

Controlled Synthesis of Luminescent Xanthene Dyes and Use of Ionic Liquid in Thermochemical Reaction

Bartłomiej Potaniec^{1,†}, Maria Zdończyk^{1,2,†} and Joanna Cybińska^{1,2,*}

¹ Advanced Materials Synthesis Group, Materials Science & Engineering Center, Łukasiewicz Research Network—PORT Polish Center for Technology Development, Stabłowska 147 Street, 54-066 Wrocław, Poland; bartlomiej.potaniec@port.lukasiewicz.gov.pl;

² Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14 Street, 50-383 Wrocław, Poland; maria.zdonczyk@chem.uni.wroc.pl

* Correspondence: joanna.cybinska@chem.uni.wroc.pl or joanna.cybinska@port.lukasiewicz.gov.pl

† These authors contributed equally to this work.

S1. Spectroscopic characterization

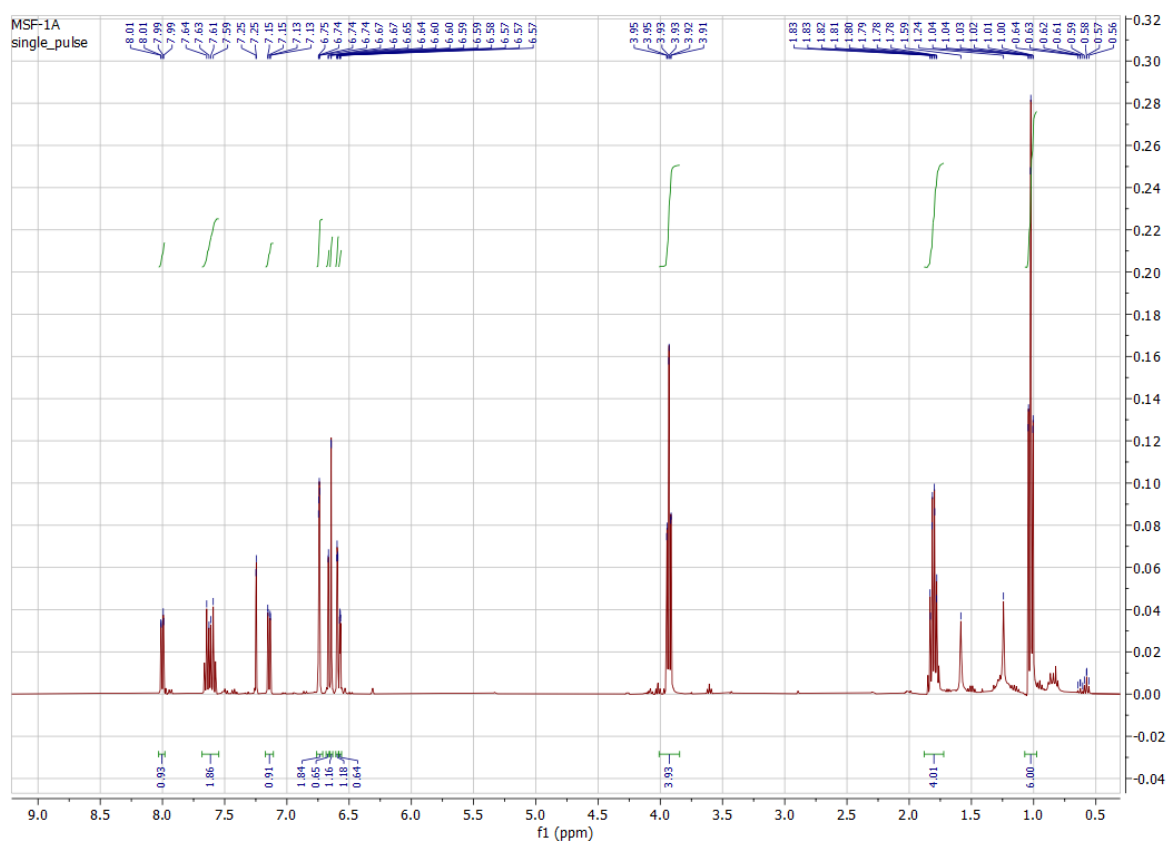


Figure S1. ¹H-NMR (600 MHz, chloroform-*d*) spectrum of product **1A**.

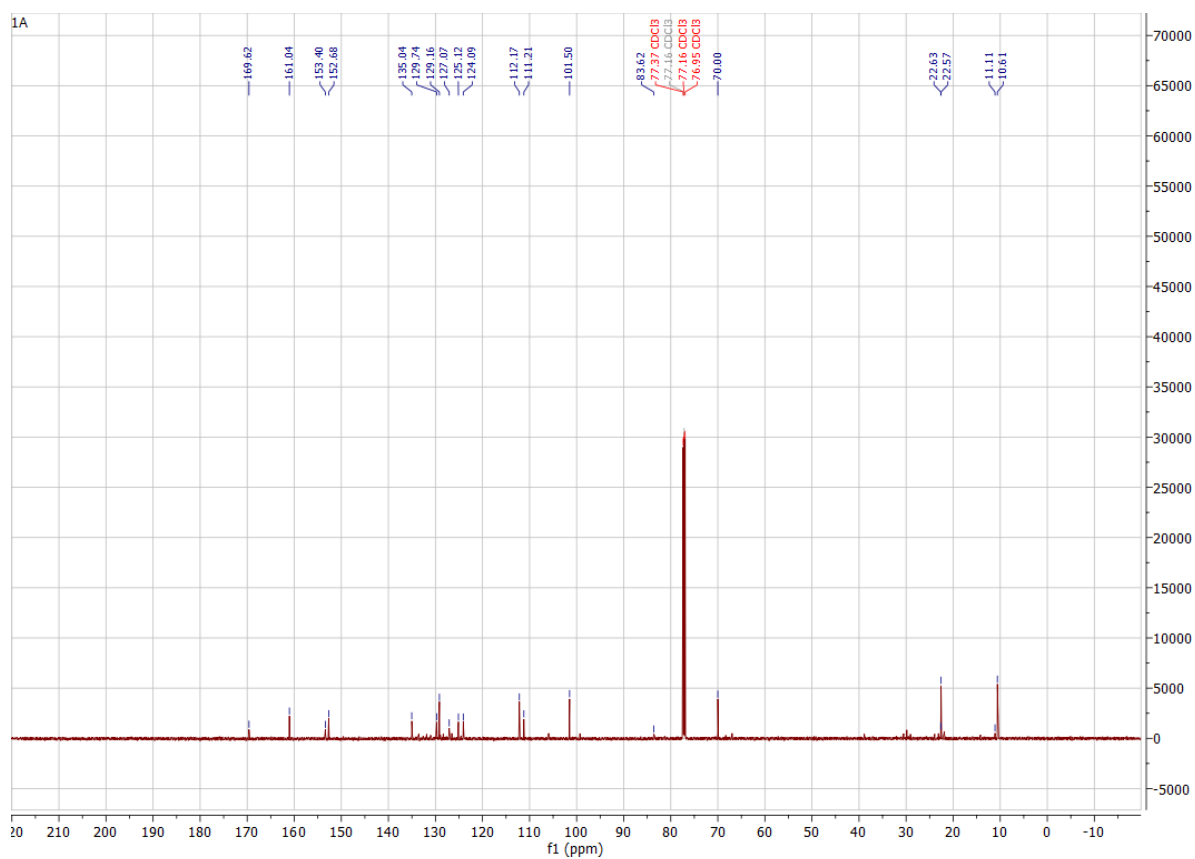


Figure S2. ^{13}C -NMR (151 MHz, chloroform- d) spectrum of product **1A**.

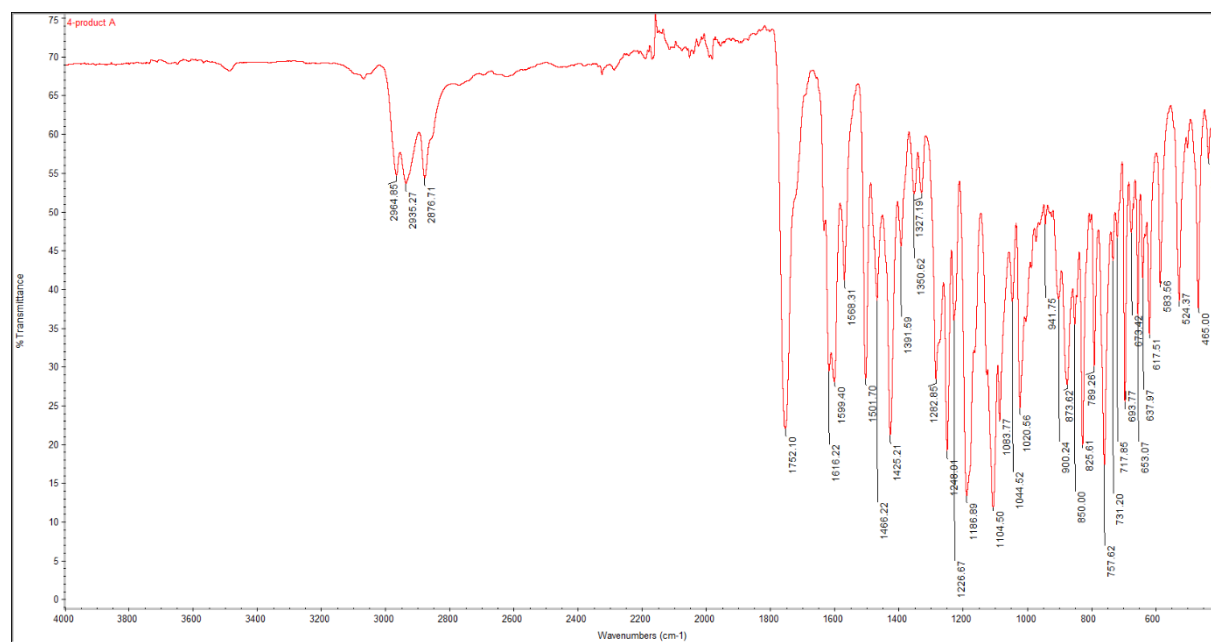


Figure S3. FTIR-ATR spectrum of product **1A**.

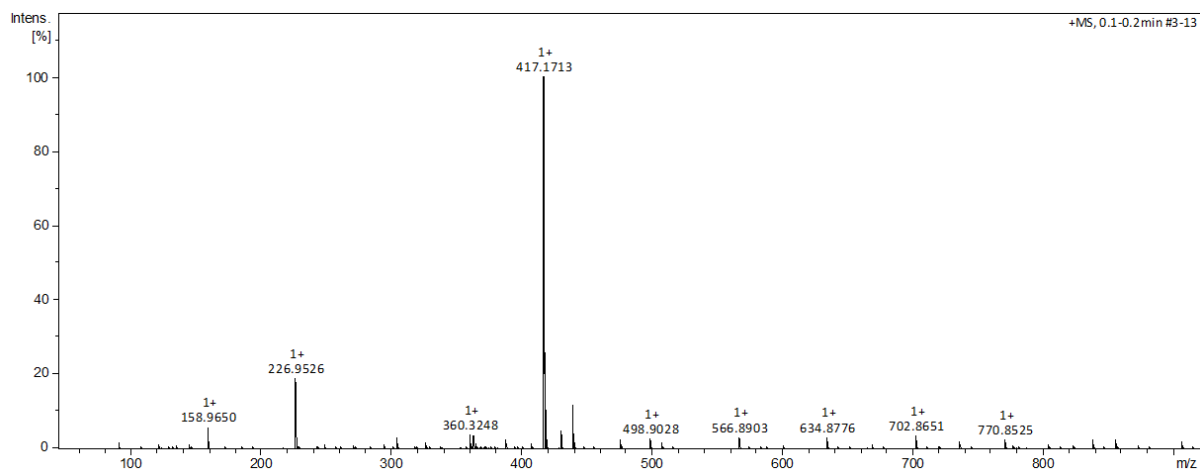


Figure S4. HR ESI-MS spectrum of product **1A**.

