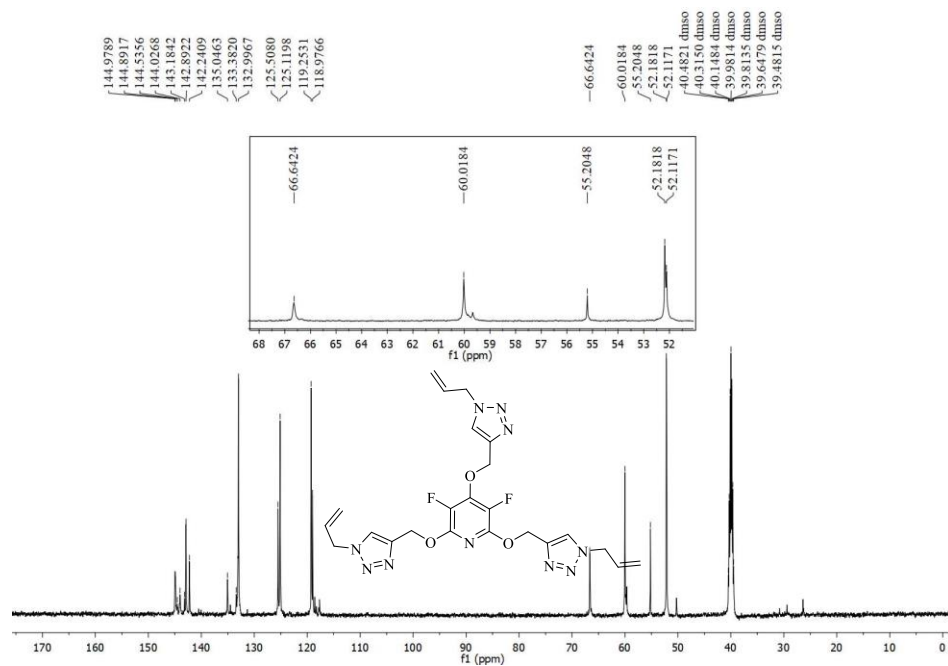
Expanded ¹³C NMR spectrum of triethyl 2,2',2''-(((3,5-difluoropyridine-2,4,6-triyl)tris(oxy))tris(methylene))tris(1H-1,2,3-triazole-4,1-diyl))triacetate **7a**



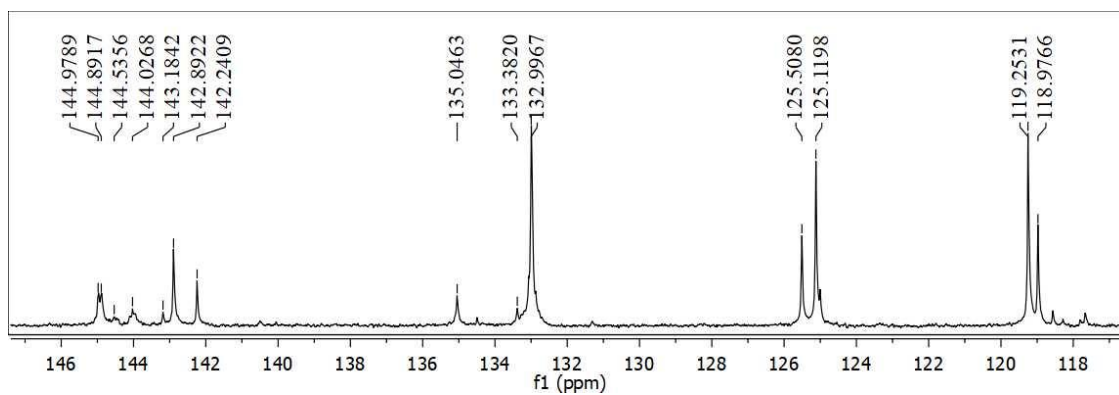
^{19}F NMR spectrum of triethyl 2,2',2''-(((3,5-difluoropyridine-2,4,6-triyl)tris(oxy))tris(methylene))tris(1H-1,2,3-triazole-4,1-diyl))triacetate **7a**



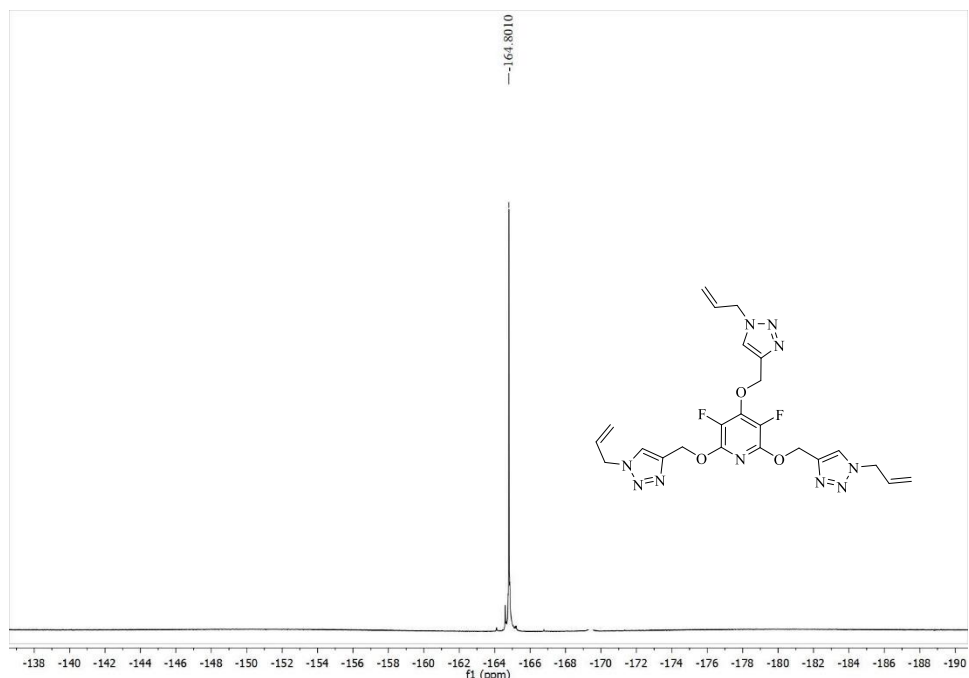
^1H NMR spectrum of 2,4,6-tris((1-allyl-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **7b**



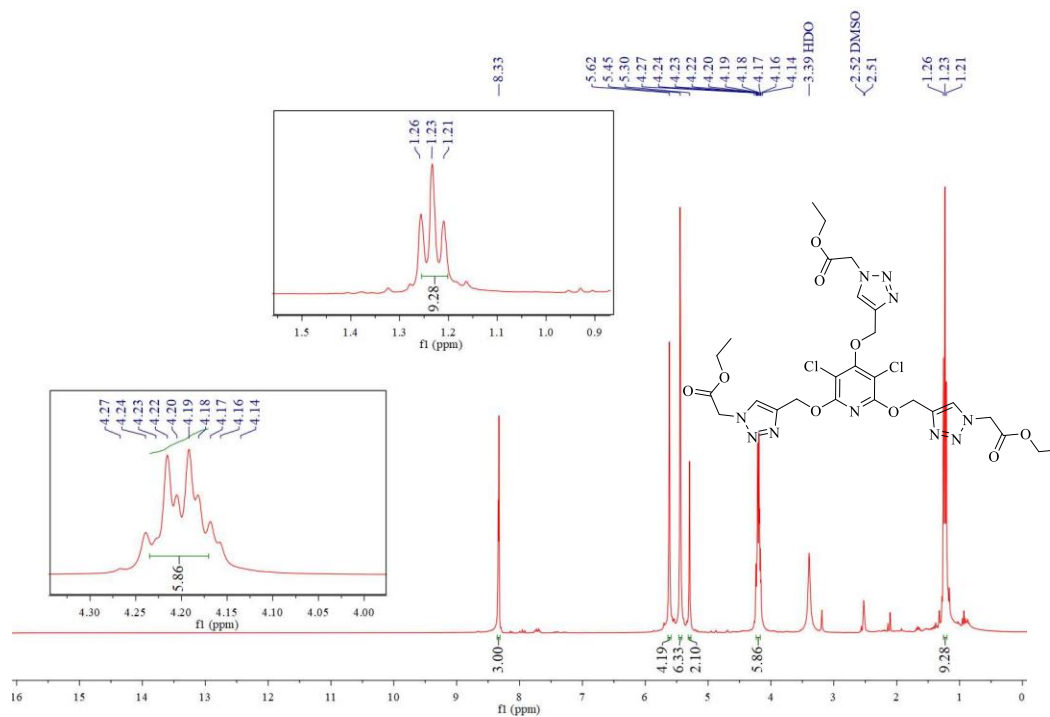
¹³C NMR spectrum of 2,4,6-tris((1-allyl-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **7b**



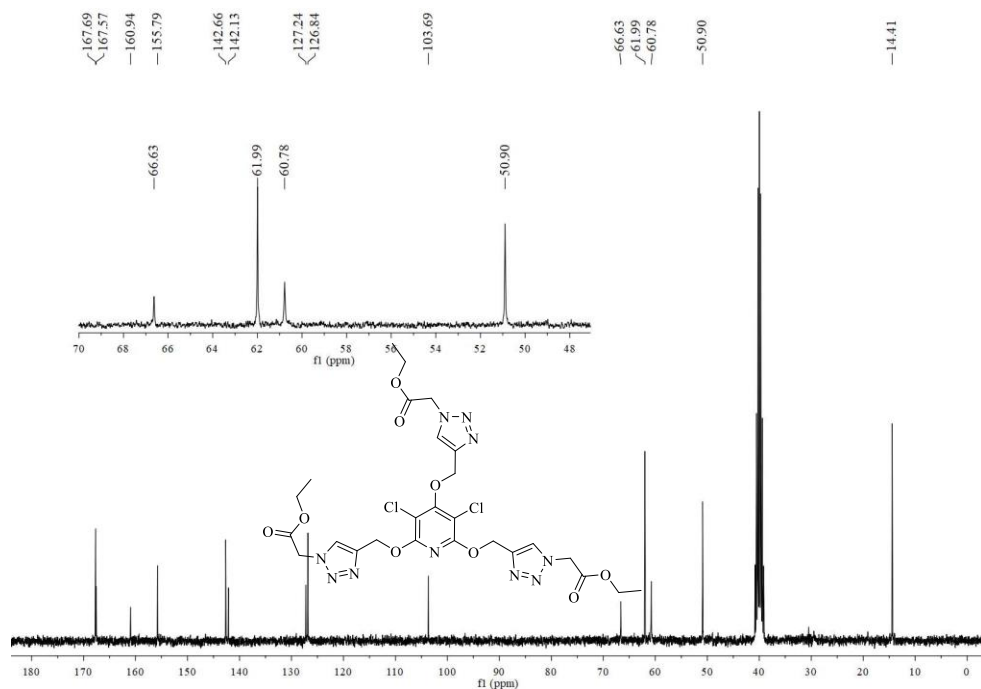
Expanded ¹³C NMR spectrum of 2,4,6-tris((1-allyl-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **7b**



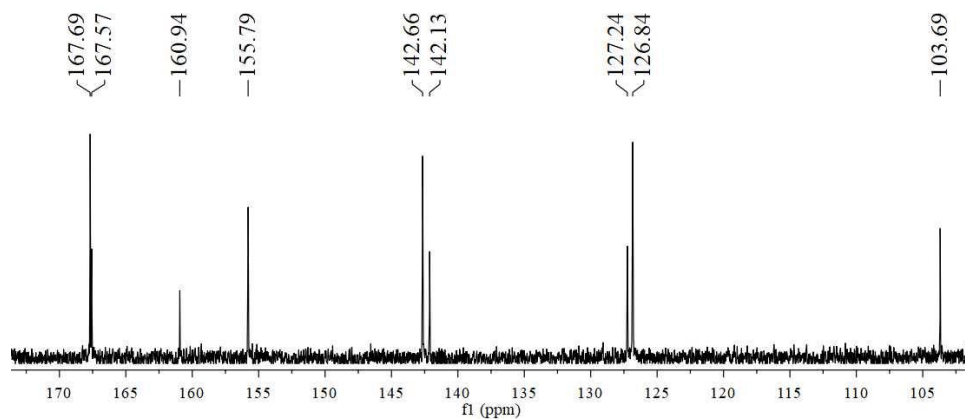
¹⁹F NMR spectrum of 2,4,6-tris((1-allyl-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **7b**



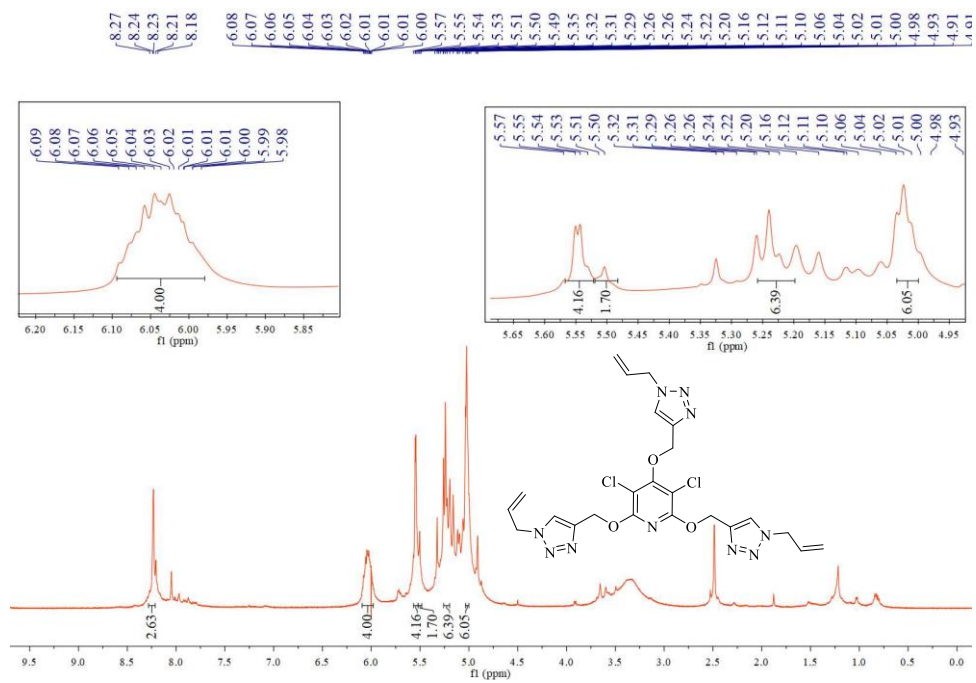
¹H NMR spectrum of triethyl 2,2',2''-(((3,5-dichloropyridine-2,4,6-triyl)tris(oxy))tris(methylene))tris(1H-1,2,3-triazole-4,1-diyl))triacetate **7c**



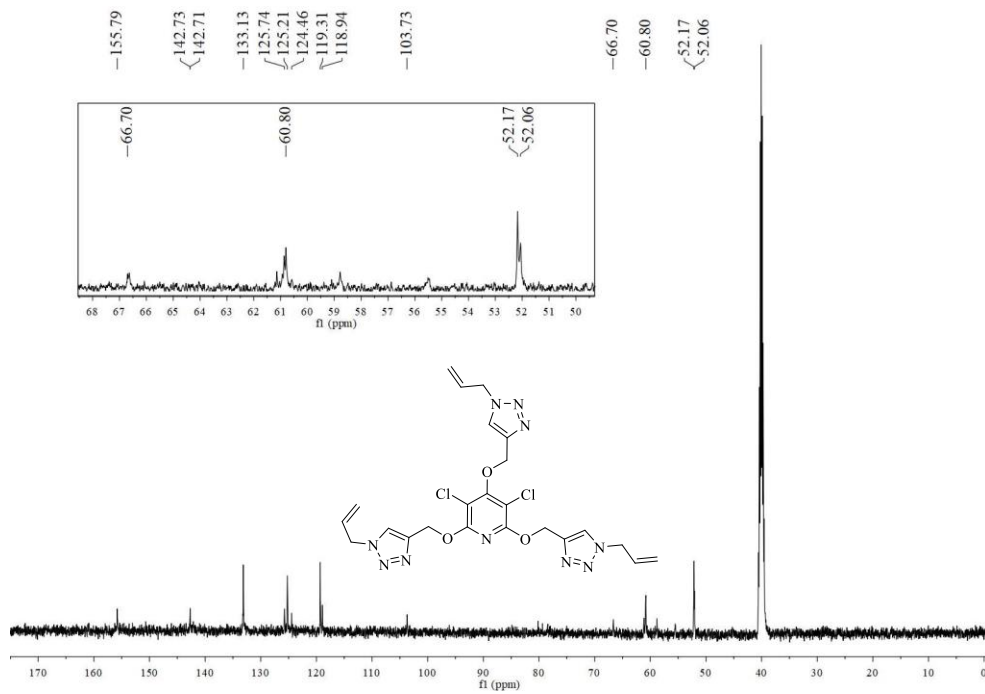
^{13}C NMR spectrum of triethyl 2,2',2''-(((3,5-dichloropyridine-2,4,6-triyl)tris(oxy))tris(methylene))tris(1H-1,2,3-triazole-4,1-diyl)triacetate **7c**



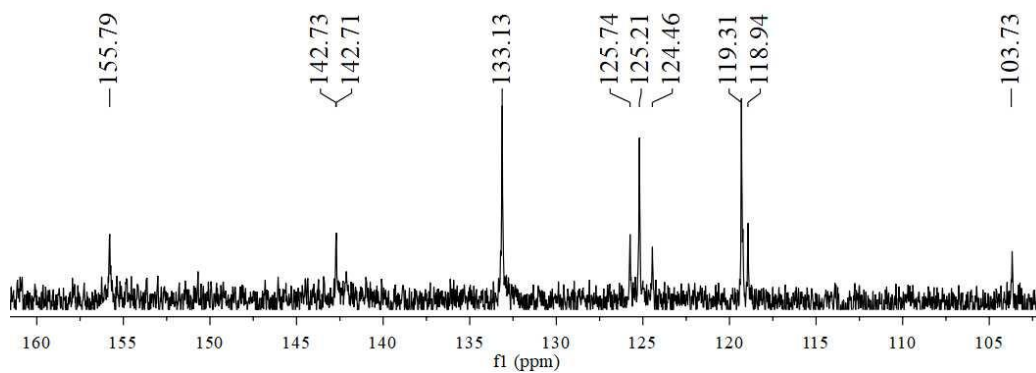
Expanded ^{13}C NMR spectrum of triethyl 2,2',2''-(((3,5-dichloropyridine-2,4,6-triyl)tris(oxy))tris(methylene))tris(1H-1,2,3-triazole-4,1-diyl)triacetate **7c**



^1H NMR spectrum of 2,4,6-tris((1-allyl-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **7d**

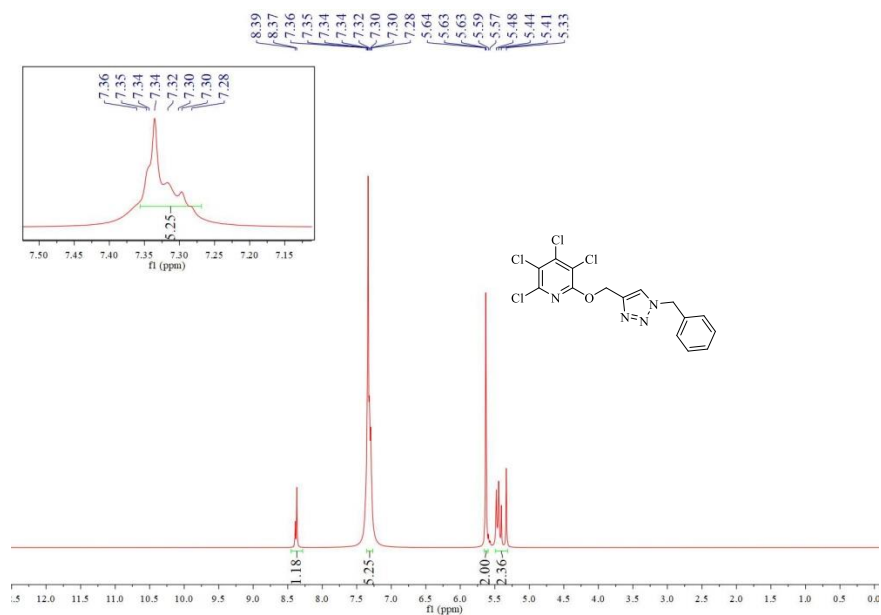


^{13}C NMR spectrum of 2,4,6-tris((1-allyl-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **7d**

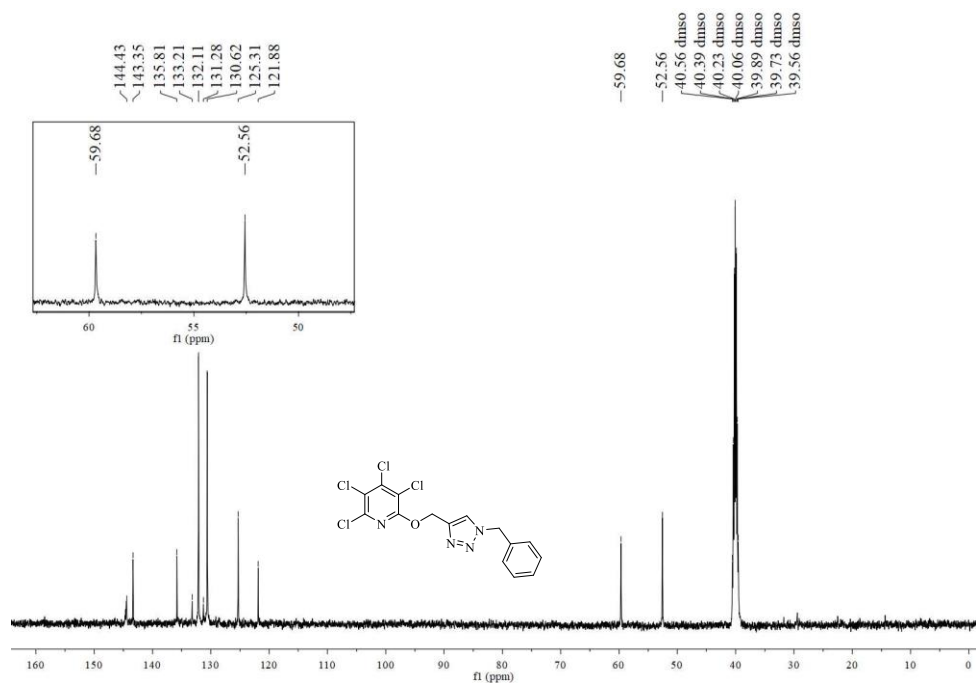


Expanded ^{13}C NMR spectrum of 2,4,6-tris((1-allyl-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **7d**

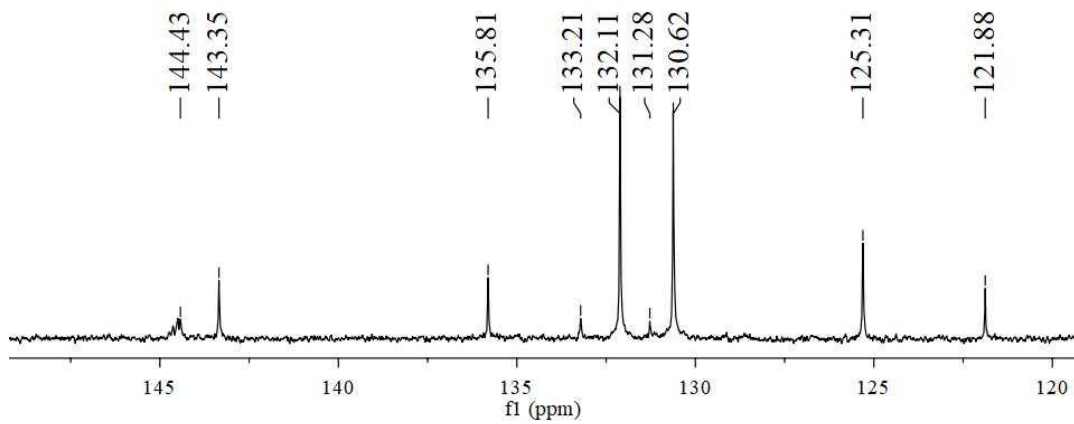
7. NMR spectra of 2-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)-3,4,5,6-tetrachloropyridine derivatives **8a-c**



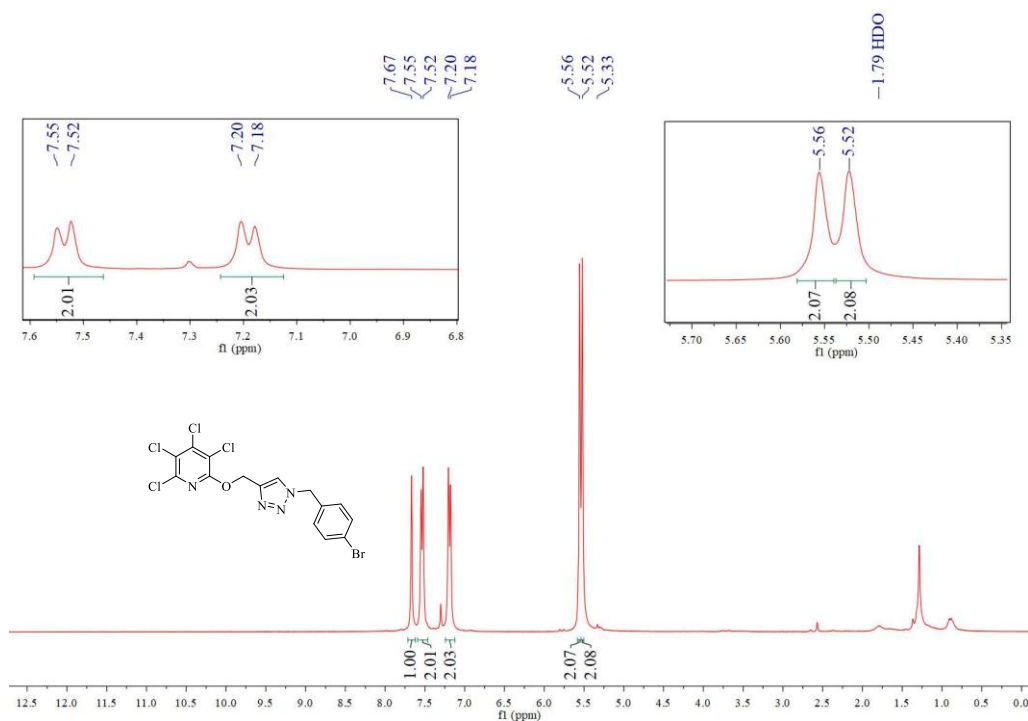
^1H NMR spectrum of 2-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)-3,4,5,6-tetrachloropyridine **8a**



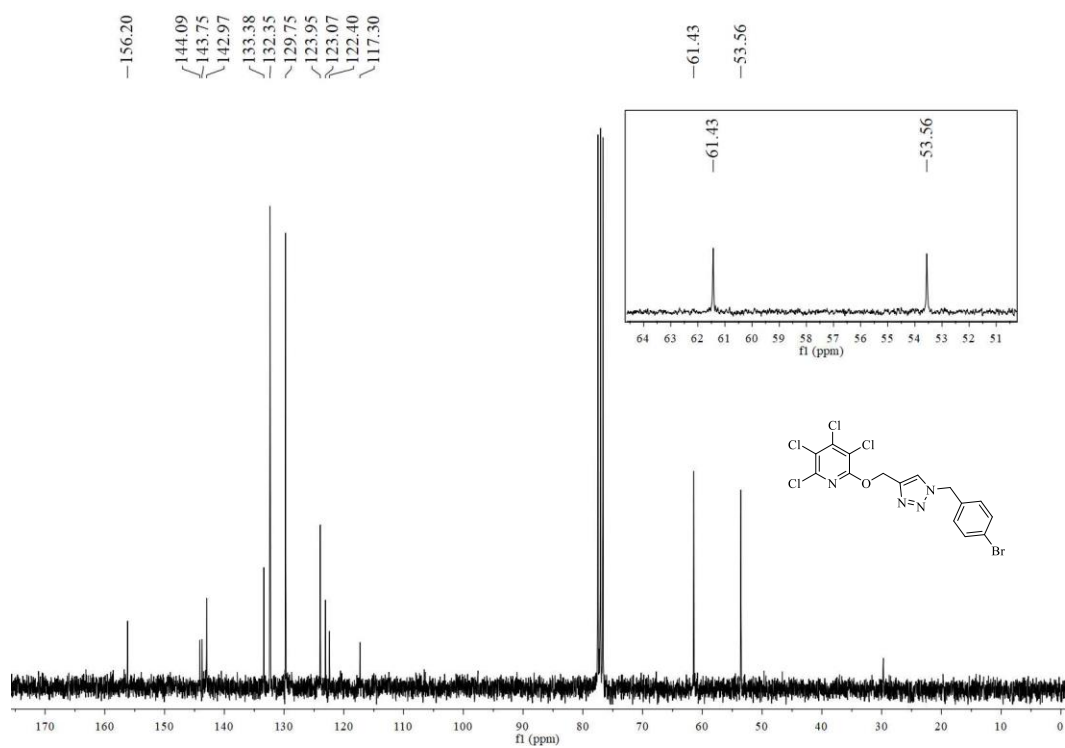
¹³C NMR spectrum of 2-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)-3,4,5,6-tetrachloropyridine **8a**



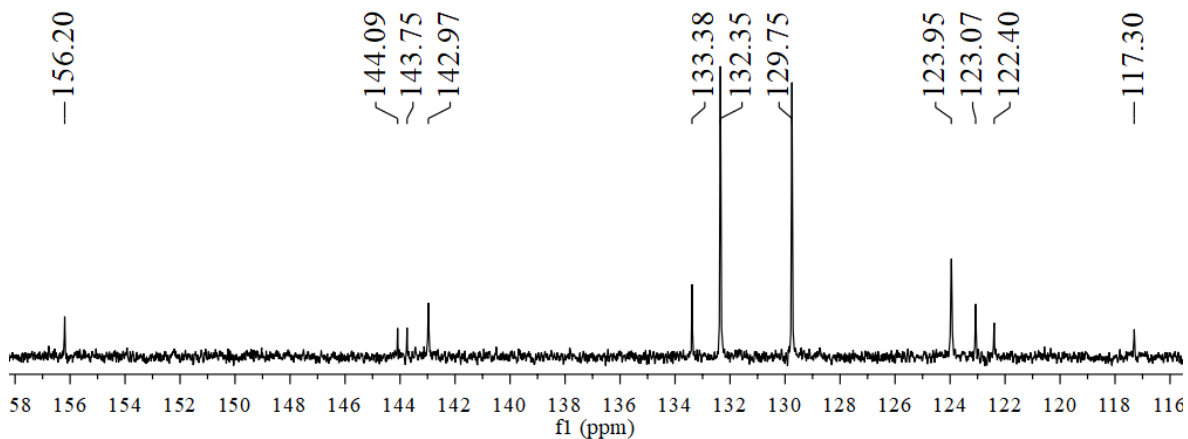
Expanded ¹³C NMR spectrum of 2-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)-3,4,5,6-tetrachloropyridine **8a**



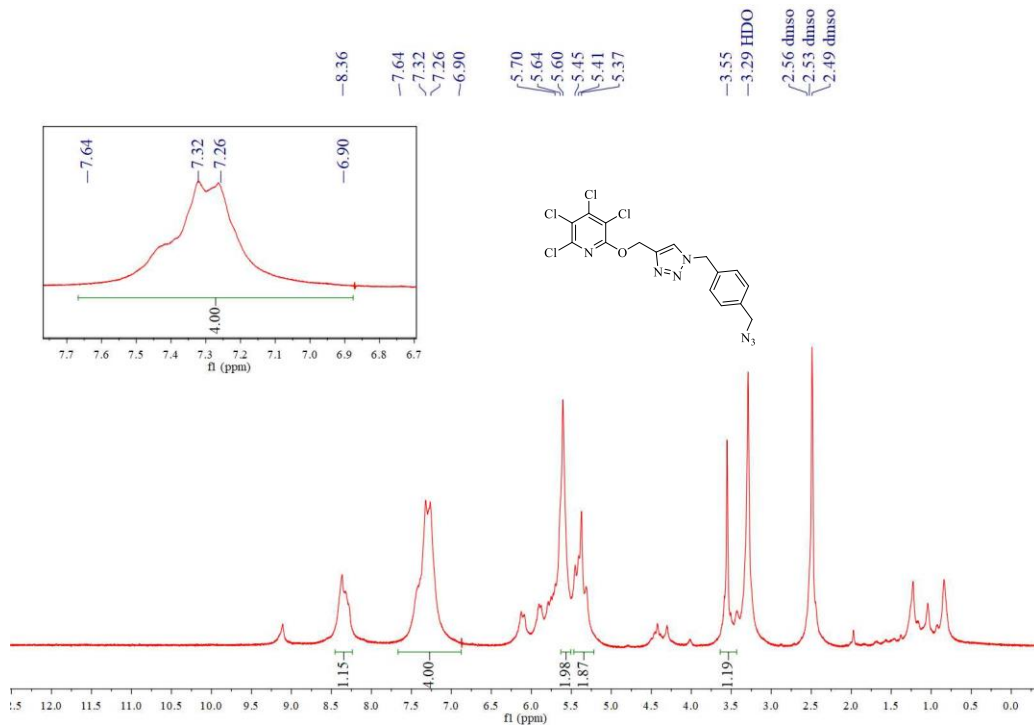
¹H NMR spectrum of 2-((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,4,5,6-tetrachloropyridine **8b**