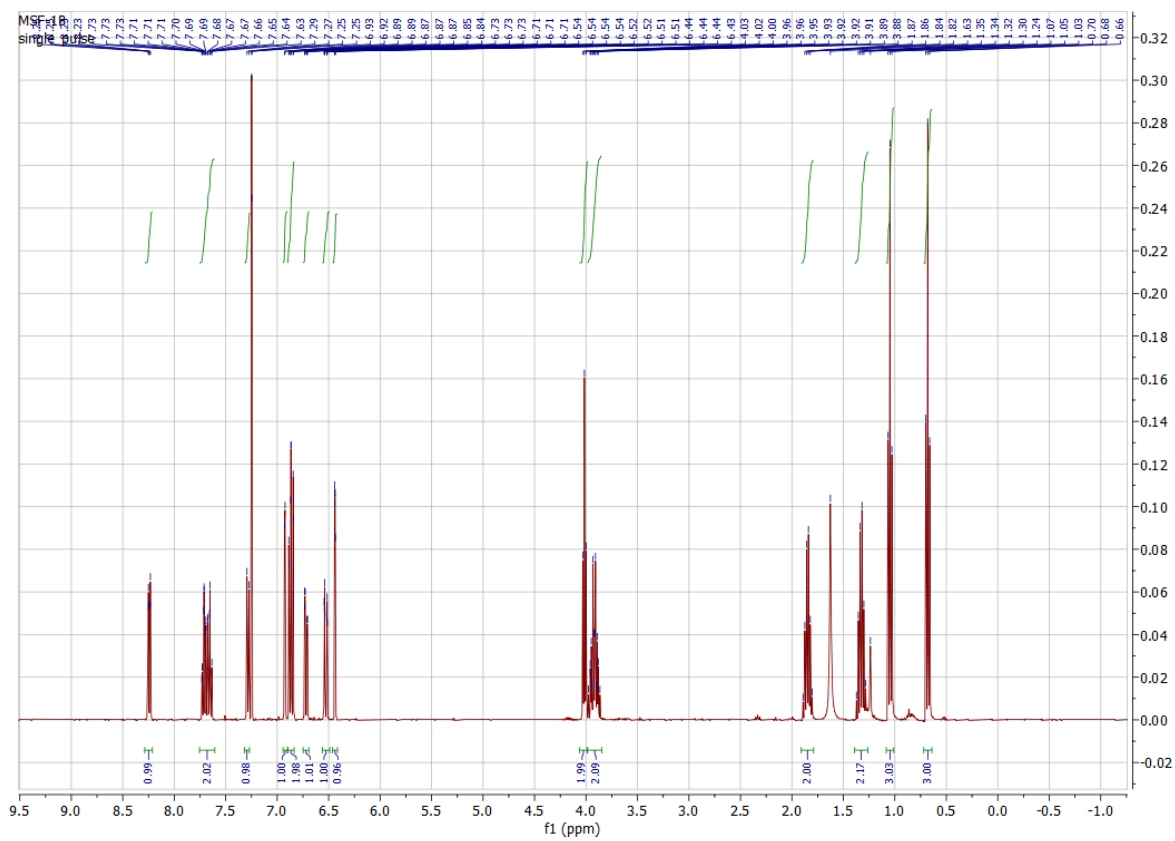


Figure S5. ¹H-NMR (600 MHz, chloroform-*d*) spectrum of product **1B**.

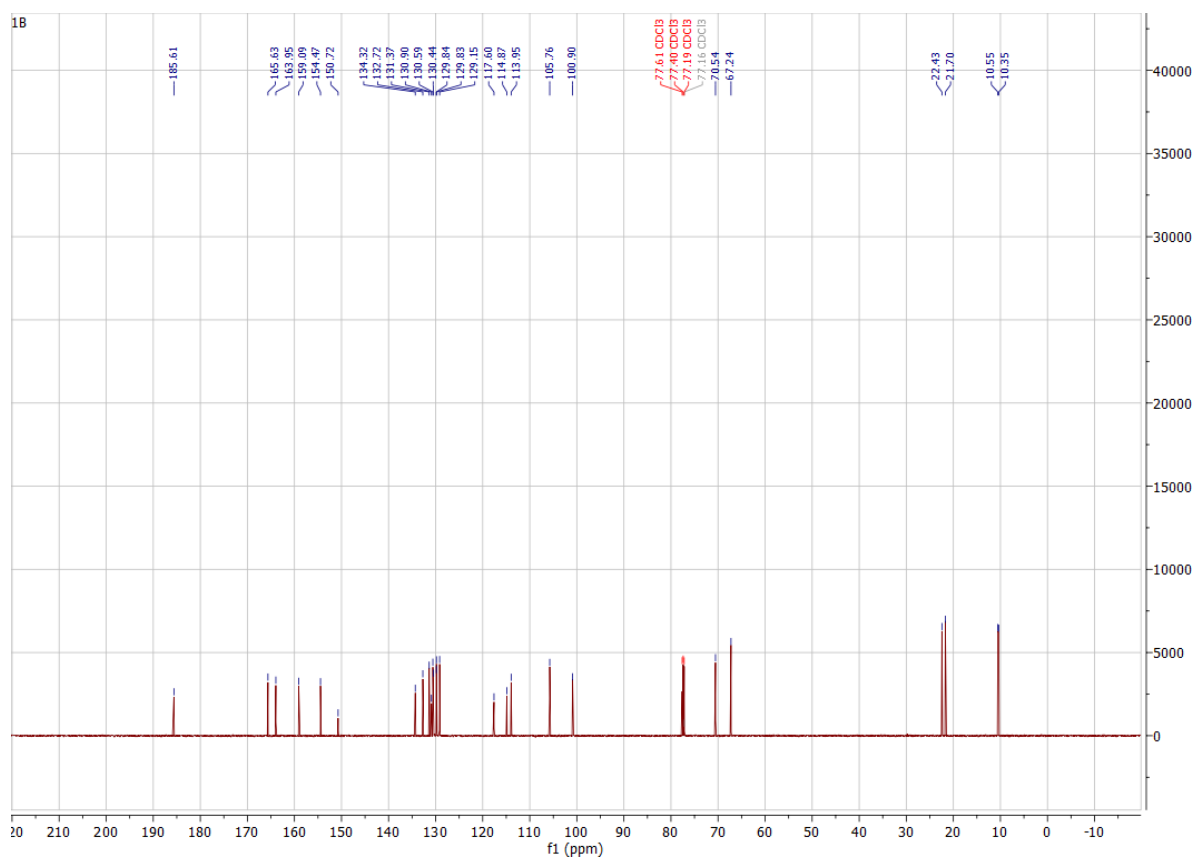


Figure S6. ^{13}C -NMR (151 MHz, chloroform- d) spectrum of product **1B**.

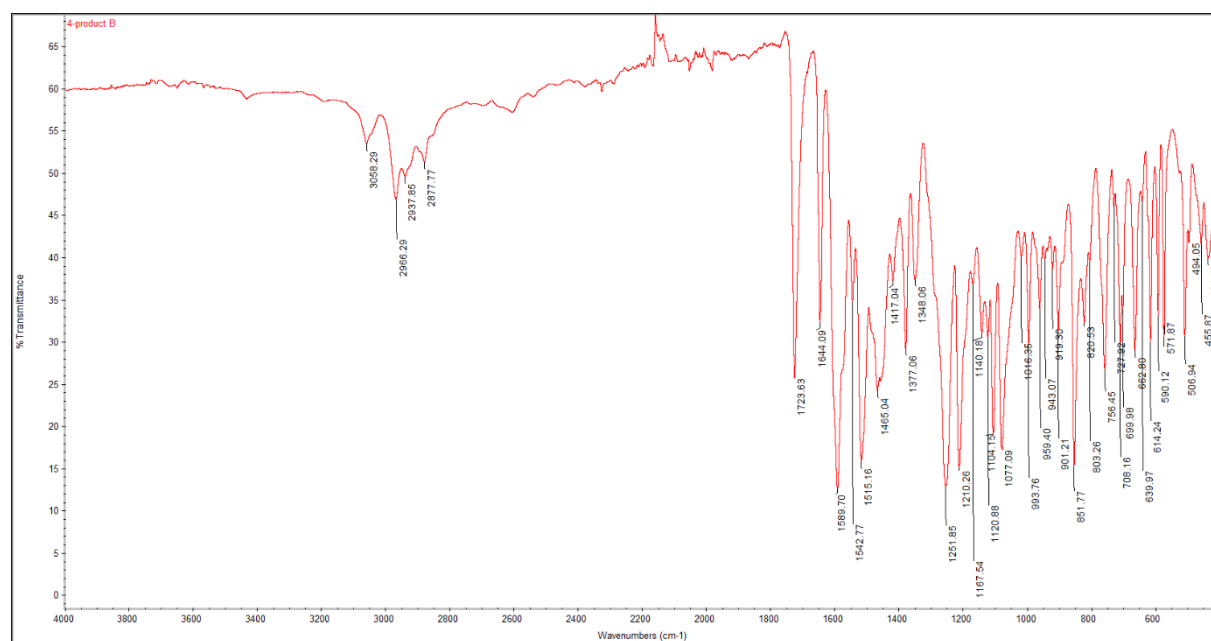


Figure S7. FTIR-ATR spectrum of product **1B**.

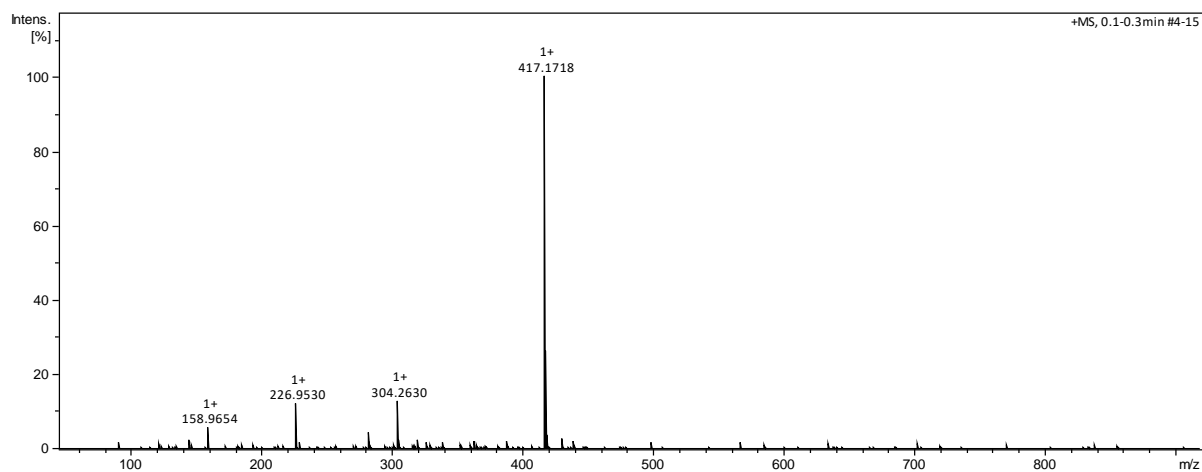


Figure S8. HR ESI-MS spectrum of product **1B**.