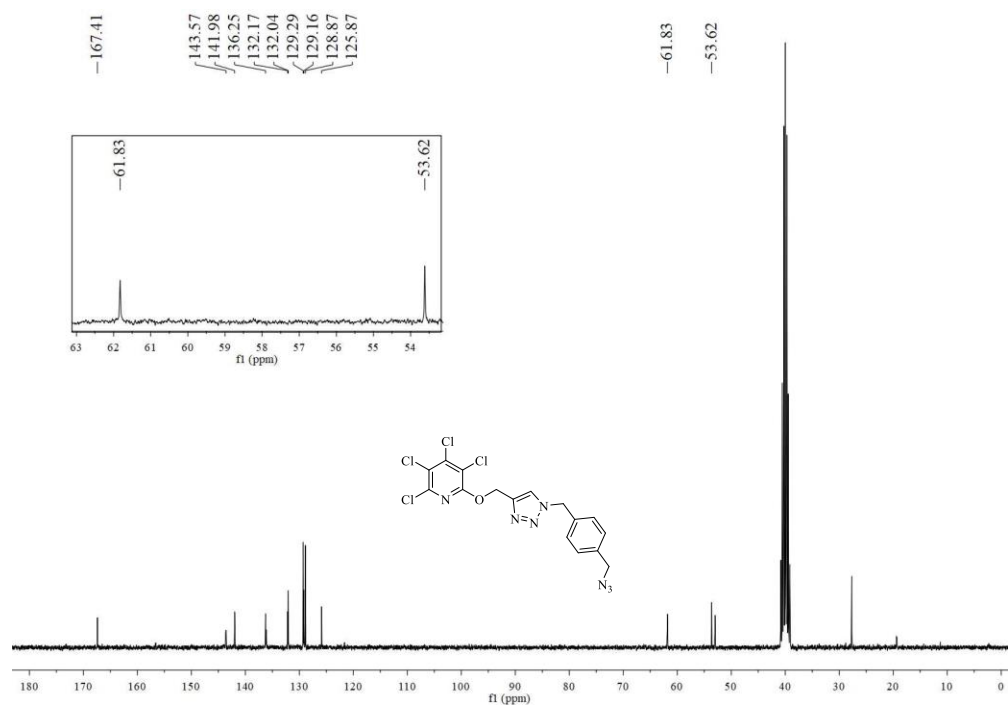
¹³C NMR spectrum of 2-((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,4,5,6-tetrachloropyridine **8b**



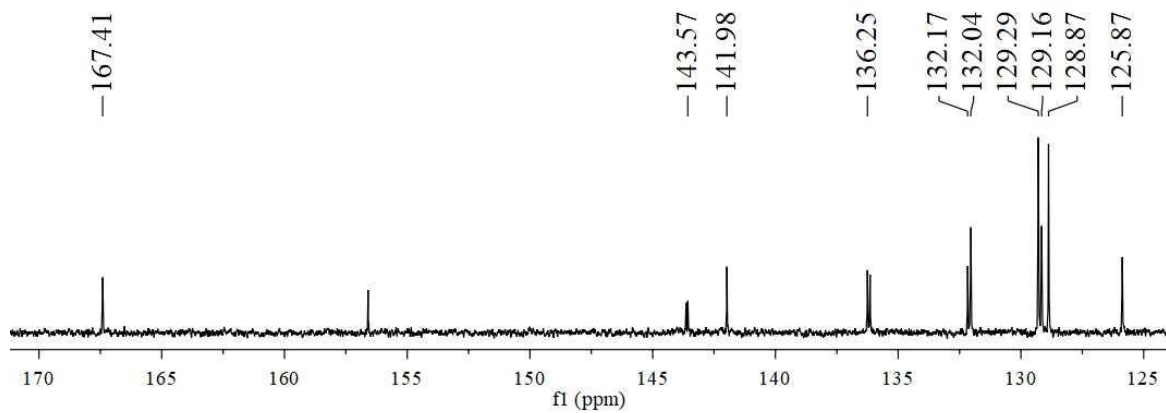
Expanded ^{13}C NMR spectrum of 2-((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,4,5,6-tetrachloropyridine **8b**



^1H NMR spectrum of 2-((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,4,5,6-tetrachloropyridine **8c**

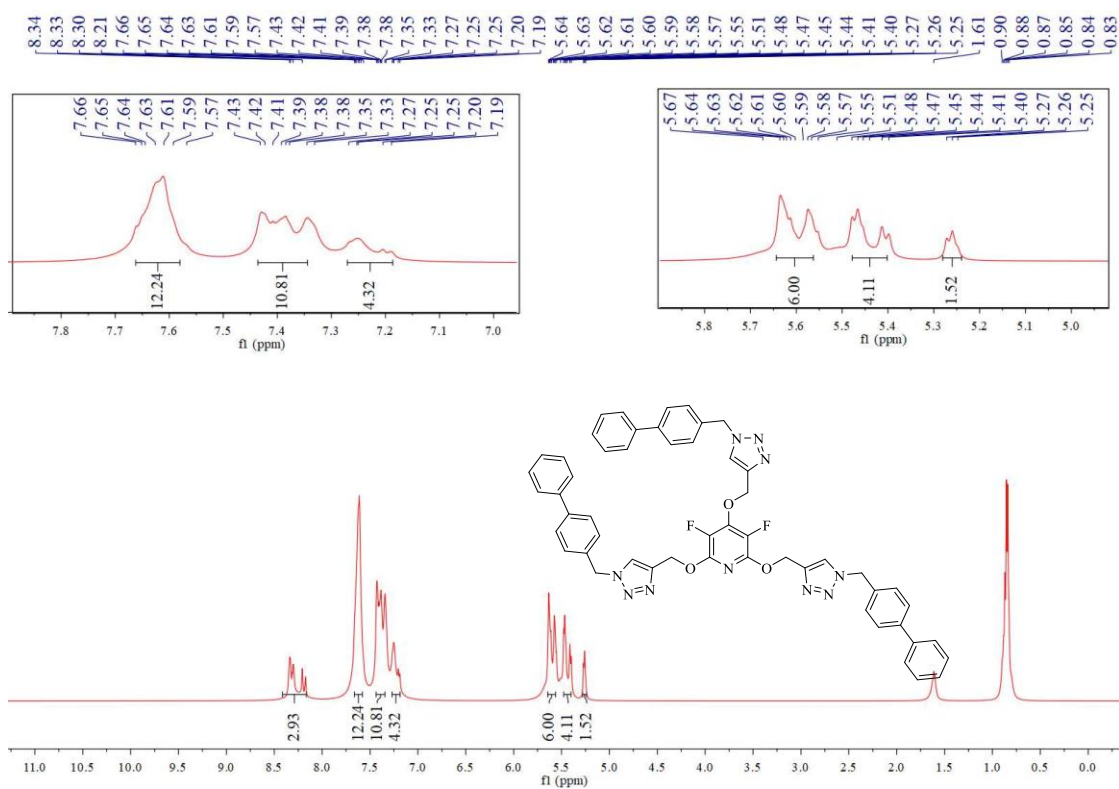


¹³C NMR spectrum of 2-((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,4,5,6-tetrachloropyridine **8c**

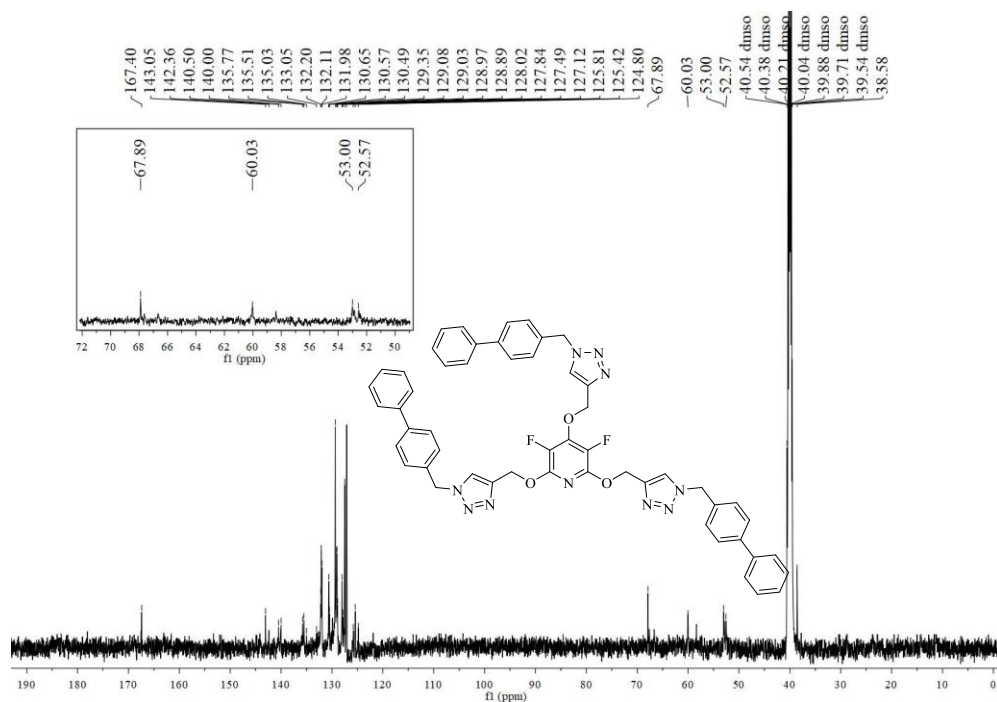


Expanded ¹³C NMR spectrum of 2-((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,4,5,6-tetrachloropyridine **8c**

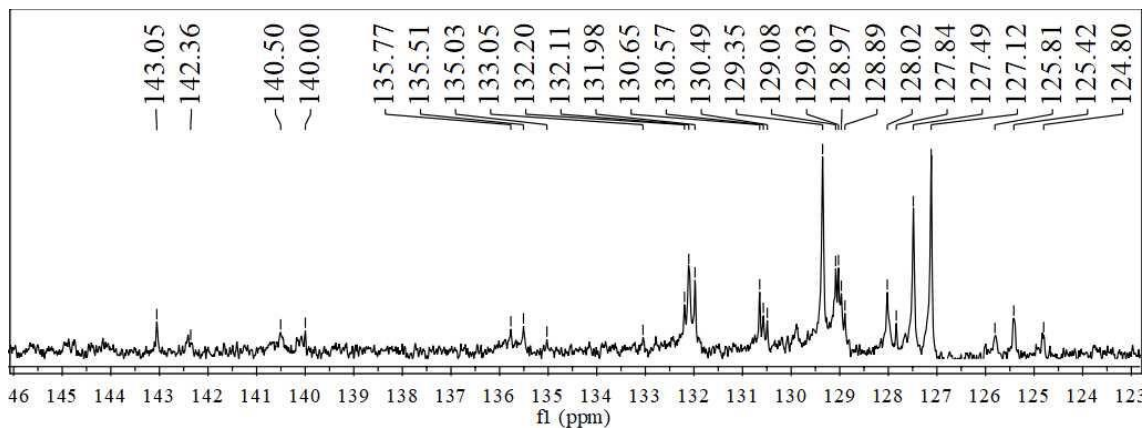
8. NMR spectra of Suzuki-Miyaura cross-coupling products 10a-f



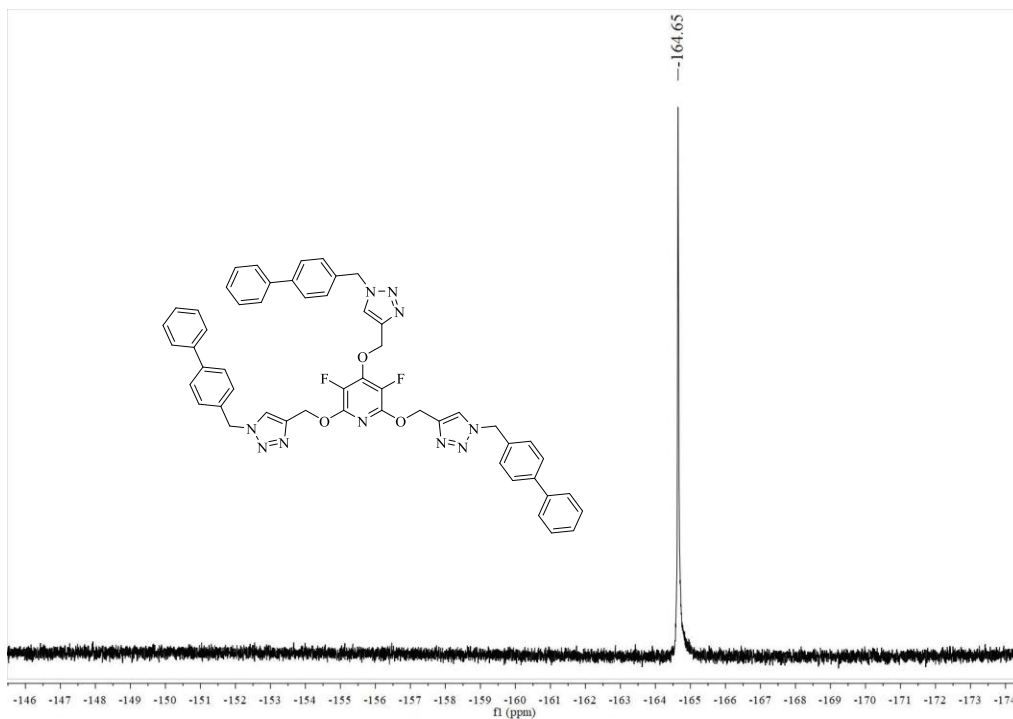
¹H NMR spectrum of 2,4-tris((1-([1,1'-biphenyl]-4-ylmethyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **10a**



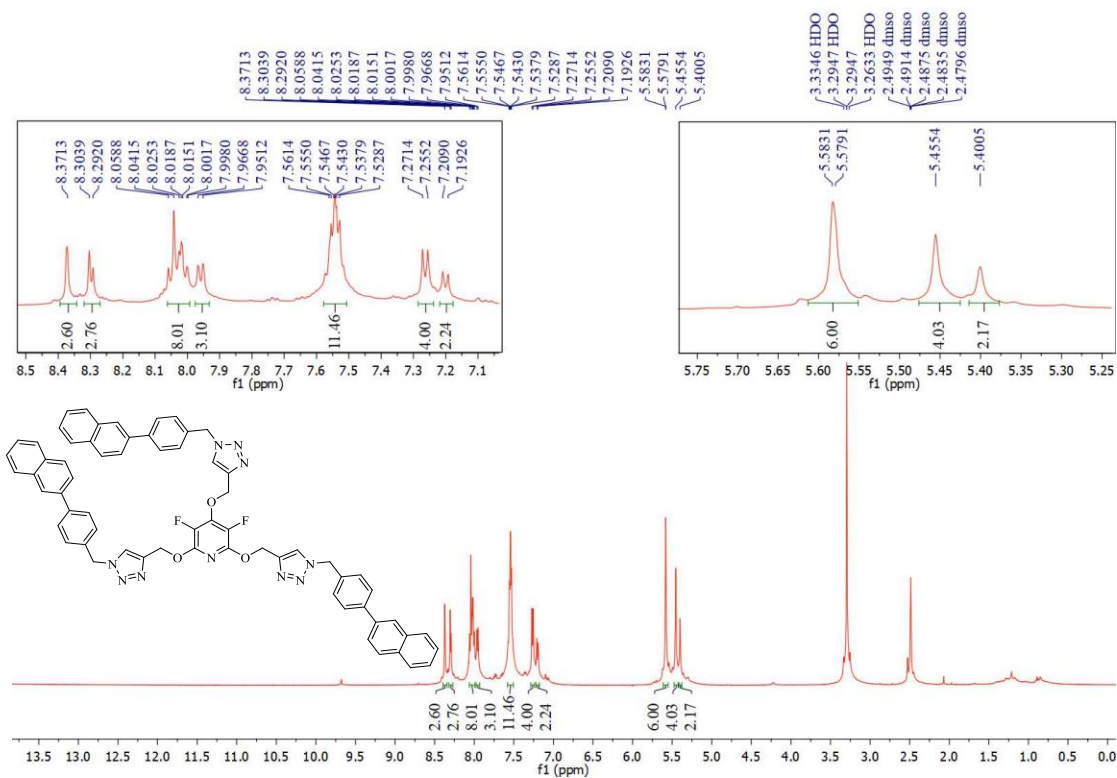
^{13}C NMR spectrum of 2,4,6-tris((1-([1,1'-biphenyl]-4-ylmethyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **10a**