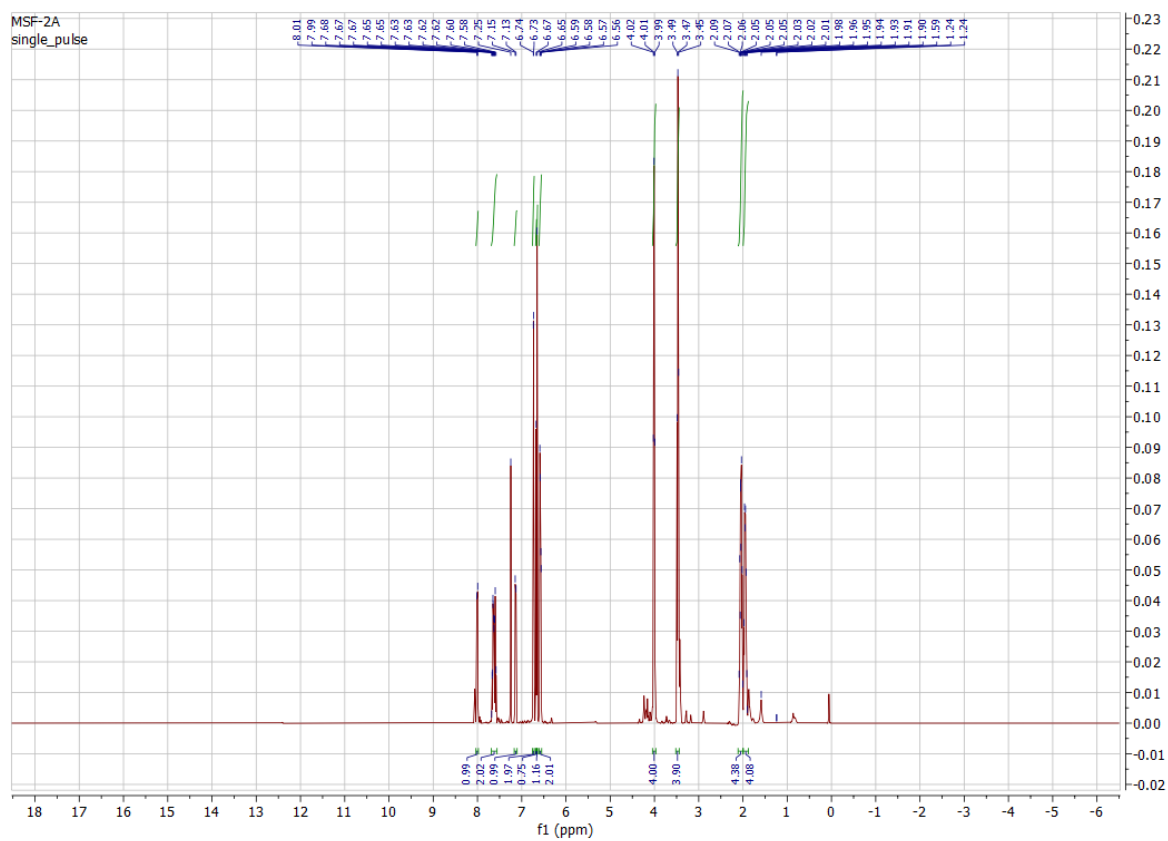


Figure S9. ^1H -NMR (600 MHz, CDCl_3) spectrum of product **2A**.

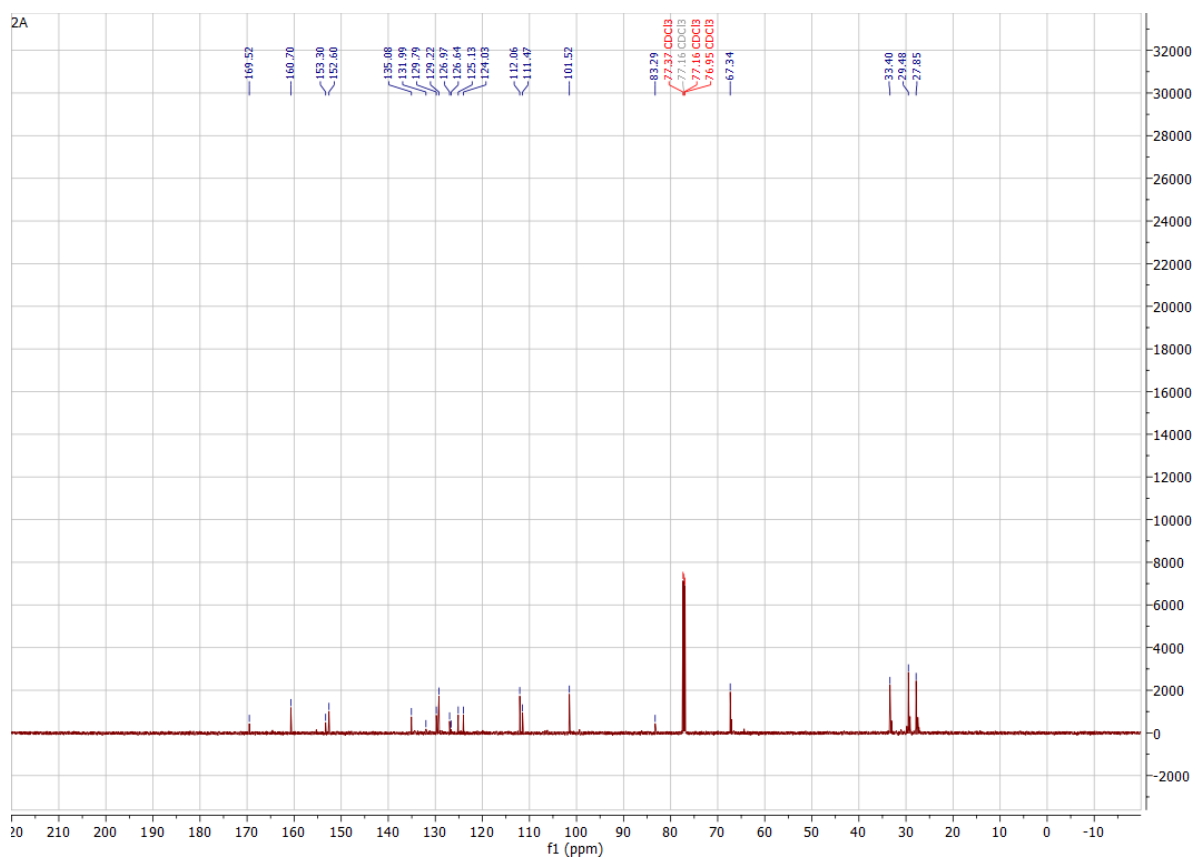


Figure S10. ^{13}C -NMR (151 MHz, chloroform-*d*) spectrum of product **2A**.

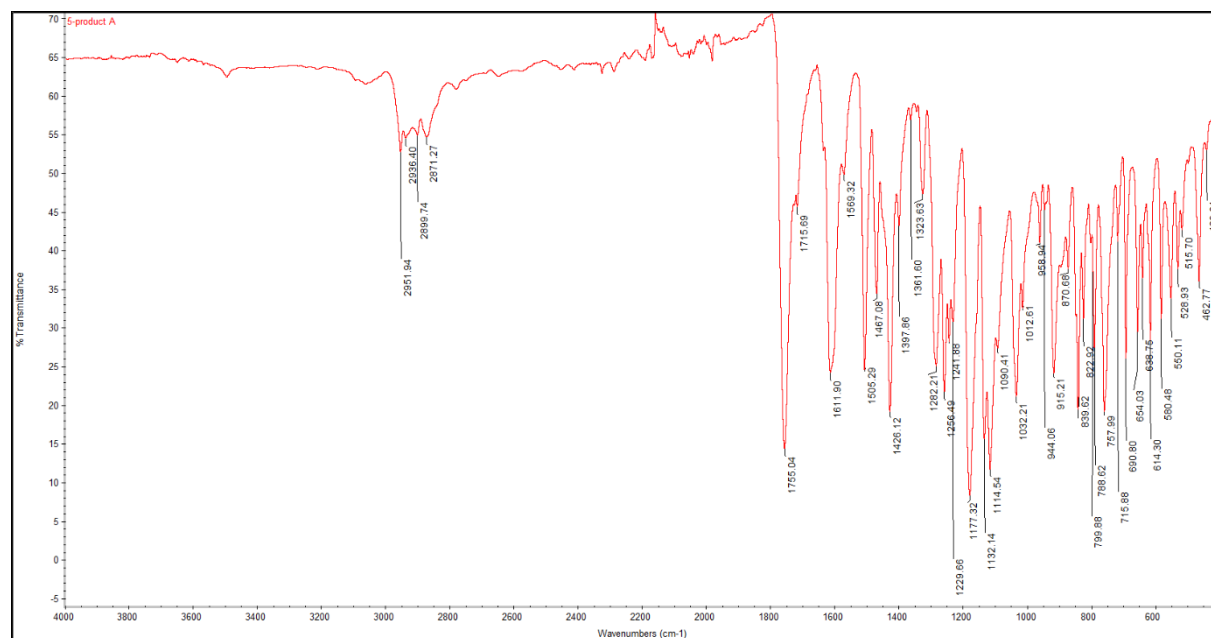


Figure S11. FTIR-ATR spectrum of product **2A**.

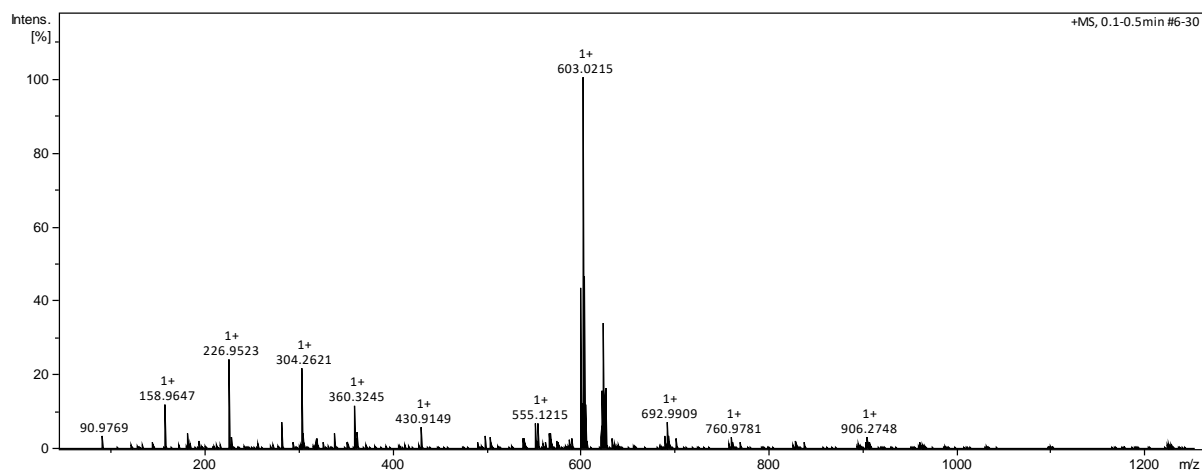


Figure S12. HR ESI-MS spectrum of product 2A.

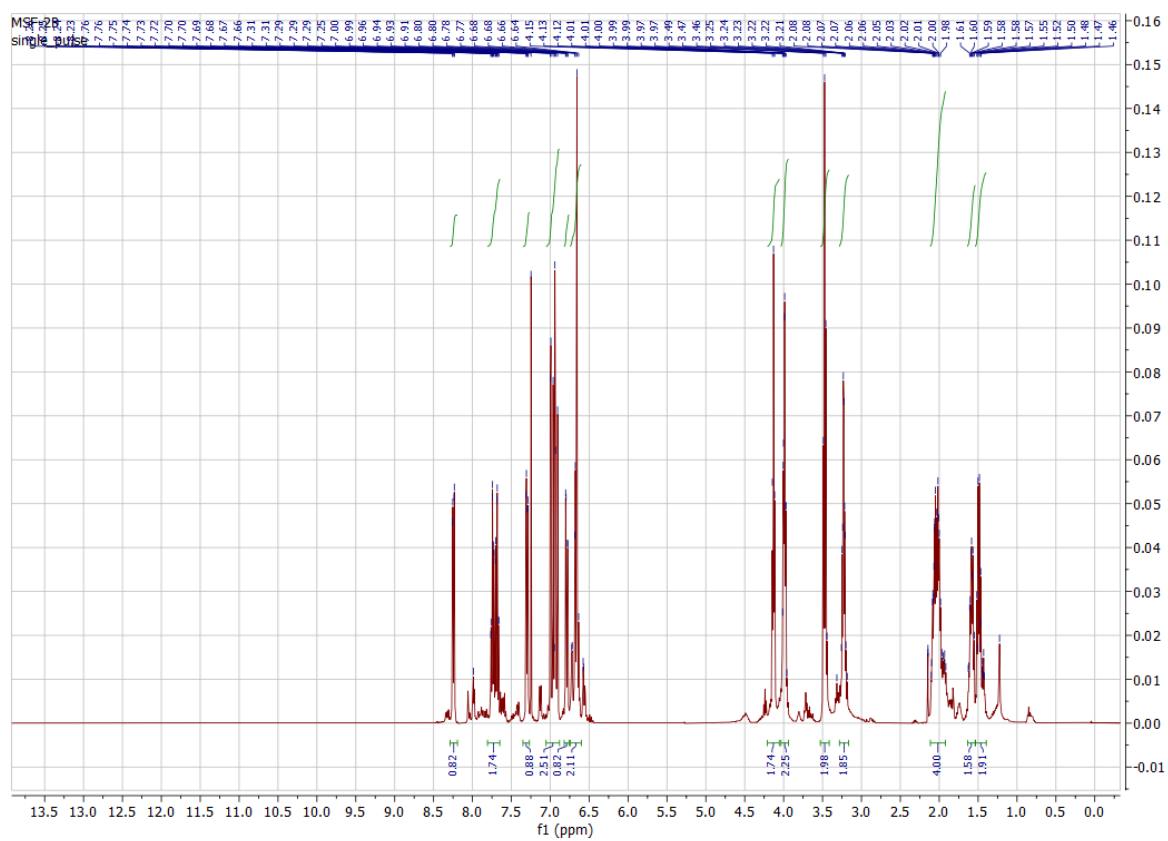


Figure S13. ¹H-NMR (600 MHz, chloroform-*d*) spectrum of product 2B.

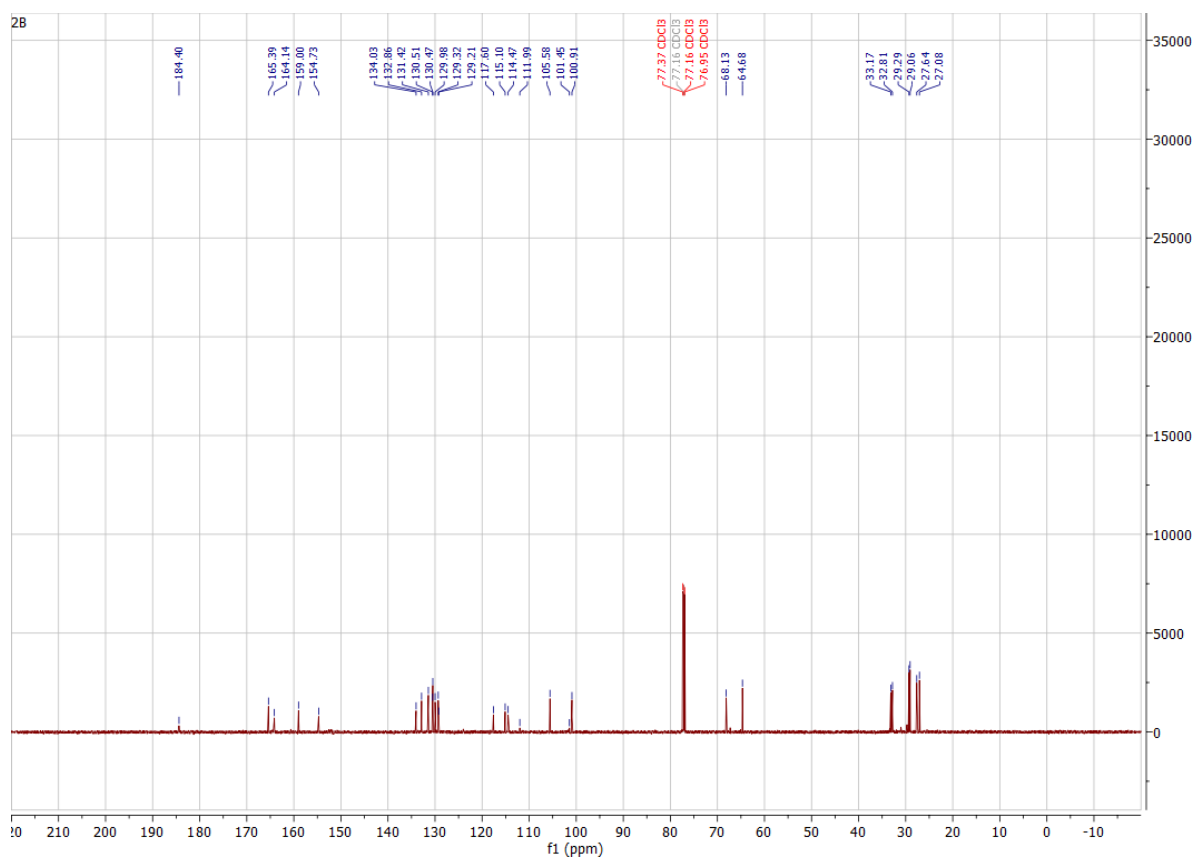


Figure S14. ^{13}C -NMR (151 MHz, chloroform- d) spectrum of product **2B**.

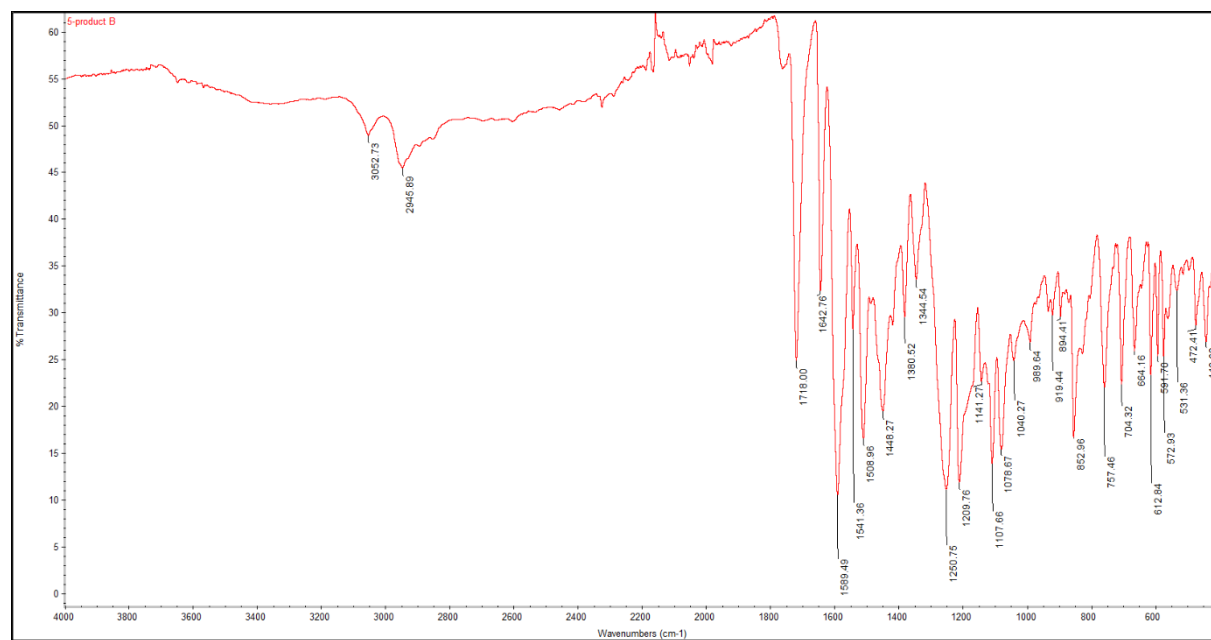


Figure S15. FTIR-ATR spectrum of product **2B**.

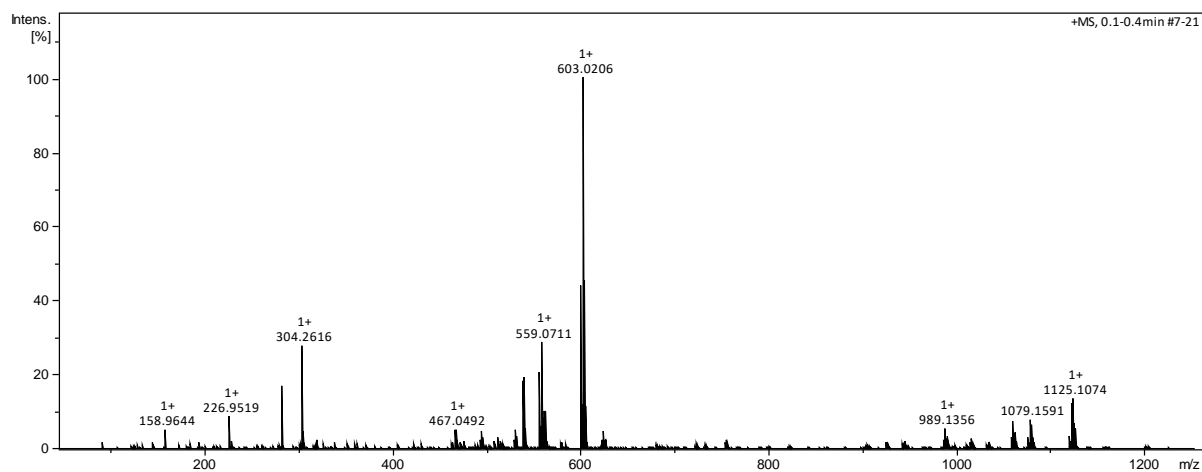


Figure S16. HR ESI-MS spectrum of product **2B**.