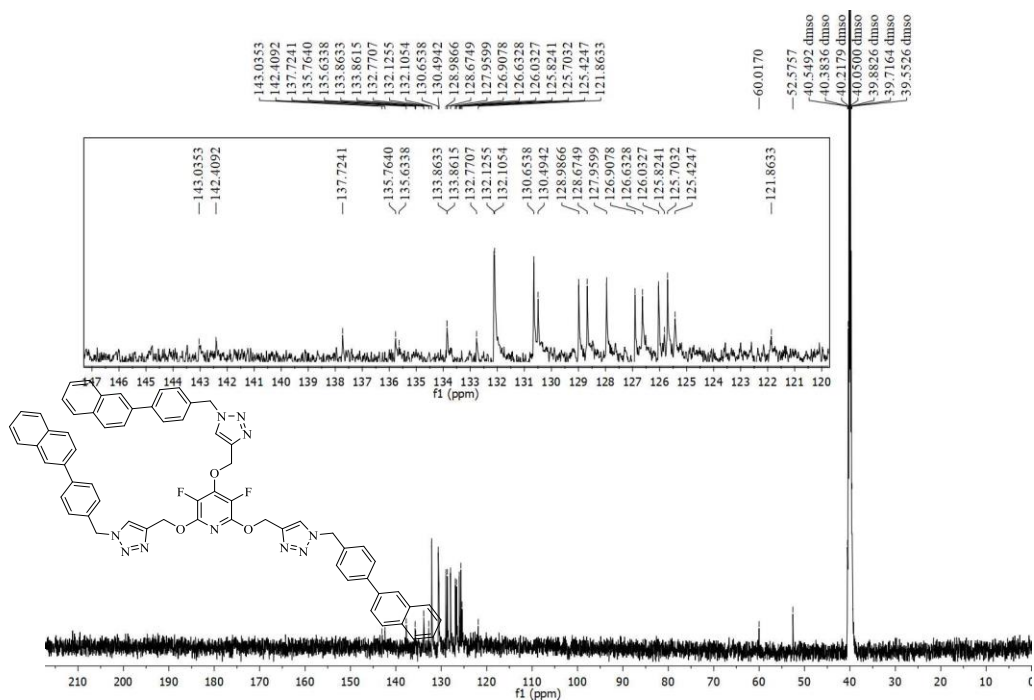
Expanded ^{13}C NMR spectrum of 2,4,6-tris((1-([1,1'-biphenyl]-4-ylmethyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **10a**



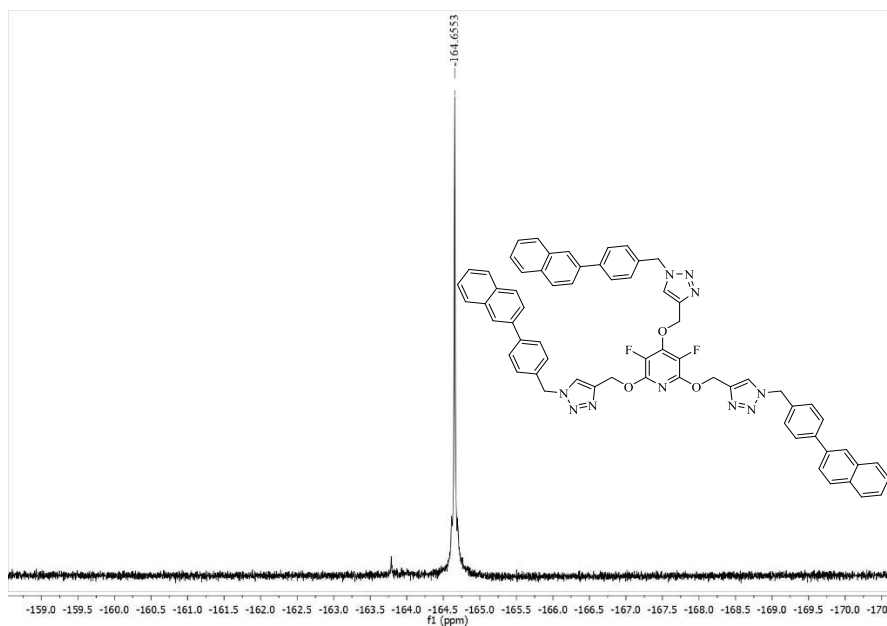
^{19}F NMR spectrum of 2,4,6-tris((1-([1,1'-biphenyl]-4-ylmethyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridine **10a**



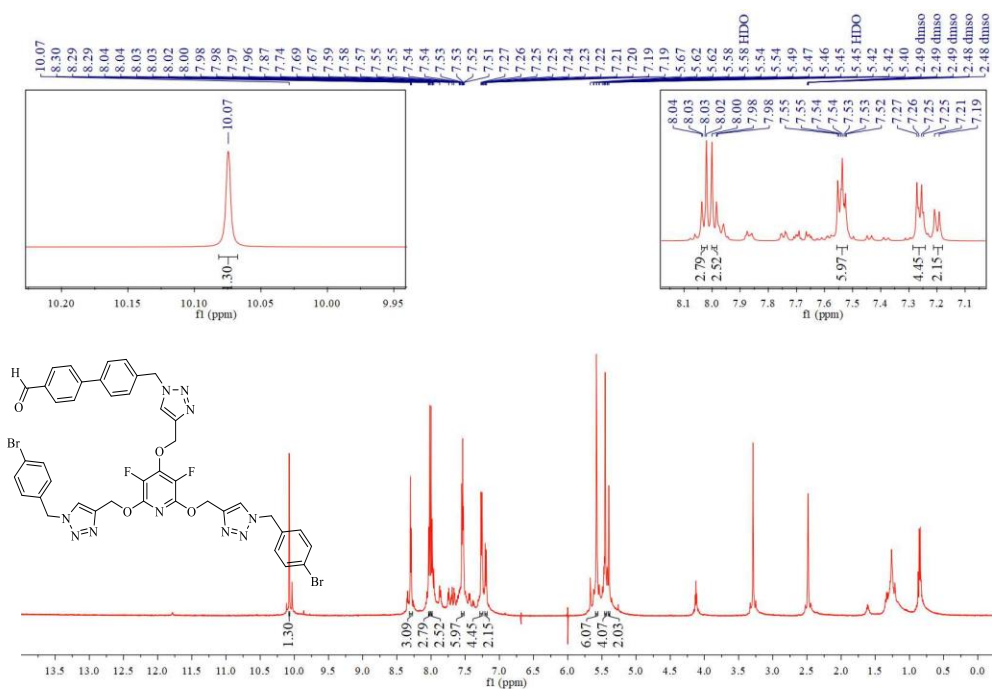
¹H NMR spectrum of 3,5-difluoro-2,4,6-tris((1-(4-(naphthalen-2-yl)benzyl)-1H-1,2,3-triazol-4-yl)methoxy)pyridine **10b**



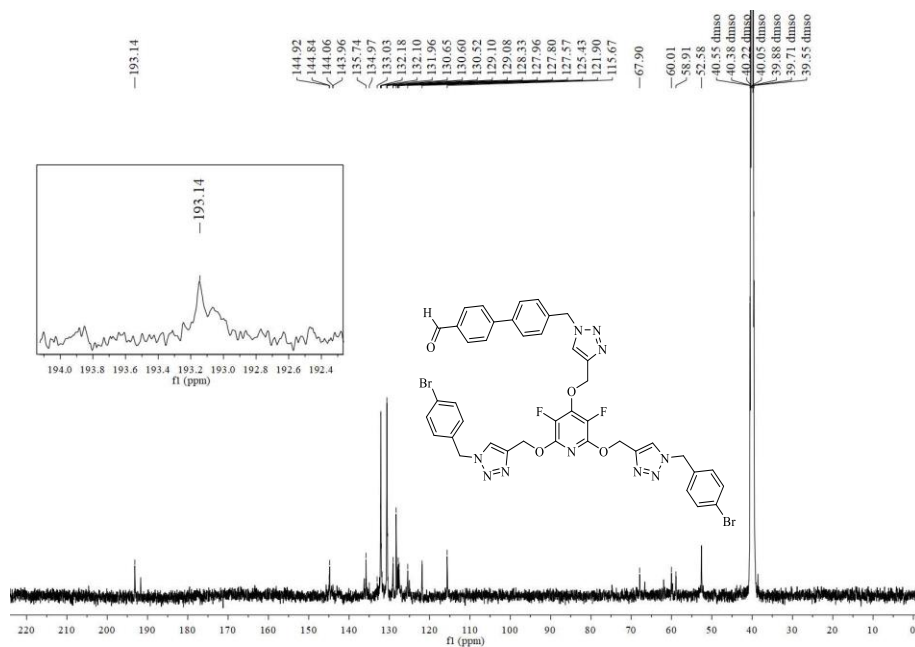
¹³C NMR spectrum of 3,5-difluoro-2,4,6-tris((1-(4-(naphthalen-2-yl)benzyl)-1H-1,2,3-triazol-4-yl)methoxy)pyridine **10b**



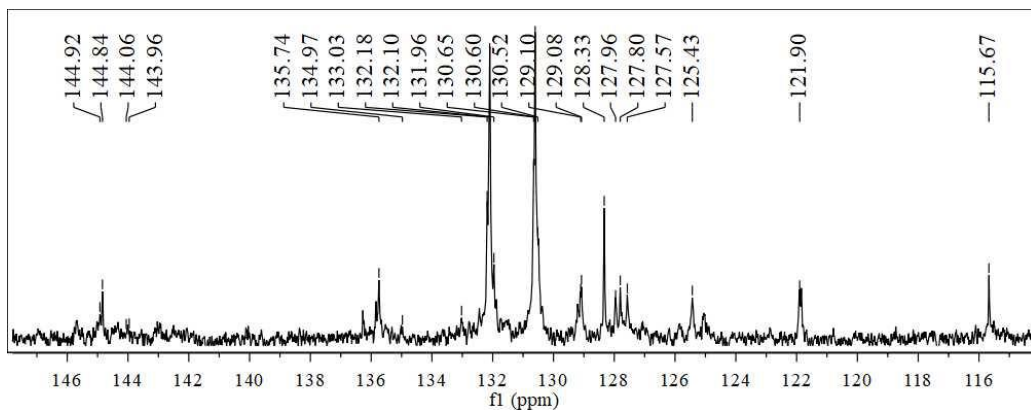
^{13}C NMR spectrum of 3,5-difluoro-2,4,6-tris((1-(4-(naphthalen-2-yl)benzyl)-1H-1,2,3-triazol-4-yl)methoxy)pyridine **10b**



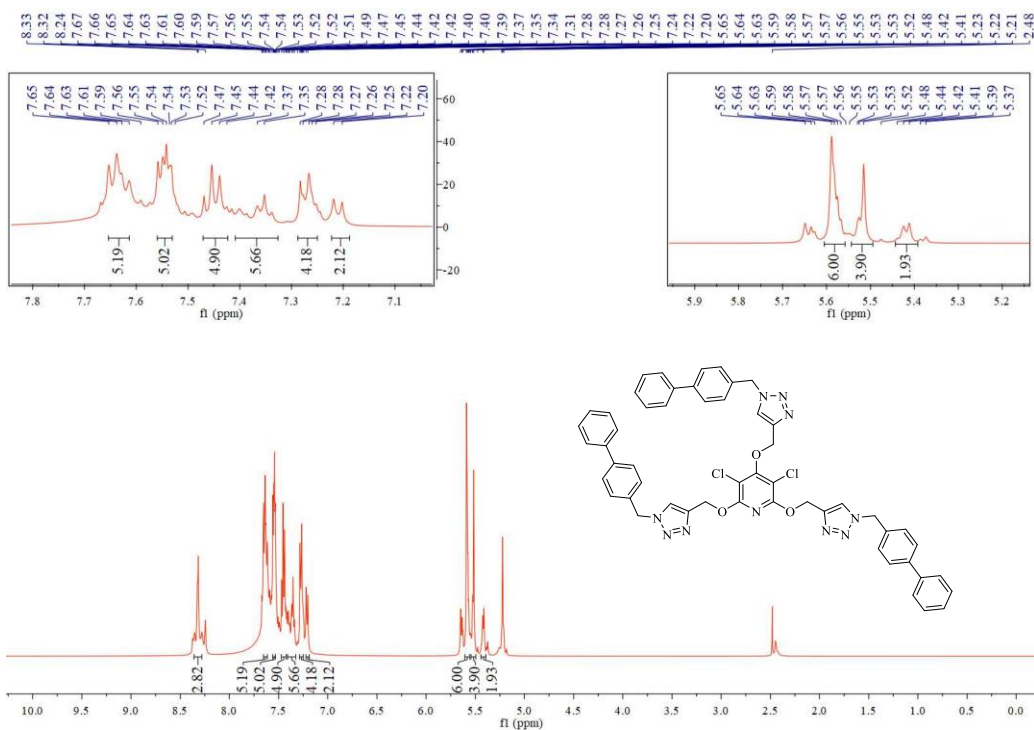
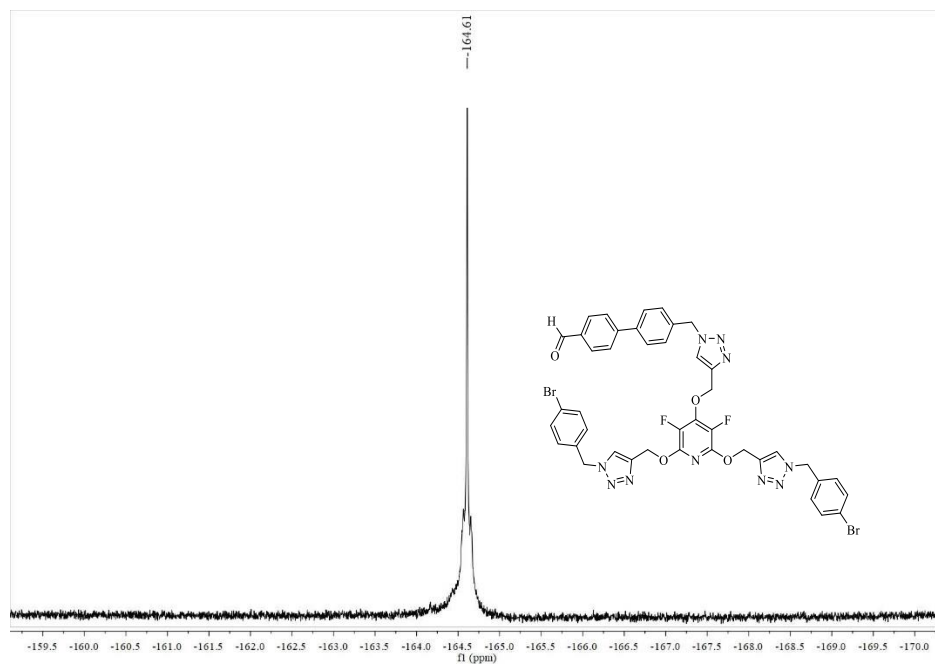
^1H NMR spectrum of 4'-((4-(((2,6-bis((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridin-4-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)methyl)-[1,1'-biphenyl]-4-carbaldehyde **10c**