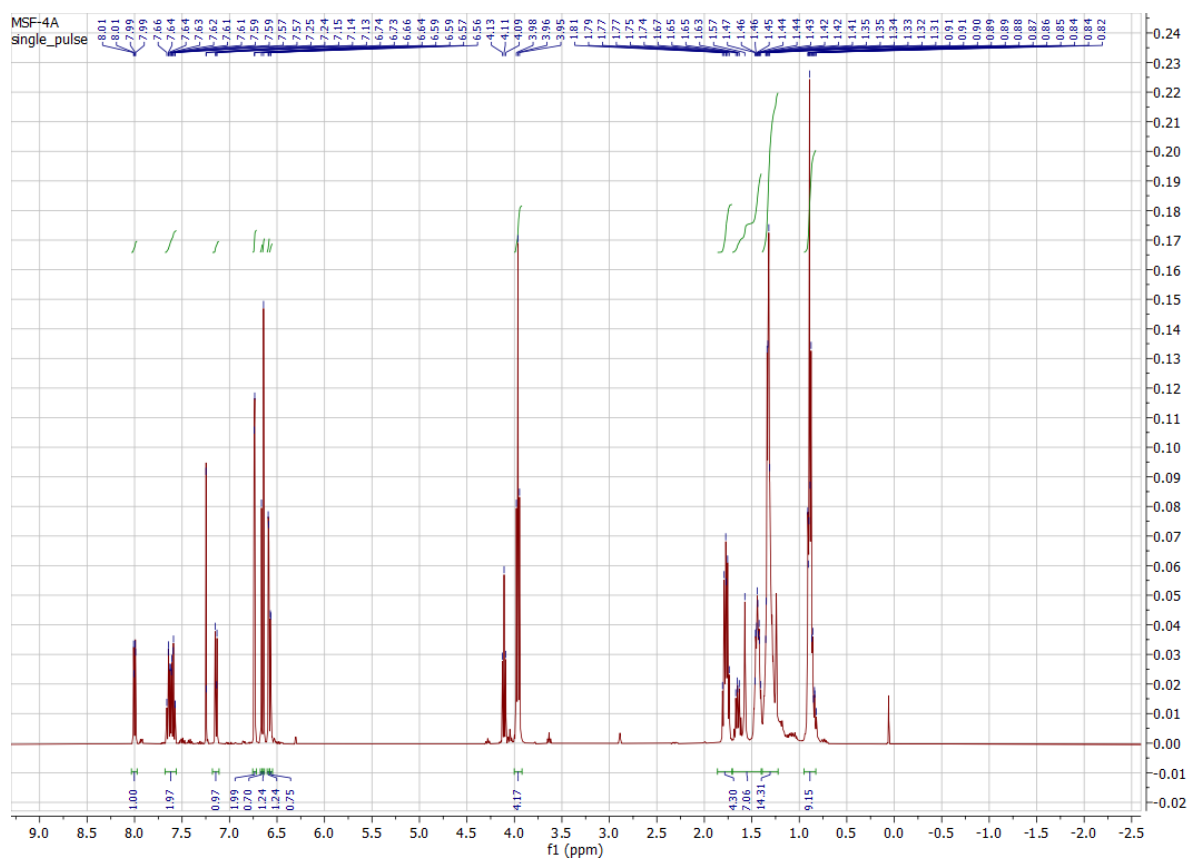


Figure S17. ^1H -NMR (600 MHz, CDCl_3) spectrum of product **3A**.

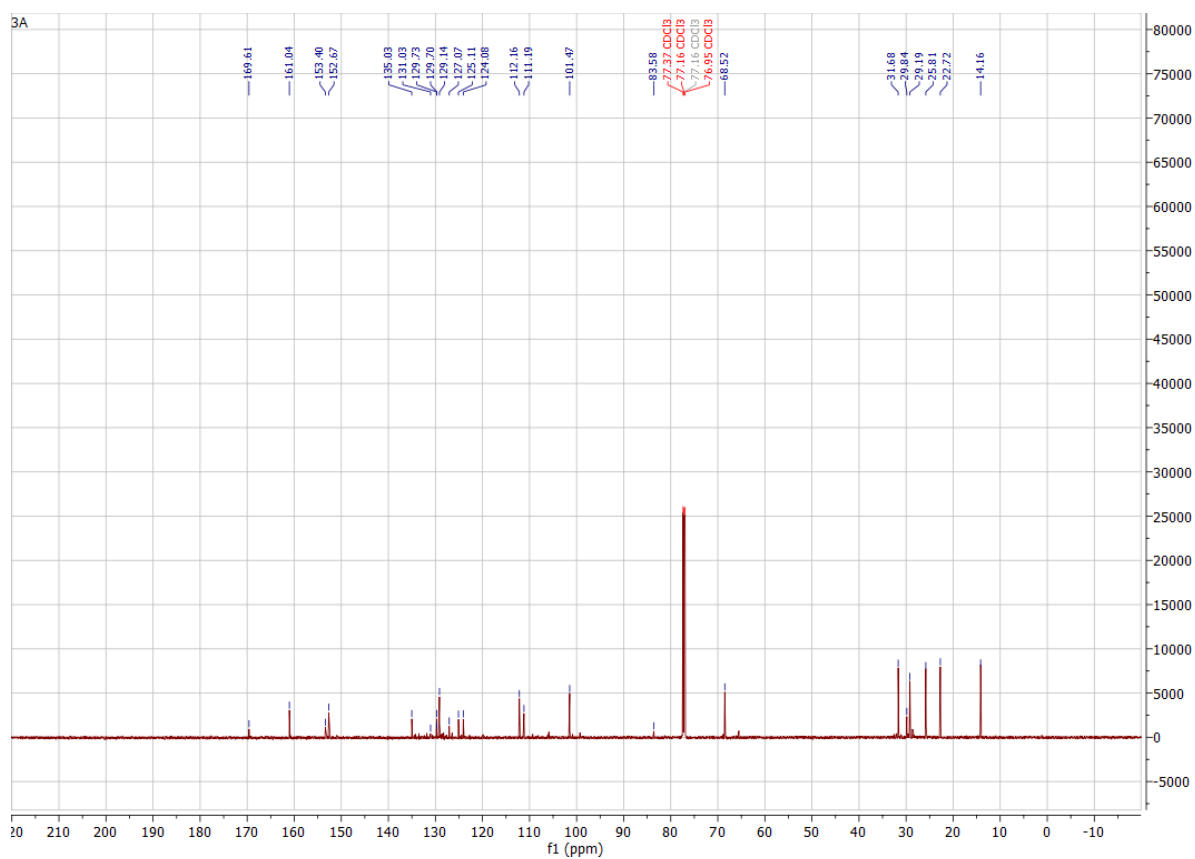


Figure S18. ^{13}C -NMR (151 MHz, chloroform-*d*) spectrum of product **3A**.

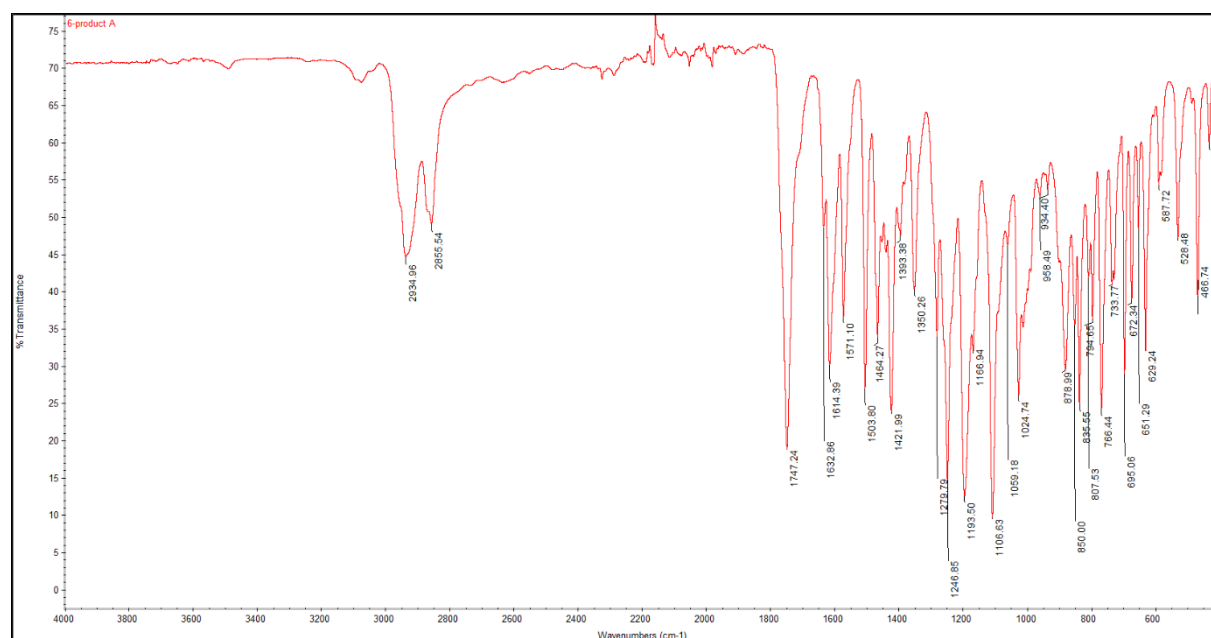


Figure S19. FTIR-ATR spectrum of product **3A**.

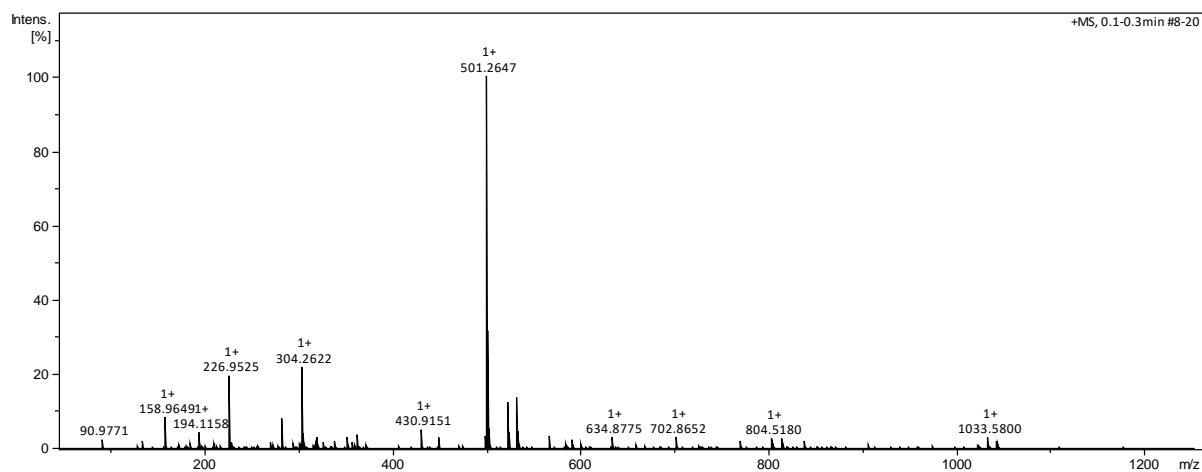


Figure S20. HR ESI-MS spectrum of product **3A**.