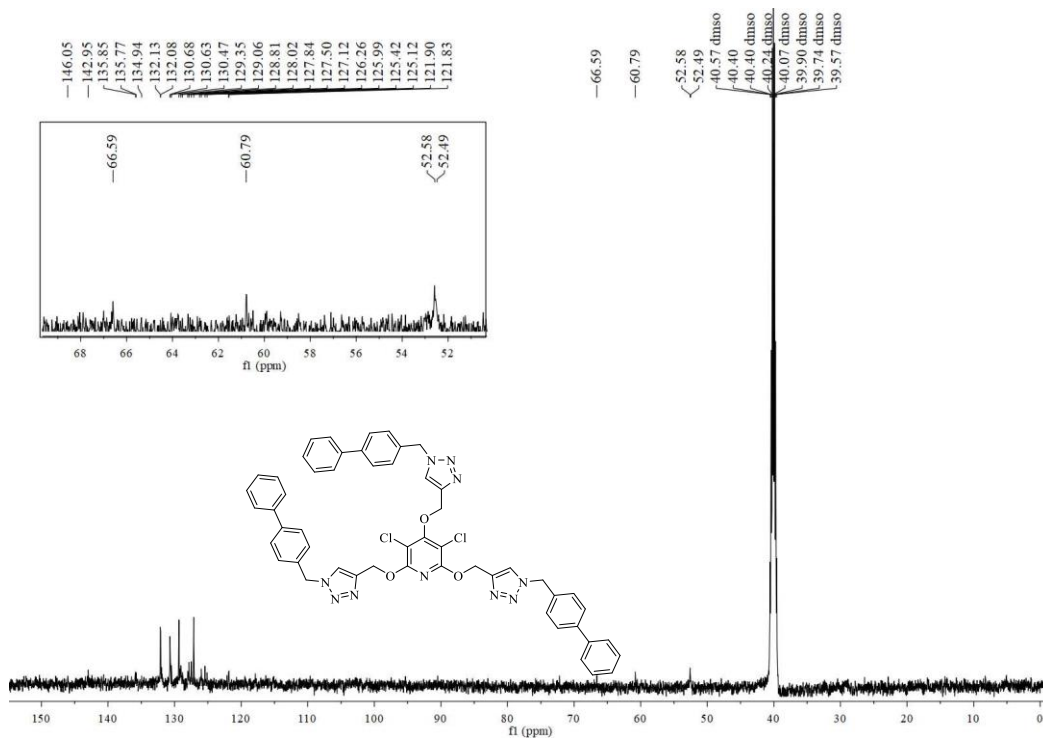


¹³C NMR spectrum of 4'-((4-(((2,6-bis((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridin-4-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)methyl)-[1,1'-biphenyl]-4-carbaldehyde) **10c**

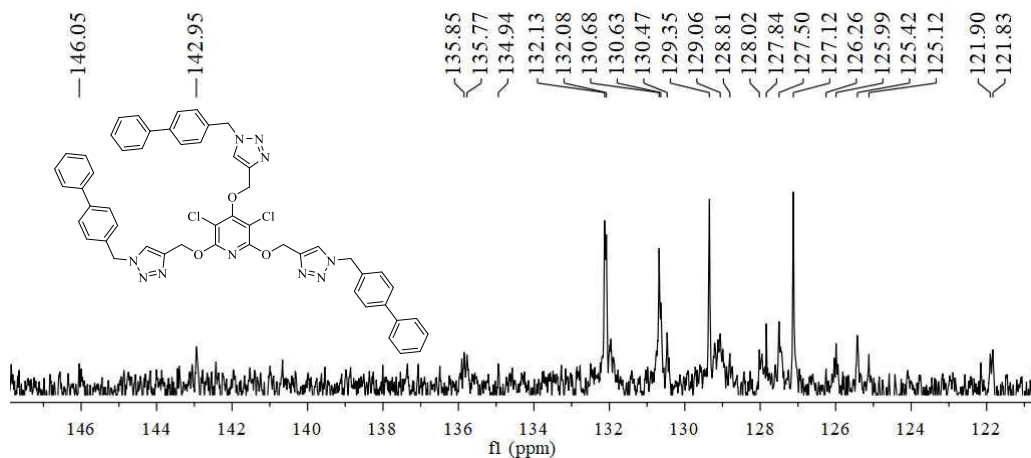


Expanded ¹³C NMR spectrum of 4'-((4-(((2,6-bis((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-difluoropyridin-4-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)methyl)-[1,1'-biphenyl]-4-carbaldehyde) **10c**

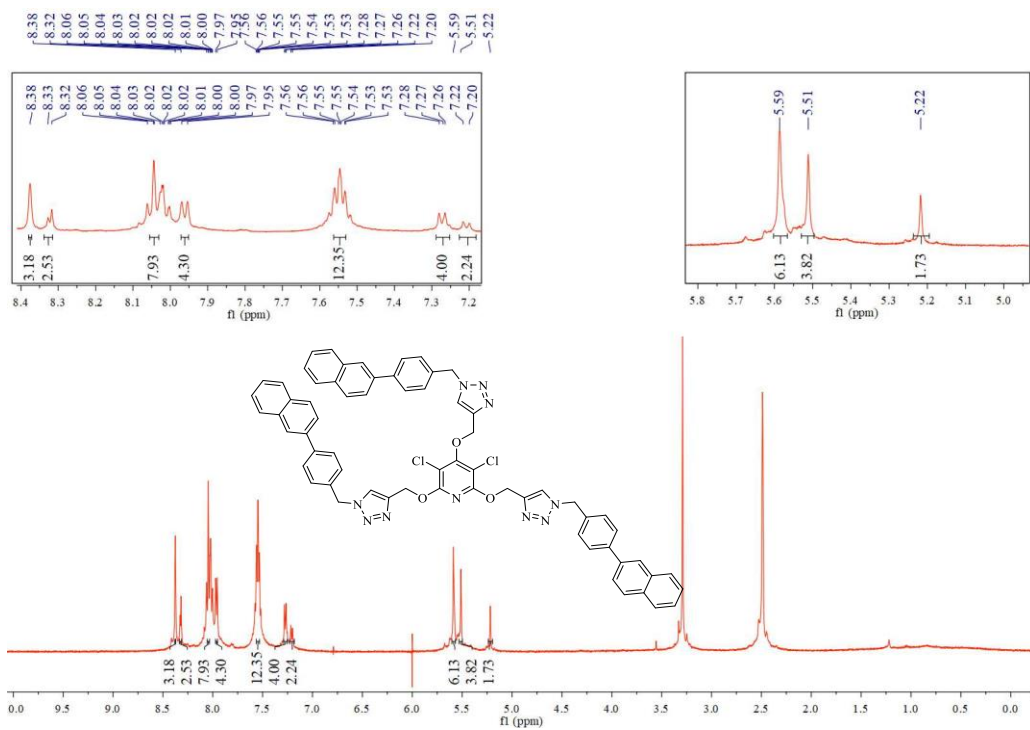




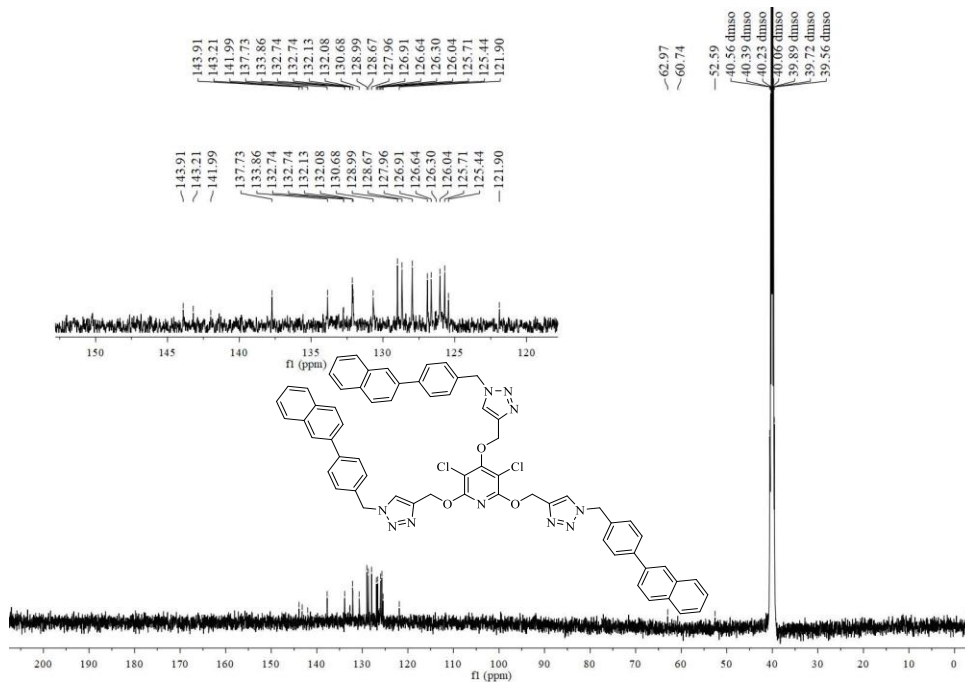
¹³C NMR spectrum of 2,4,6-tris((1-([1,1'-biphenyl]-4-yl)methyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-dichloropyridine **10d**



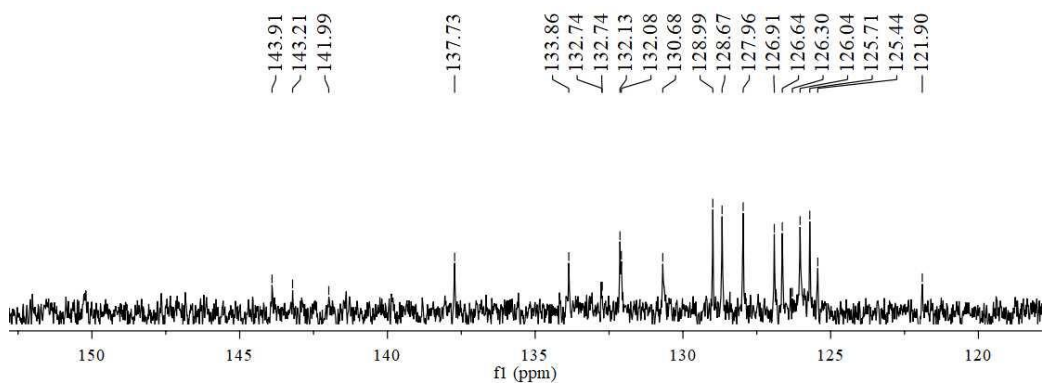
Expanded ¹³C NMR spectrum of 2,4,6-tris((1-([1,1'-biphenyl]-4-yl)methyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-dichloropyridine **10d**



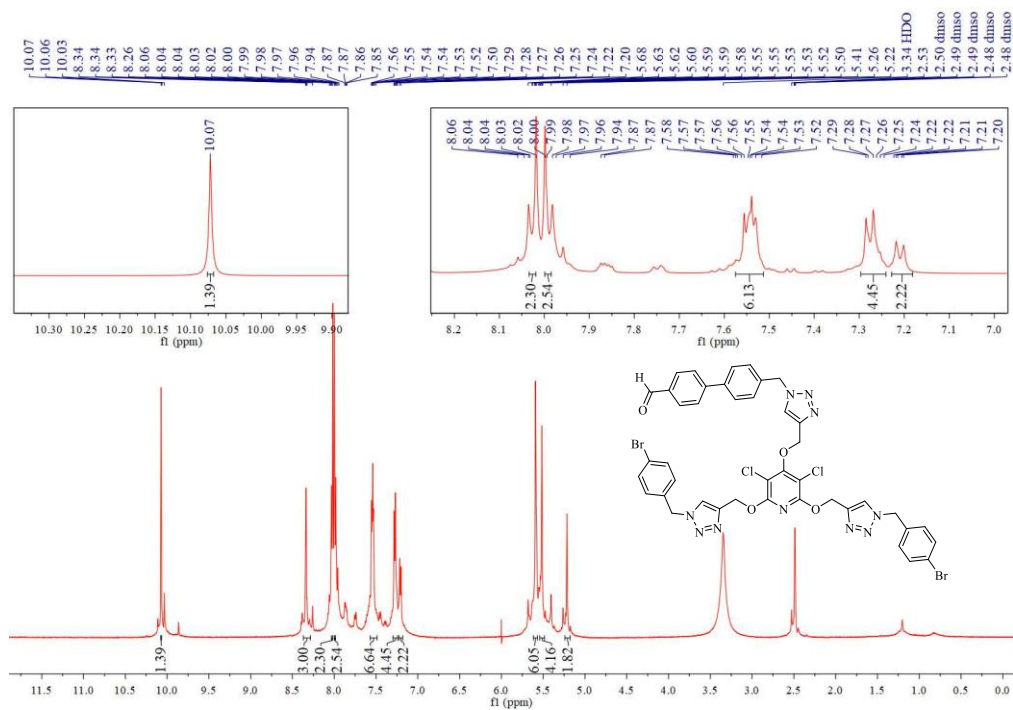
¹H NMR spectrum of 3,5-dichloro-2,4,6-tris((1-(4-(naphthalen-2-yl)benzyl)-1H-1,2,3-triazol-4-yl)methoxy)pyridine **10e**



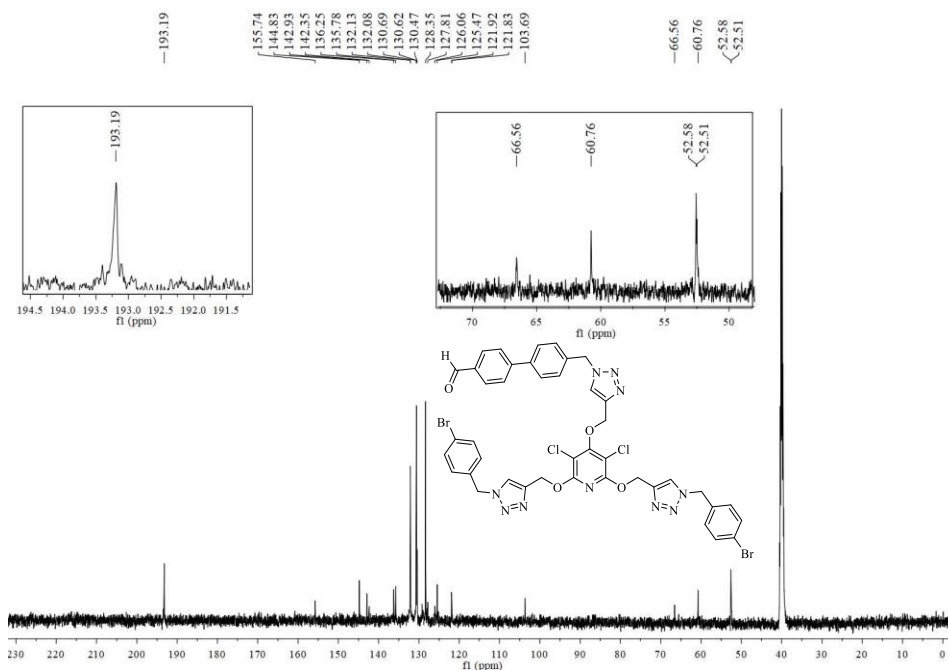
¹³C NMR spectrum of 3,5-dichloro-2,4,6-tris((1-(4-(naphthalen-2-yl)benzyl)-1H-1,2,3-triazol-4-yl)methoxy)pyridine **10e**



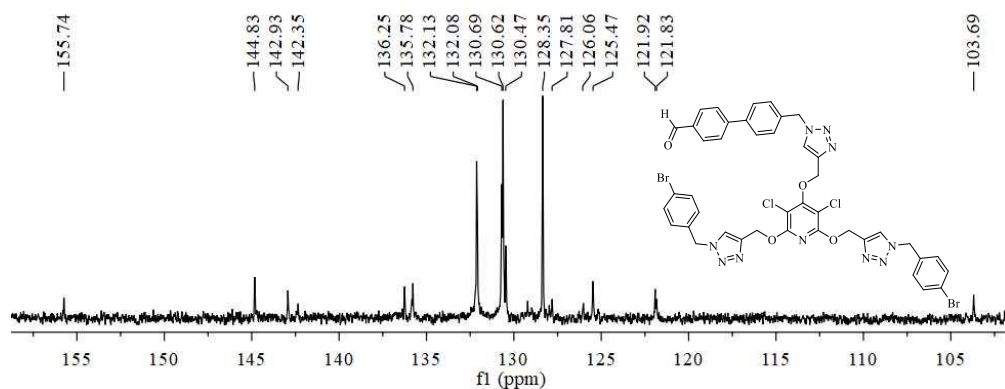
Expanded ^{13}C NMR spectrum of 3,5-dichloro-2,4,6-tris((1-(4-(naphthalen-2-yl)benzyl)-1H-1,2,3-triazol-4-yl)methoxy)pyridine **10e**