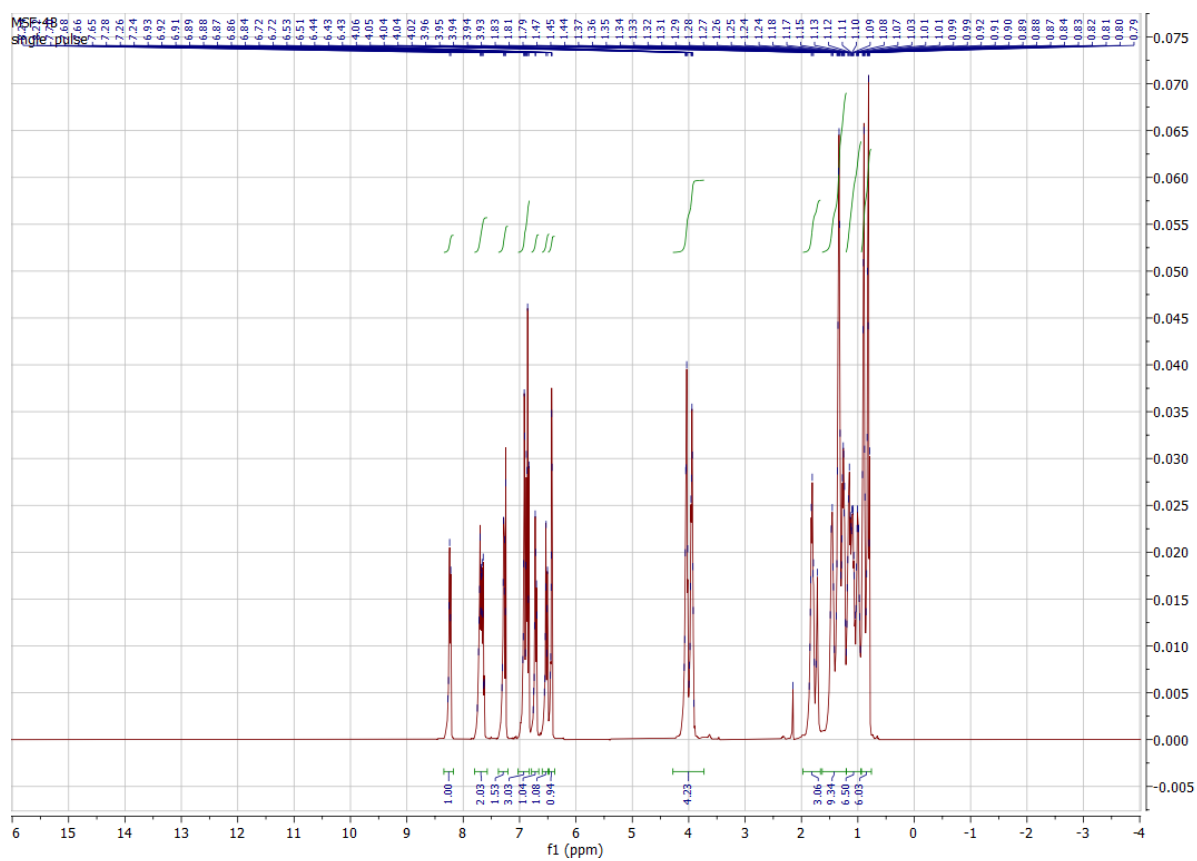


Figure S21. ^1H -NMR (600 MHz, CDCl_3) spectrum of product **3B**.

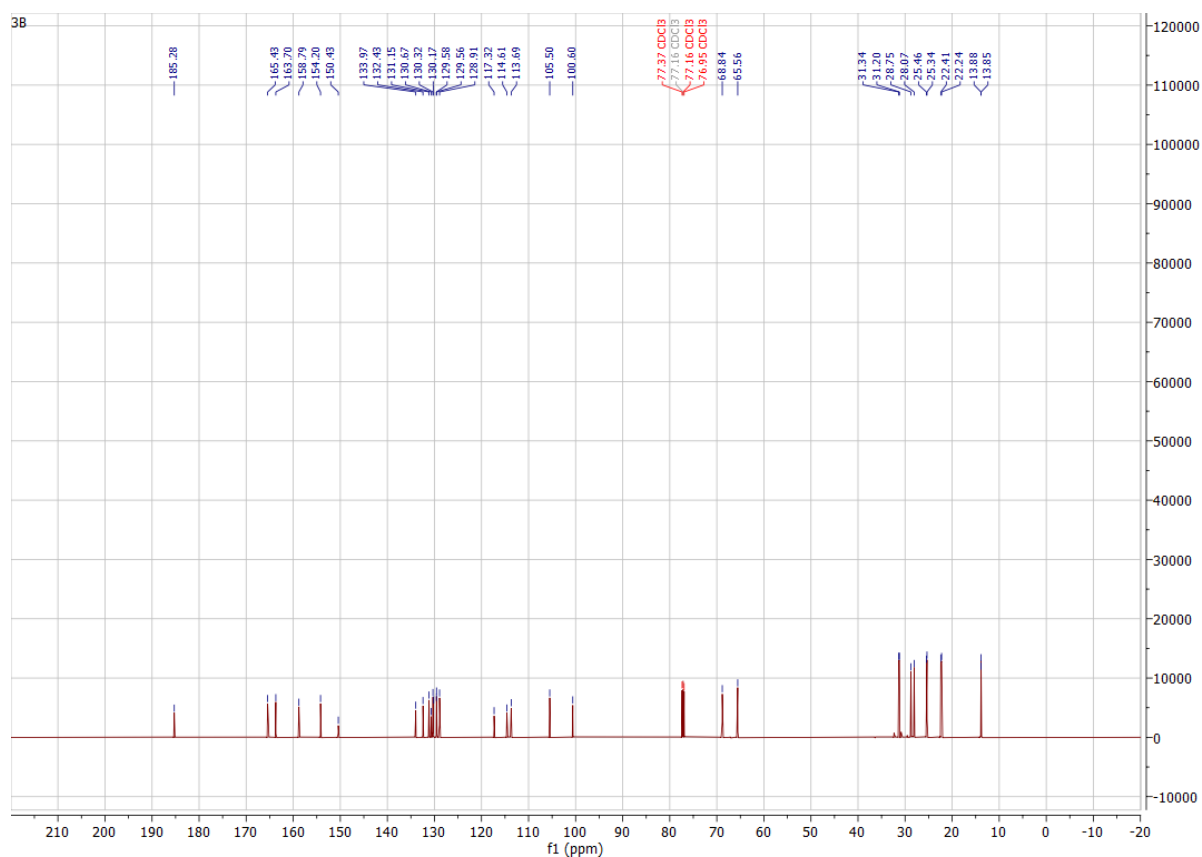


Figure S22. ^{13}C -NMR (151 MHz, chloroform- d) spectrum of product **3B**.

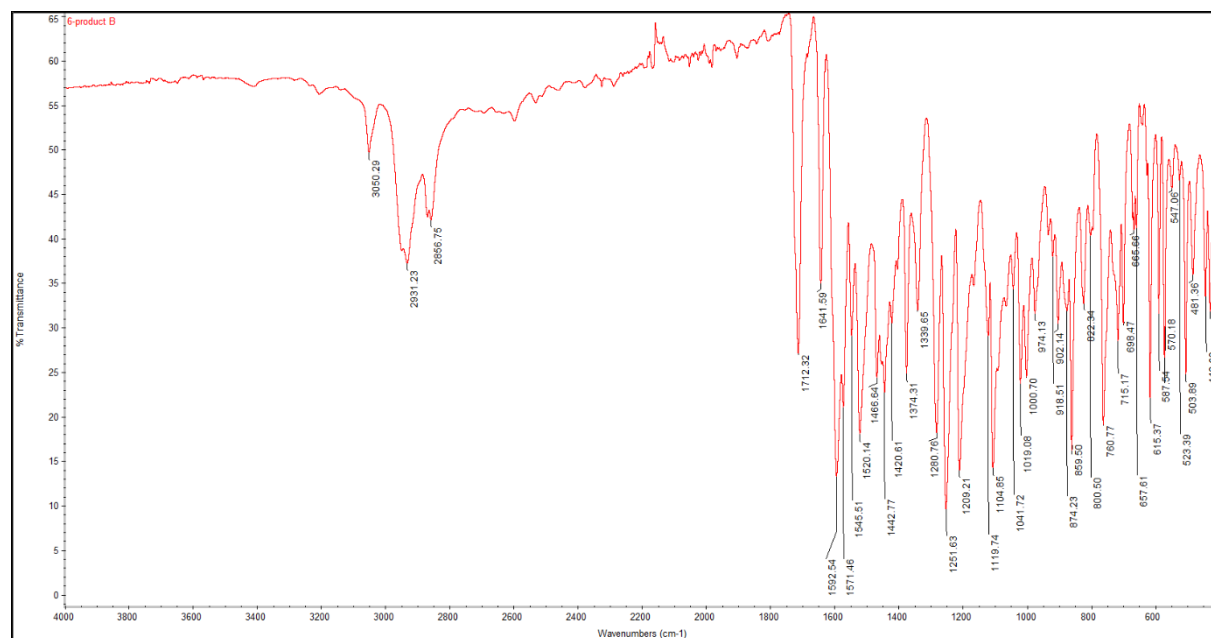


Figure S23. FTIR-ATR spectrum of product **3B**.

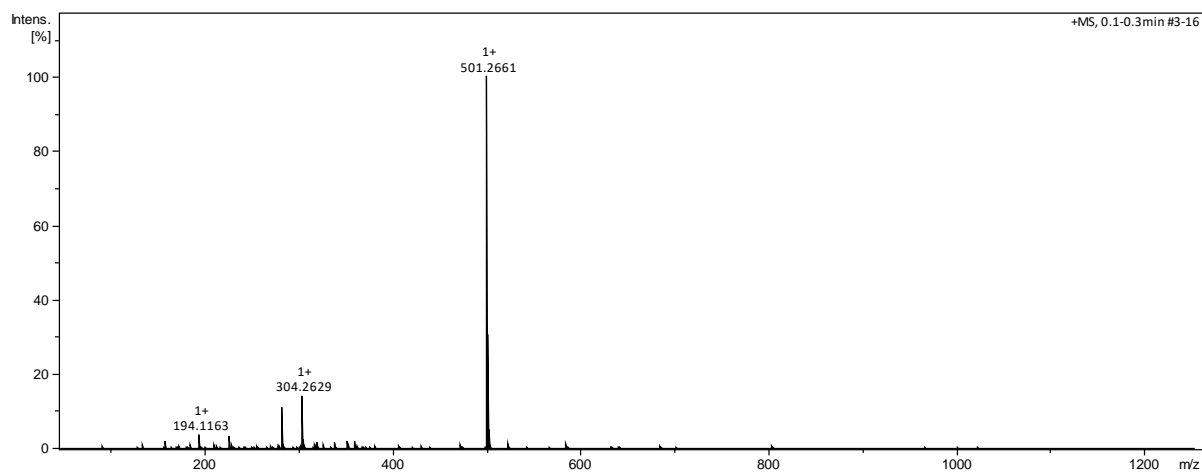


Figure S24. HR ESI-MS spectrum of product **3B**.

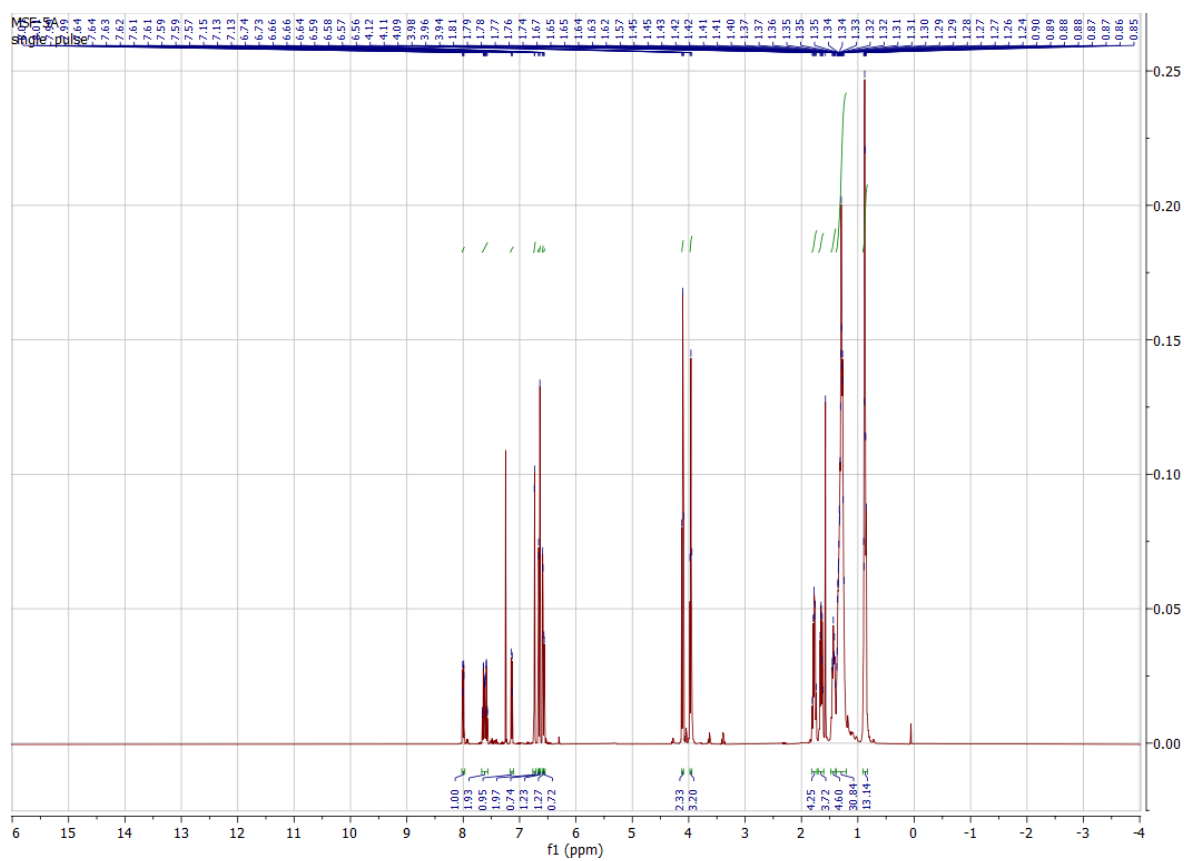


Figure S25. ^1H -NMR (600 MHz, CDCl_3) spectrum of product **4A**.

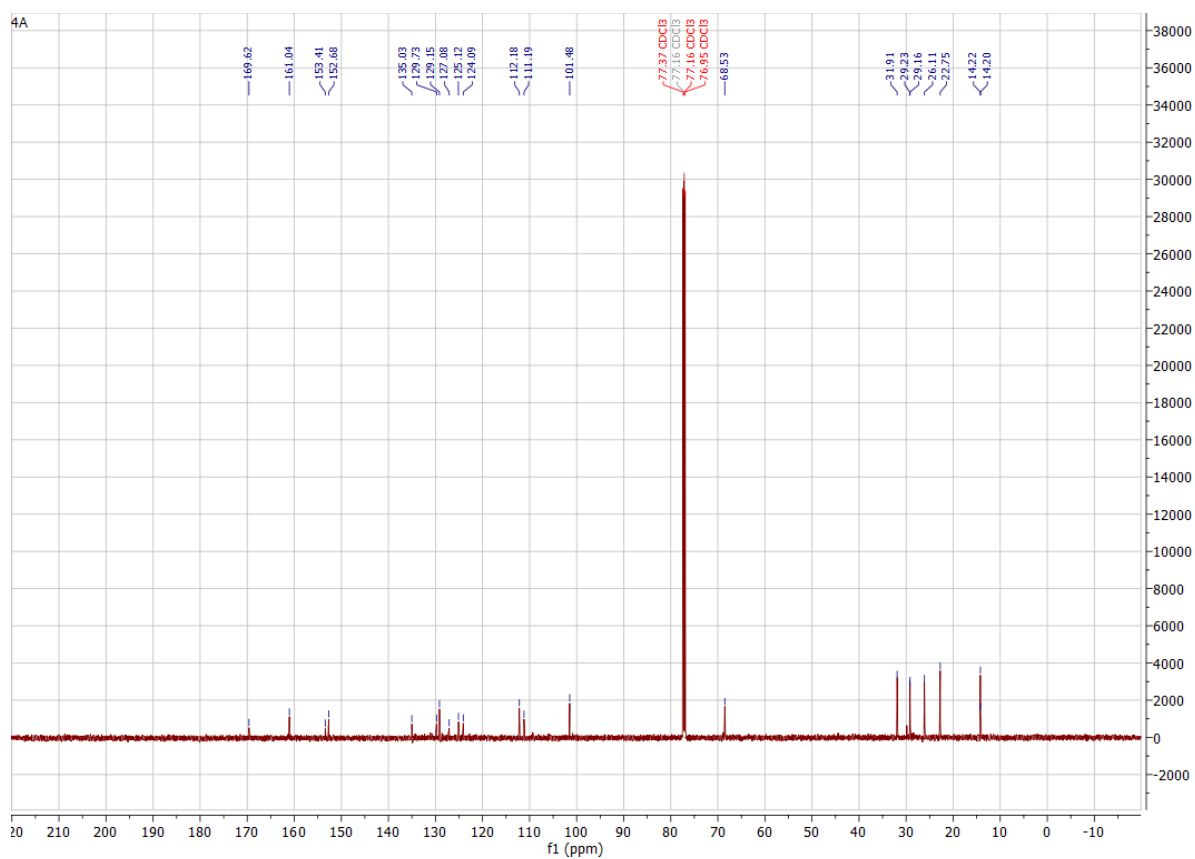


Figure S26. ^{13}C -NMR (151 MHz, chloroform- d) spectrum of product 4A.

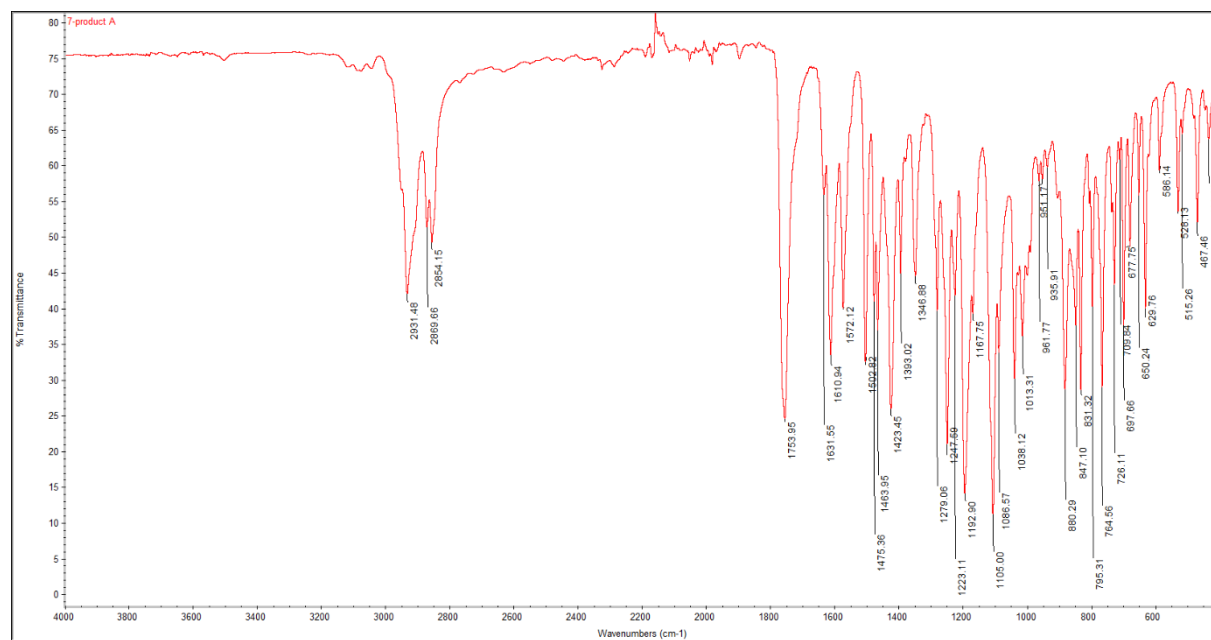


Figure S27. FTIR-ATR spectrum of product 4A.

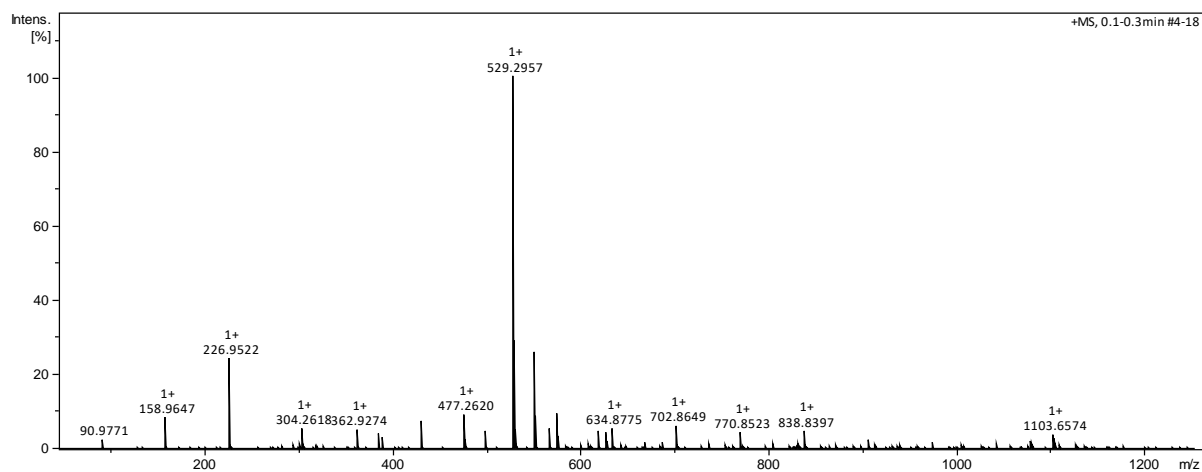


Figure S28. HR ESI-MS spectrum of product **4A**.