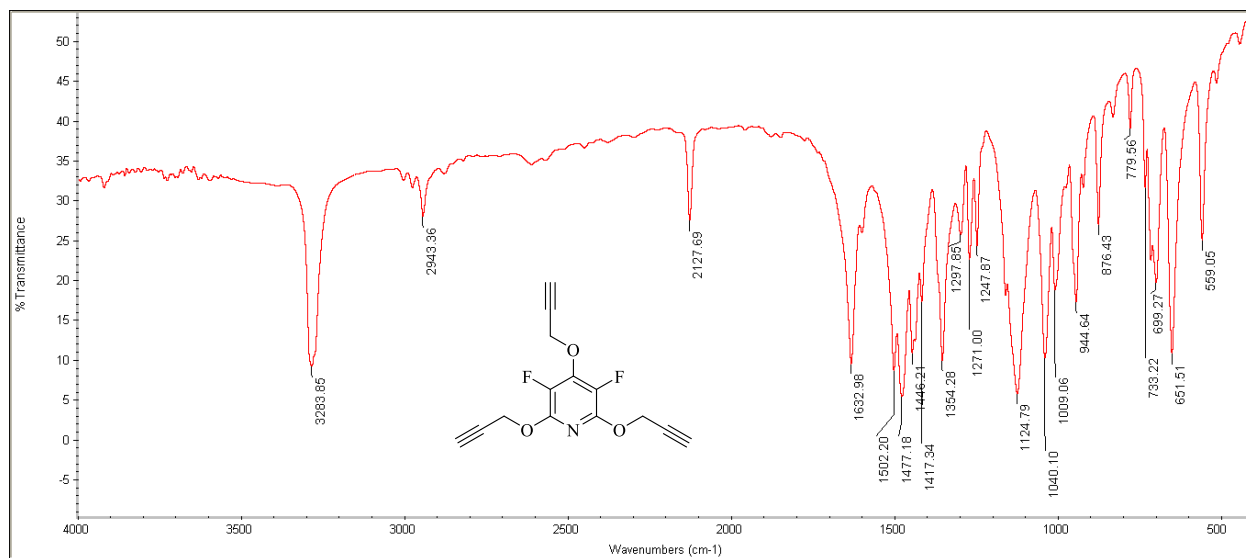
^1H NMR spectrum of 4'-((4-(((2,6-bis((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-dichloropyridin-4-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)methyl)-[1,1'-biphenyl]-4-carbaldehyde **10f**



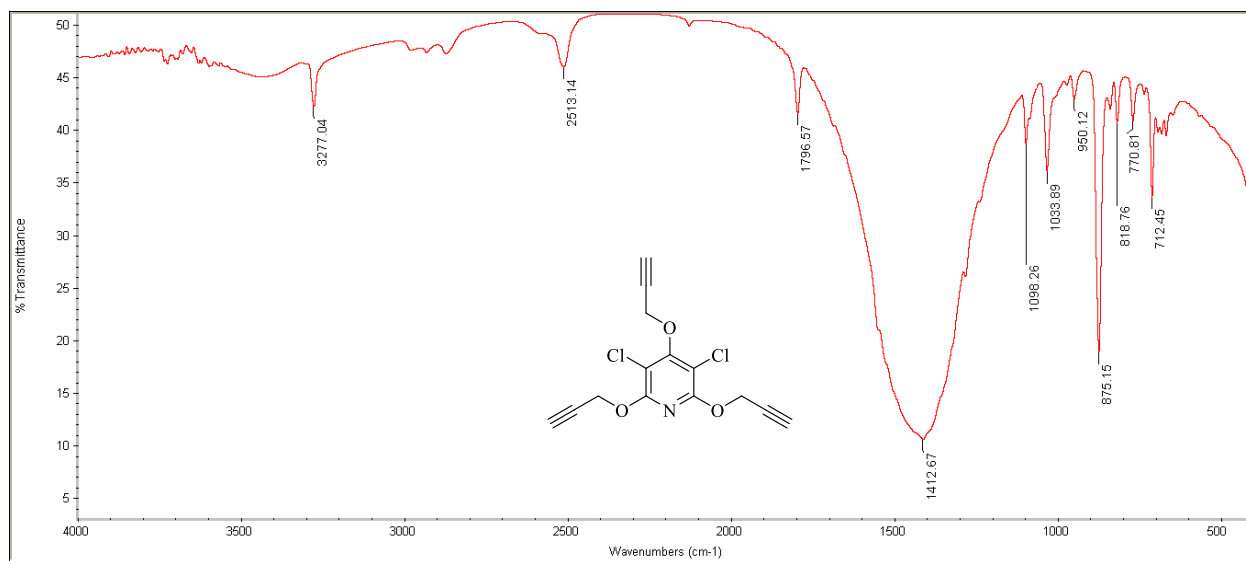
¹³C NMR spectrum of 4'-((4-(((2,6-bis((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-dichloropyridin-4-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)methyl)-[1,1'-biphenyl]-4-carbaldehyde **10f**



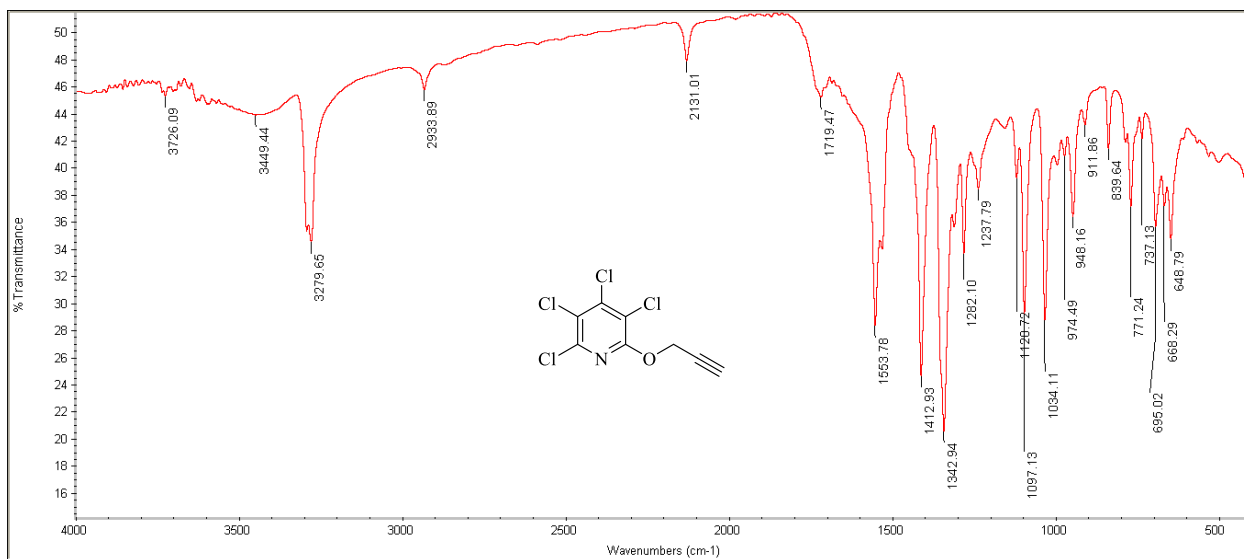
Expanded ¹³C NMR spectrum of 4'-((4-(((2,6-bis((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)-3,5-dichloropyridin-4-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)methyl)-[1,1'-biphenyl]-4-carbaldehyde **10f**



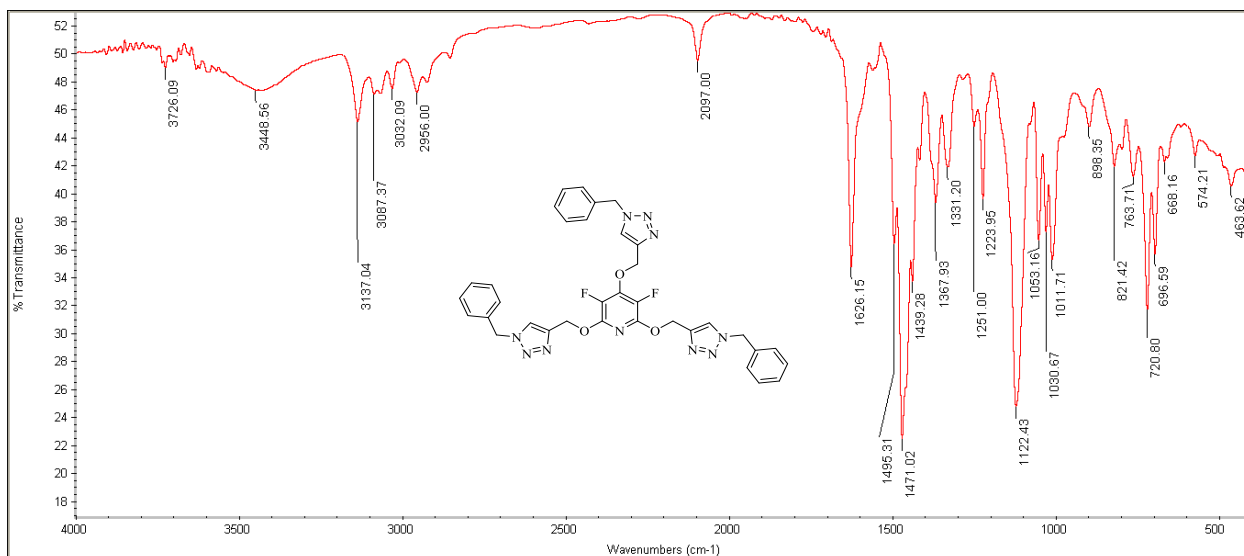
FT-IR spectrum of **3a**



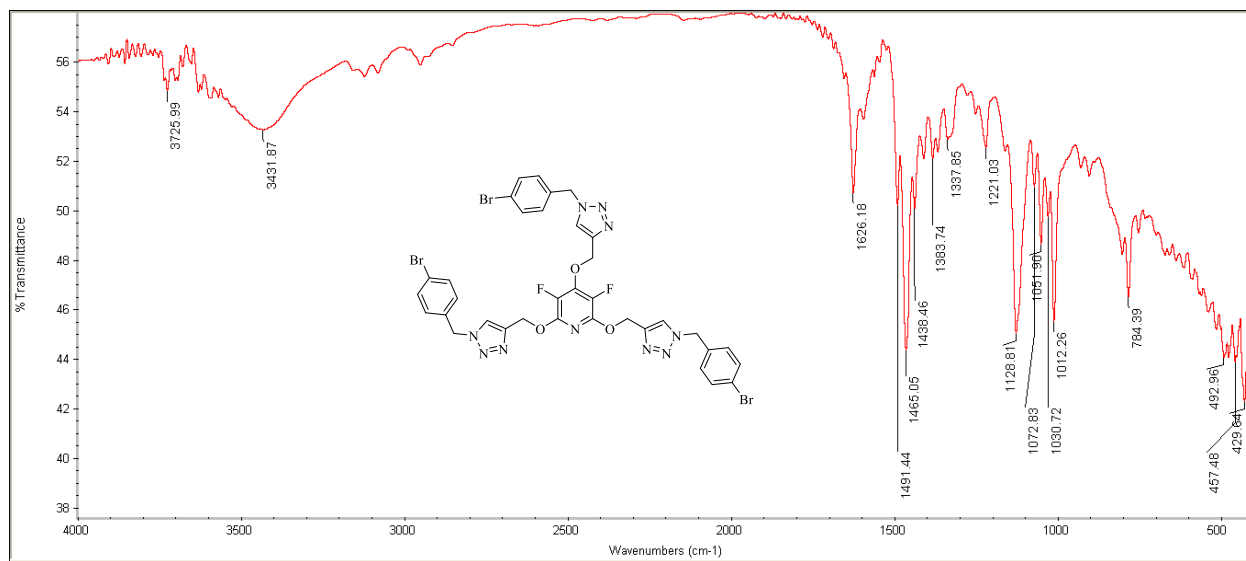
FT-IR spectrum of **3b**



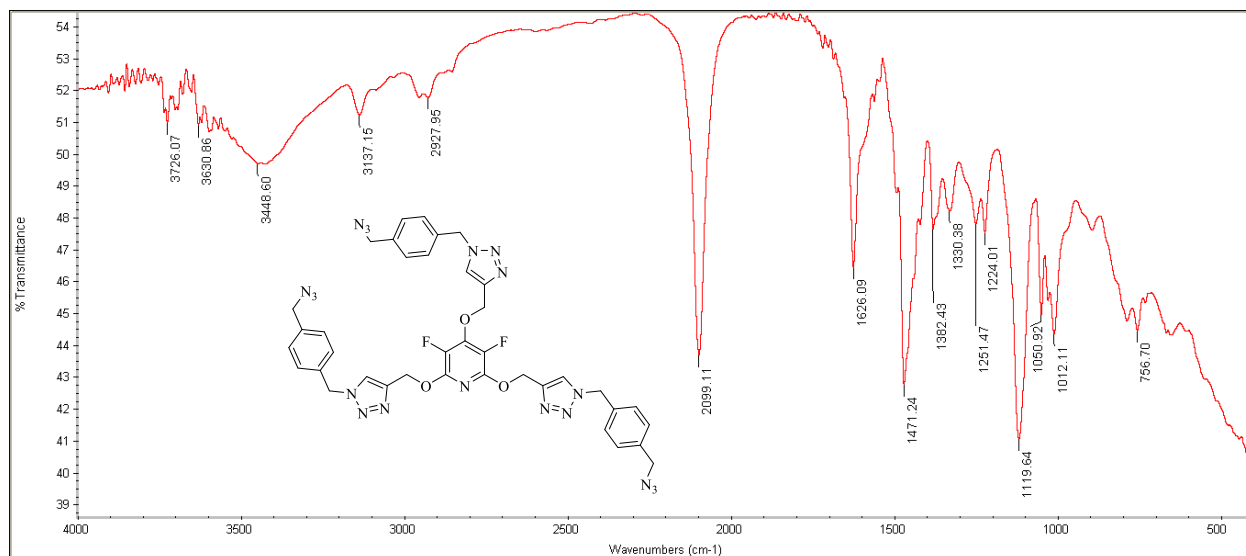
FT-IR spectrum of **3c**



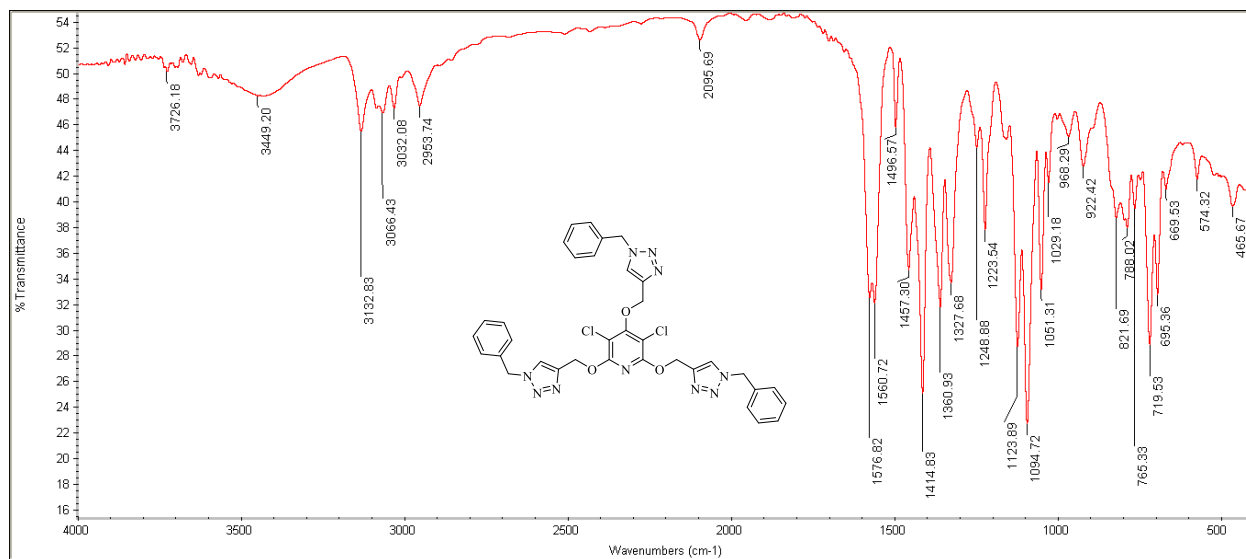
FT-IR spectrum of **5a**



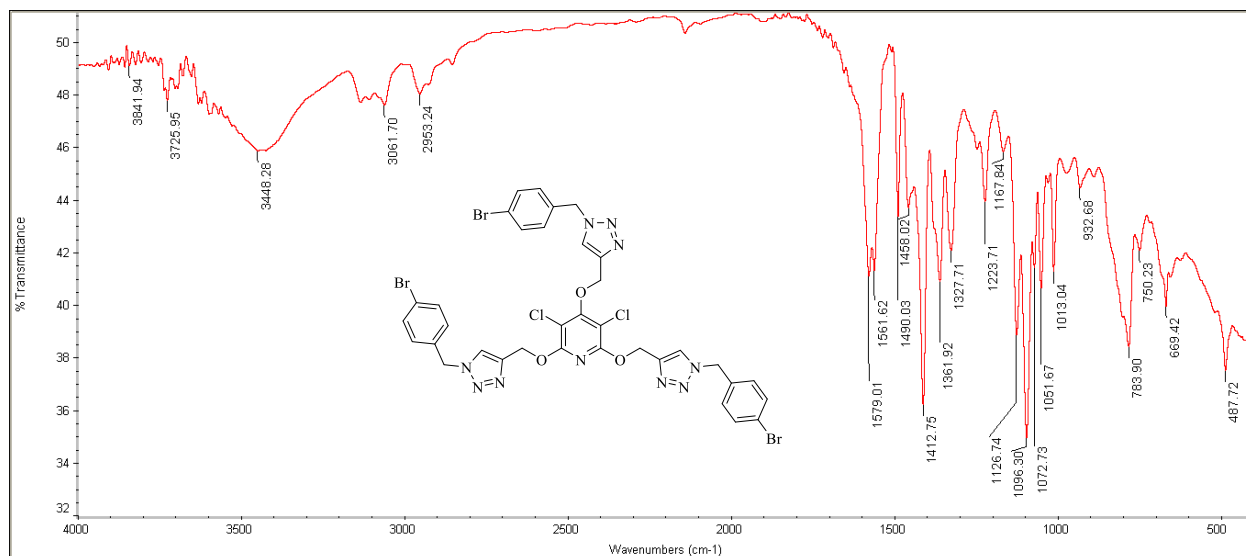
FT-IR spectrum of **5b**



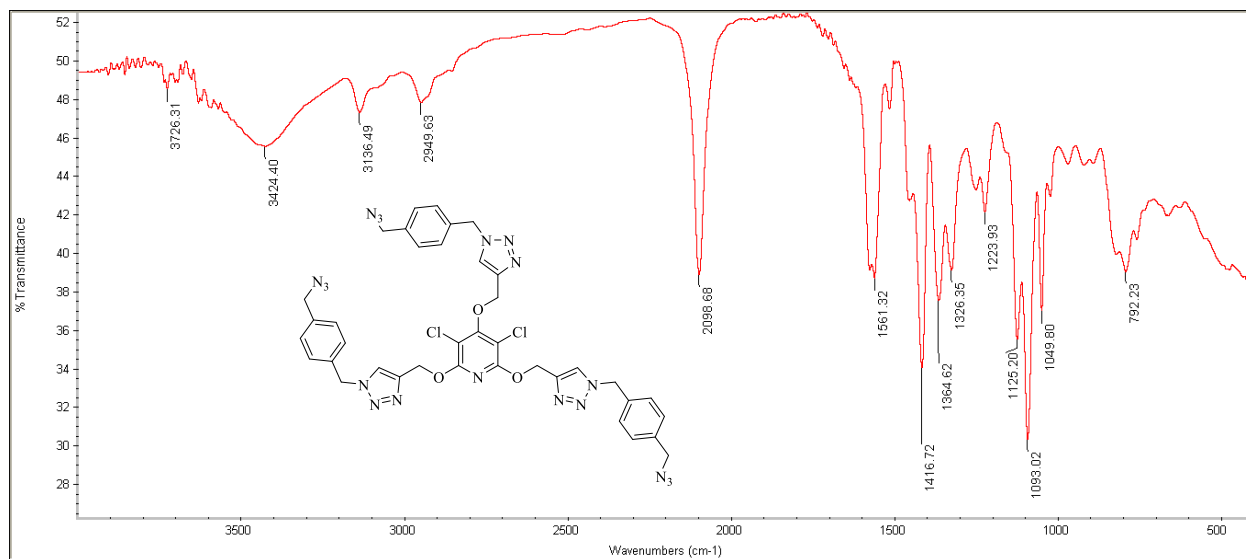
FT-IR spectrum of **5c**



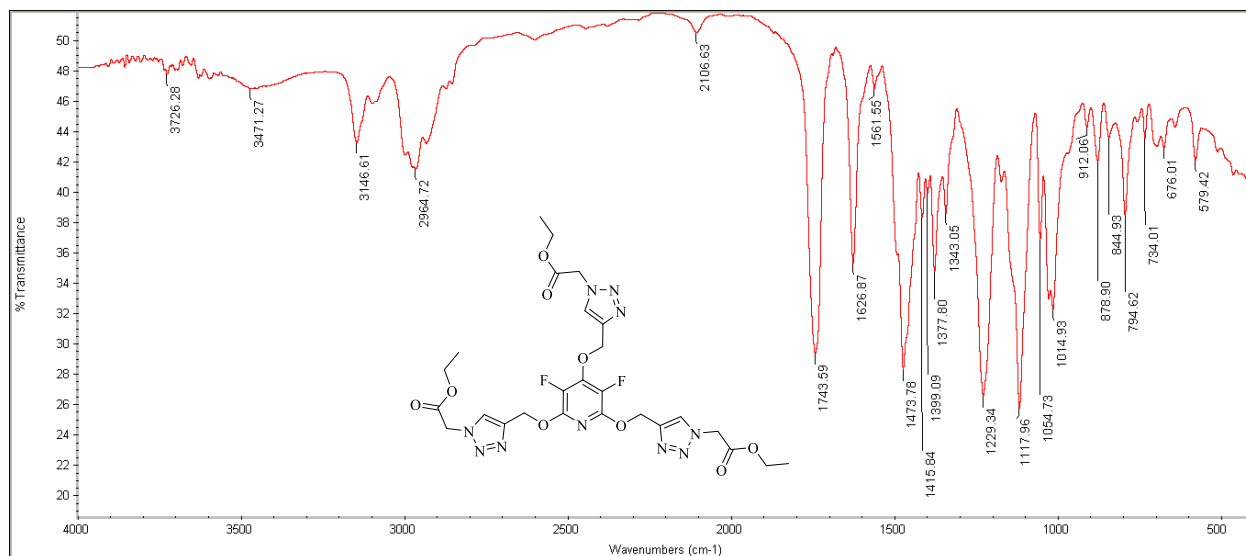
FT-IR spectrum of **5d**



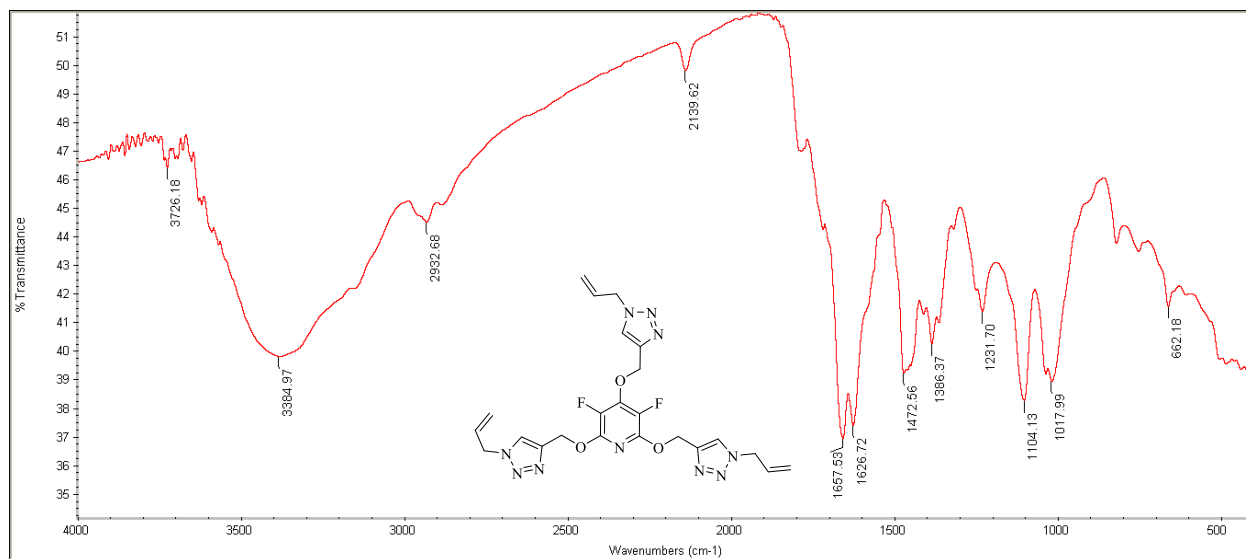
FT-IR spectrum of **5e**



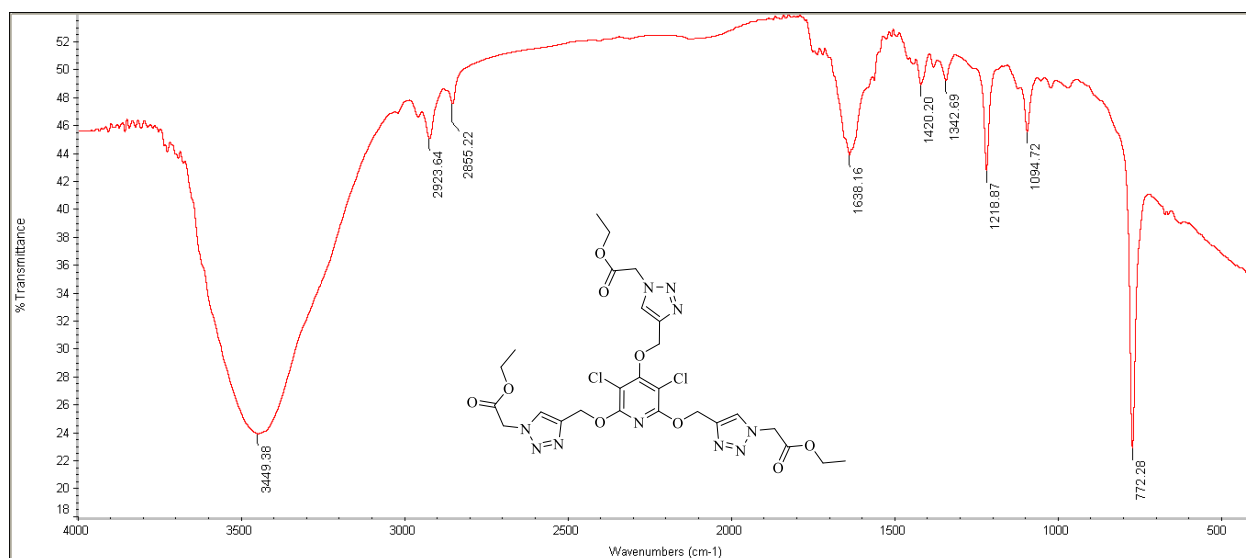
FT-IR spectrum of **5f**



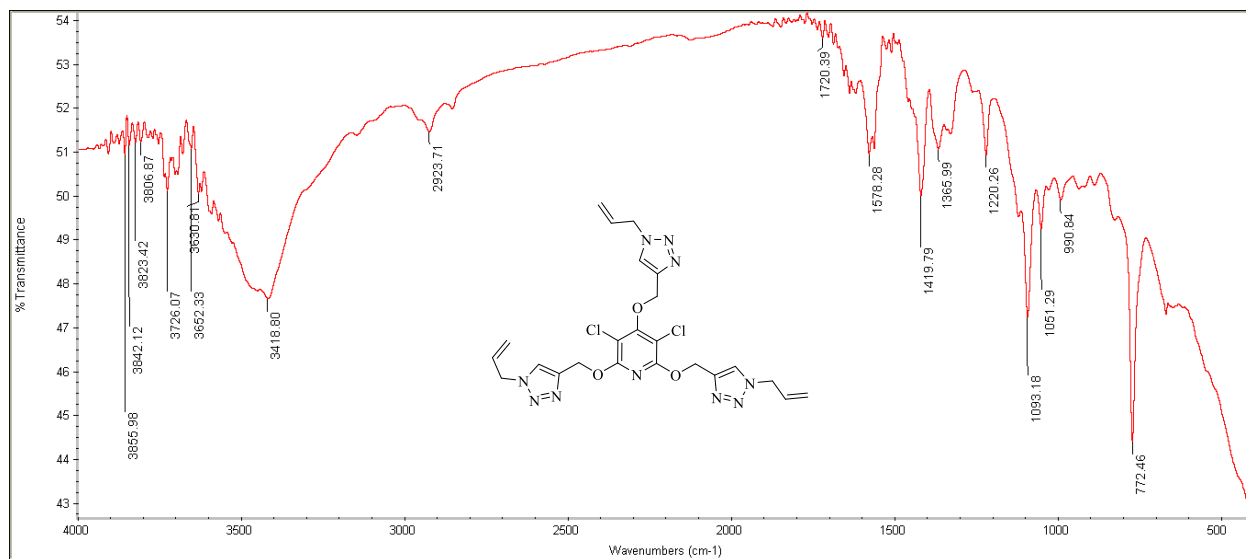
FT-IR spectrum of **7a**



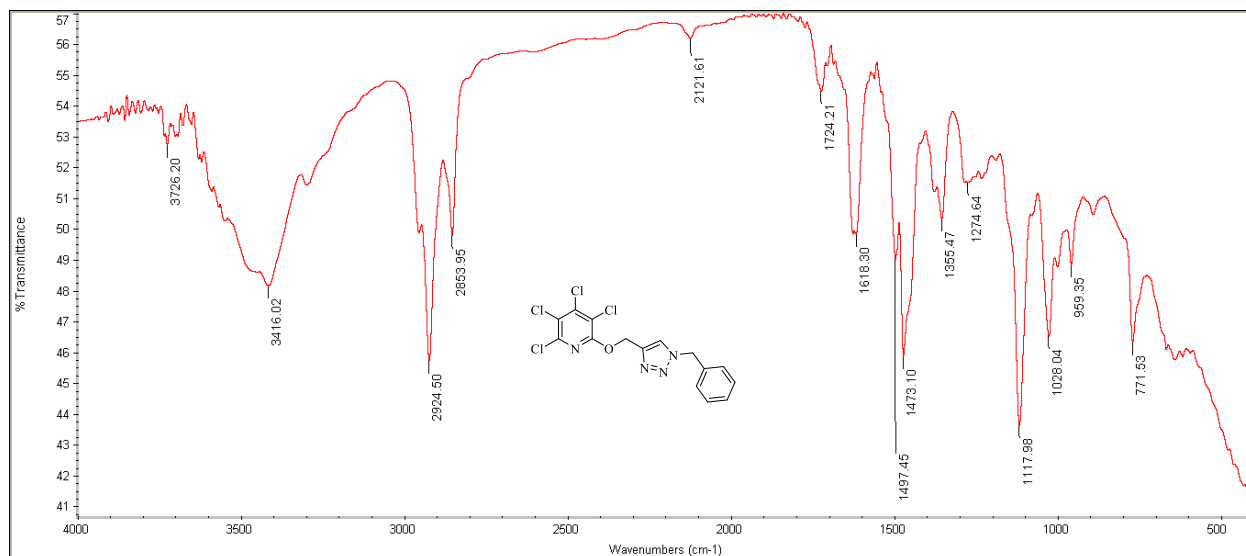
FT-IR spectrum of **7b**



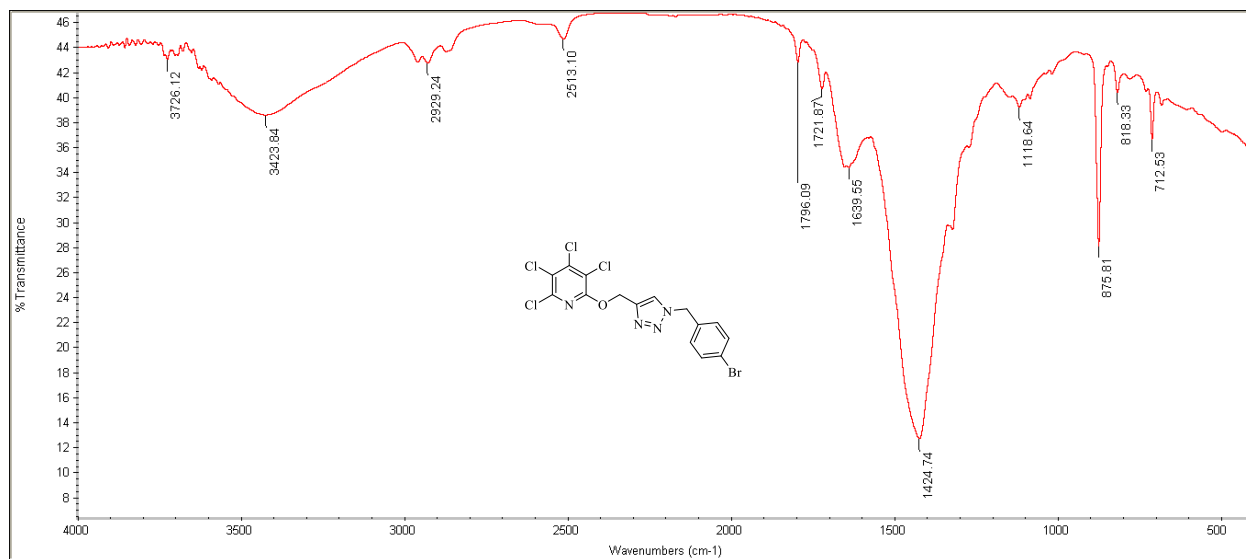
FT-IR spectrum of **7c**



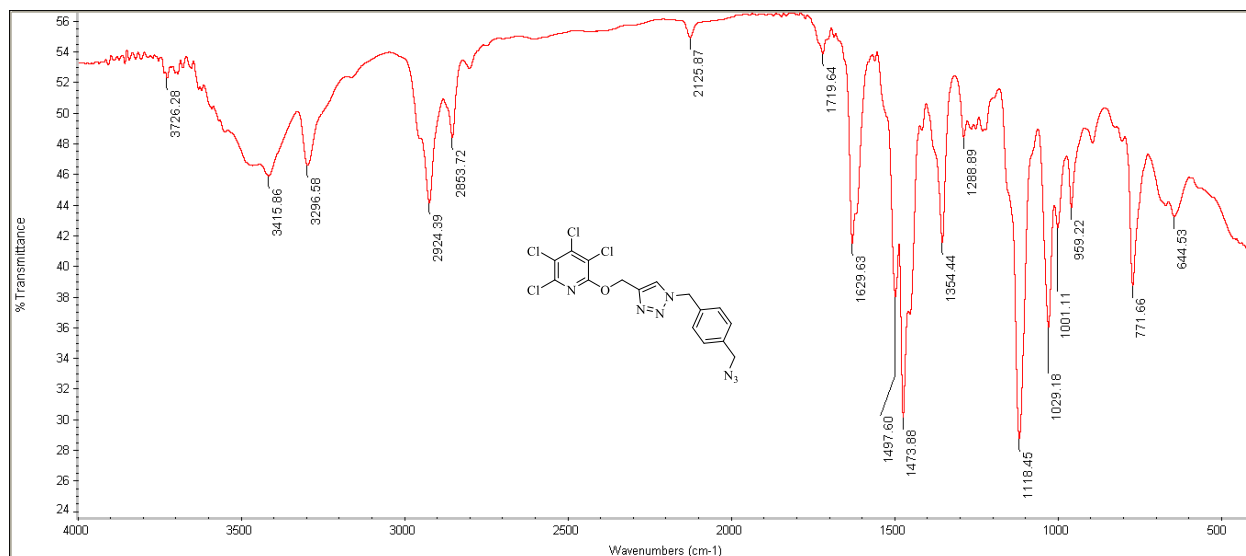
FT-IR spectrum of **7d**

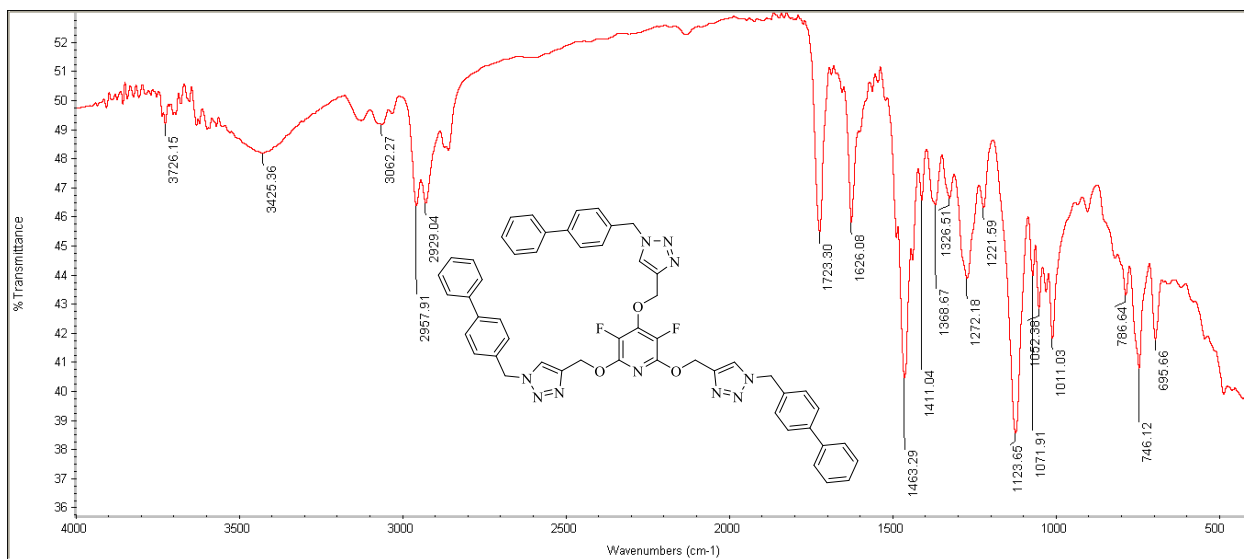


FT-IR spectrum of **8a**

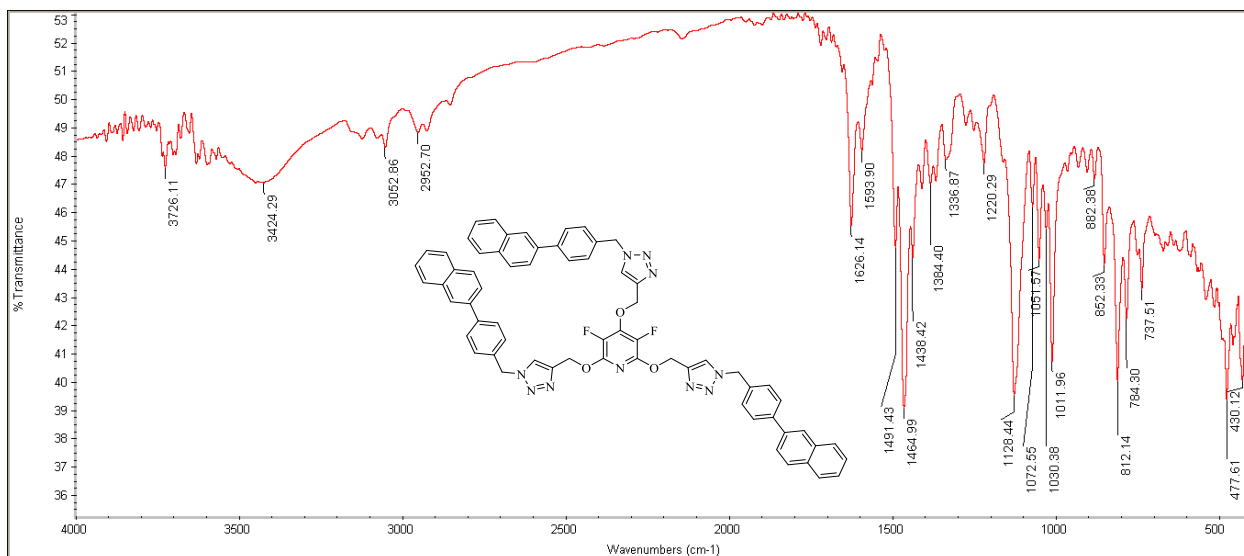


FT-IR spectrum of **8b**

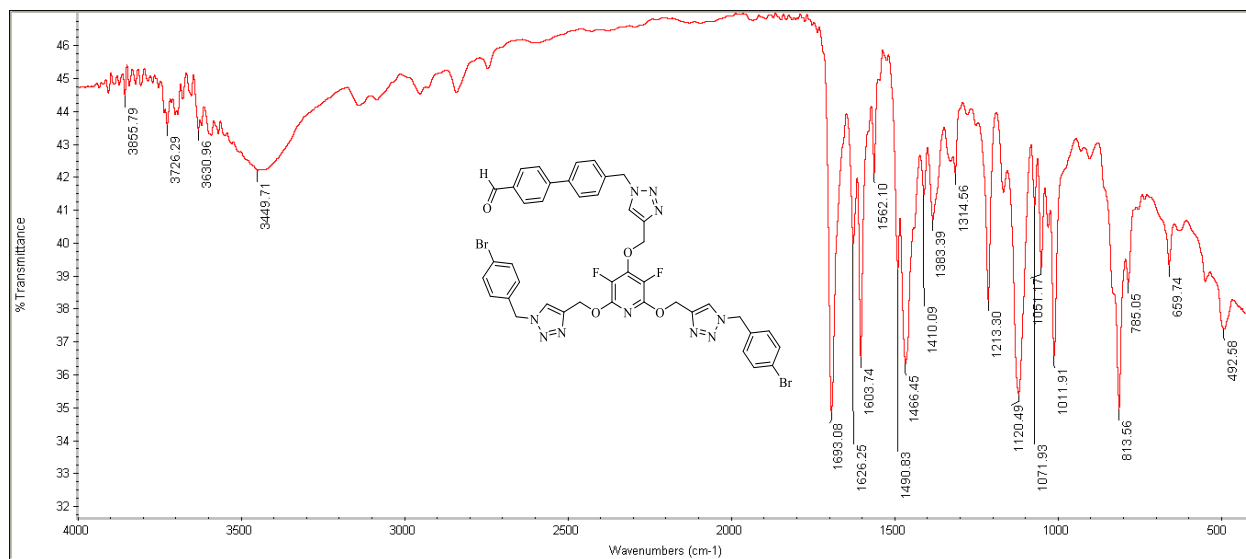




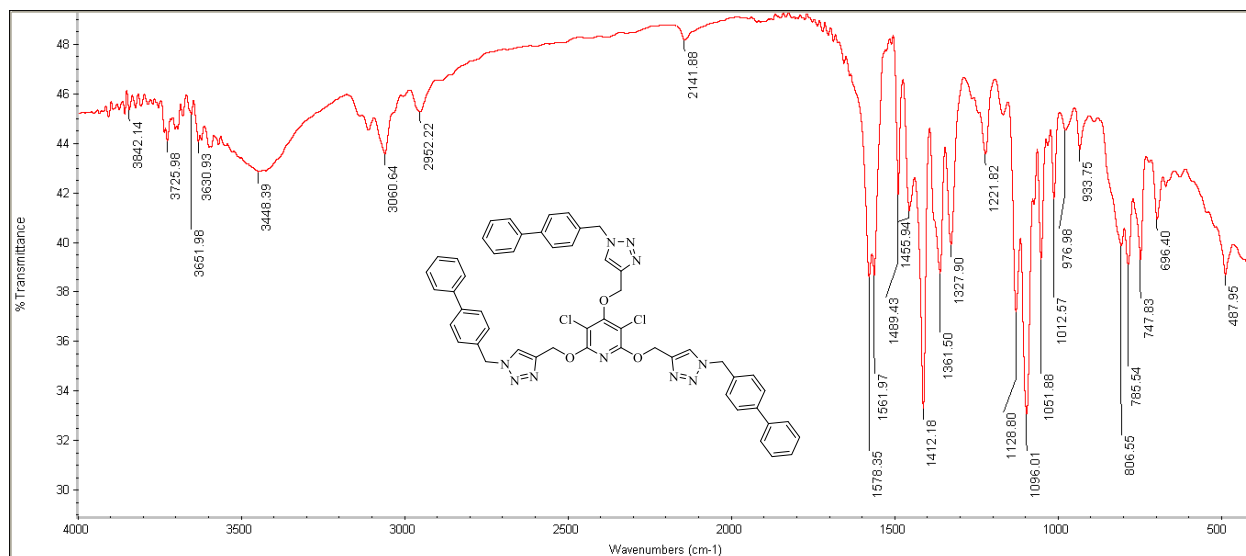
FT-IR spectrum of **10a**



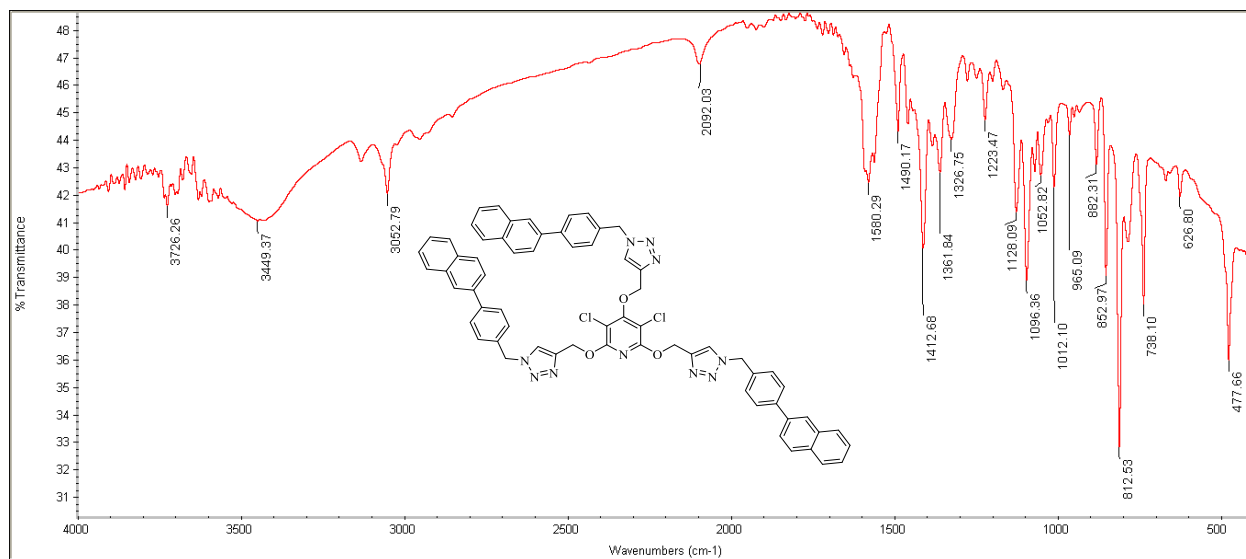
FT-IR spectrum of **10b**



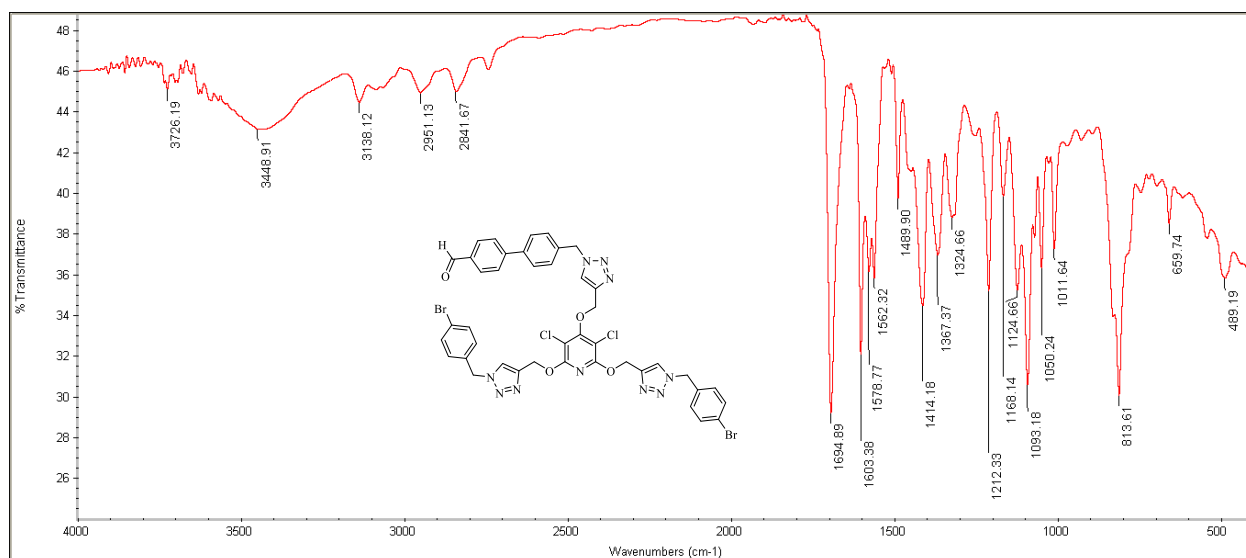
FT-IR spectrum of **10c**



FT-IR spectrum of **10d**



FT-IR spectrum of **10e**



FT-IR spectrum of **10f**