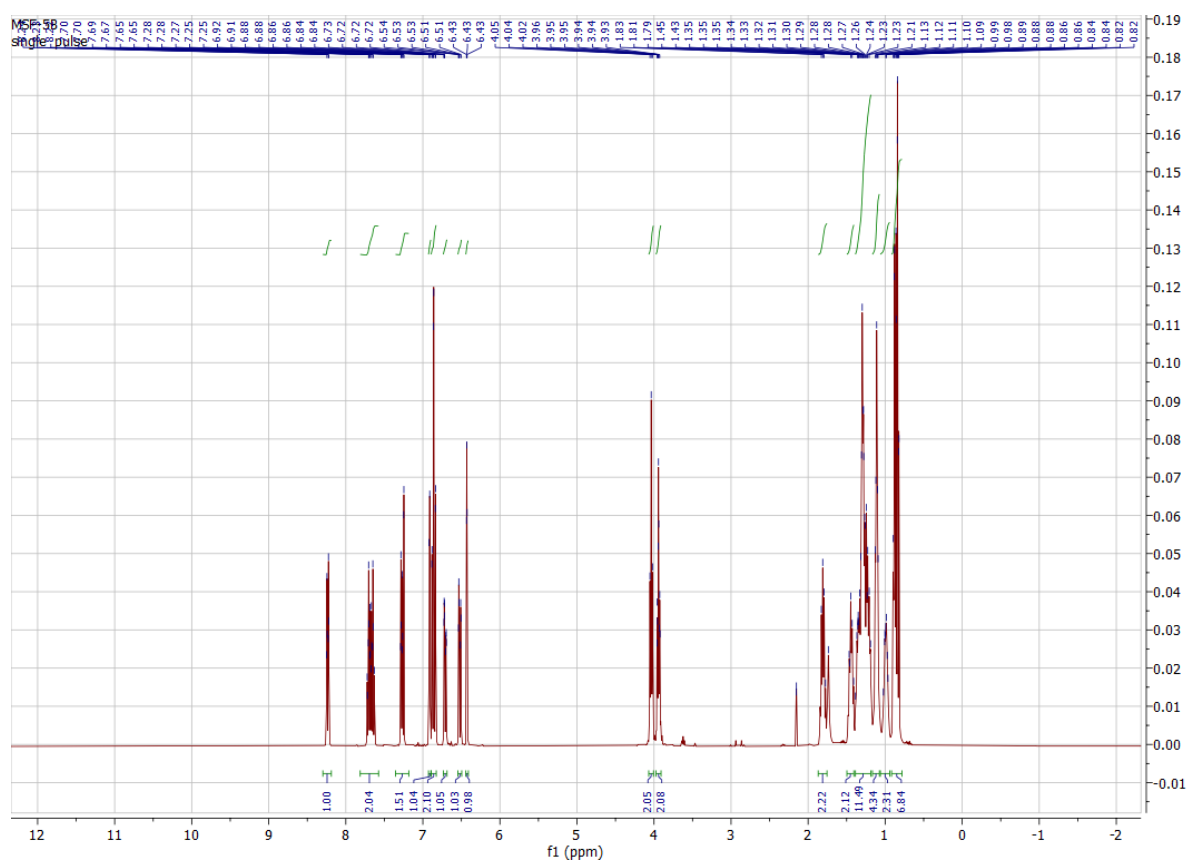


Figure S29. ¹H-NMR (600 MHz, chloroform-*d*) spectrum of product **4B**.

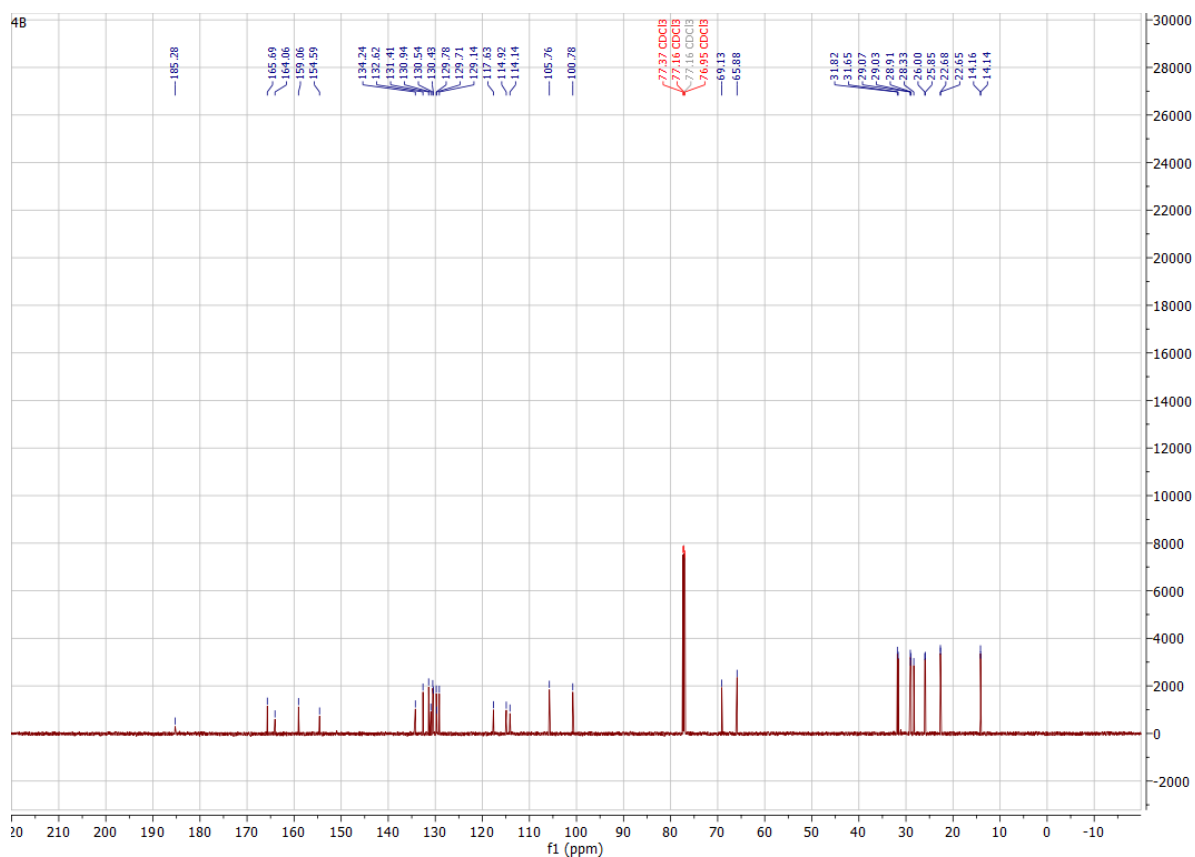


Figure S30. ^{13}C -NMR (151 MHz, chloroform-*d*) spectrum of product **4B**.

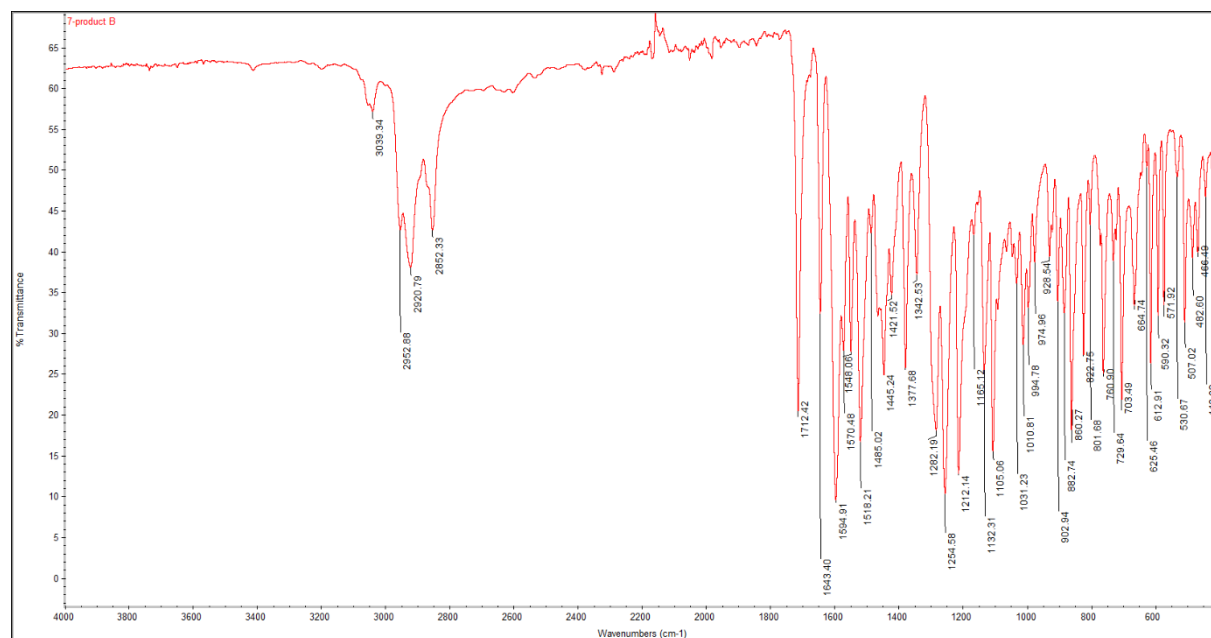


Figure S31. FTIR-ATR spectrum of product **4B**.

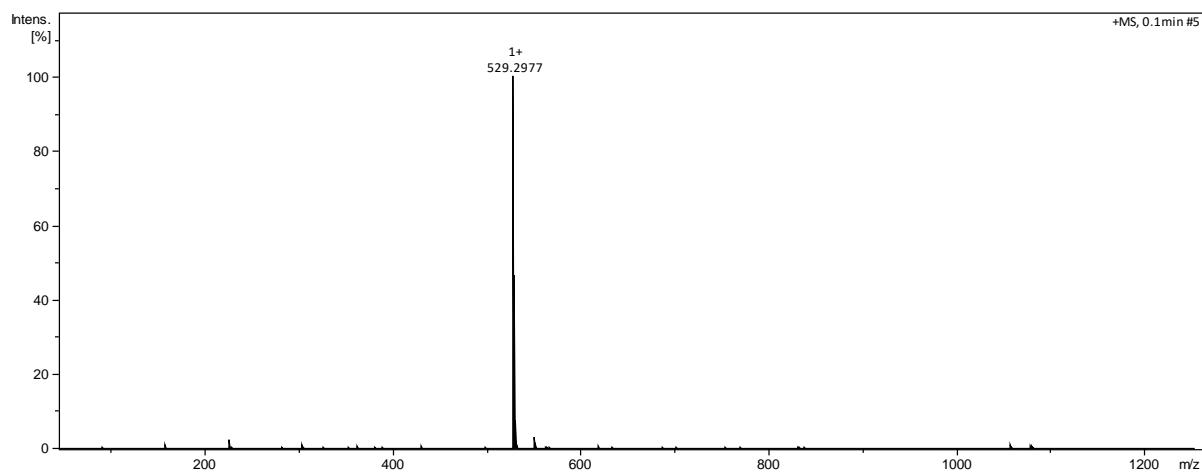


Figure S32. HR ESI-MS spectrum of product **4B**.

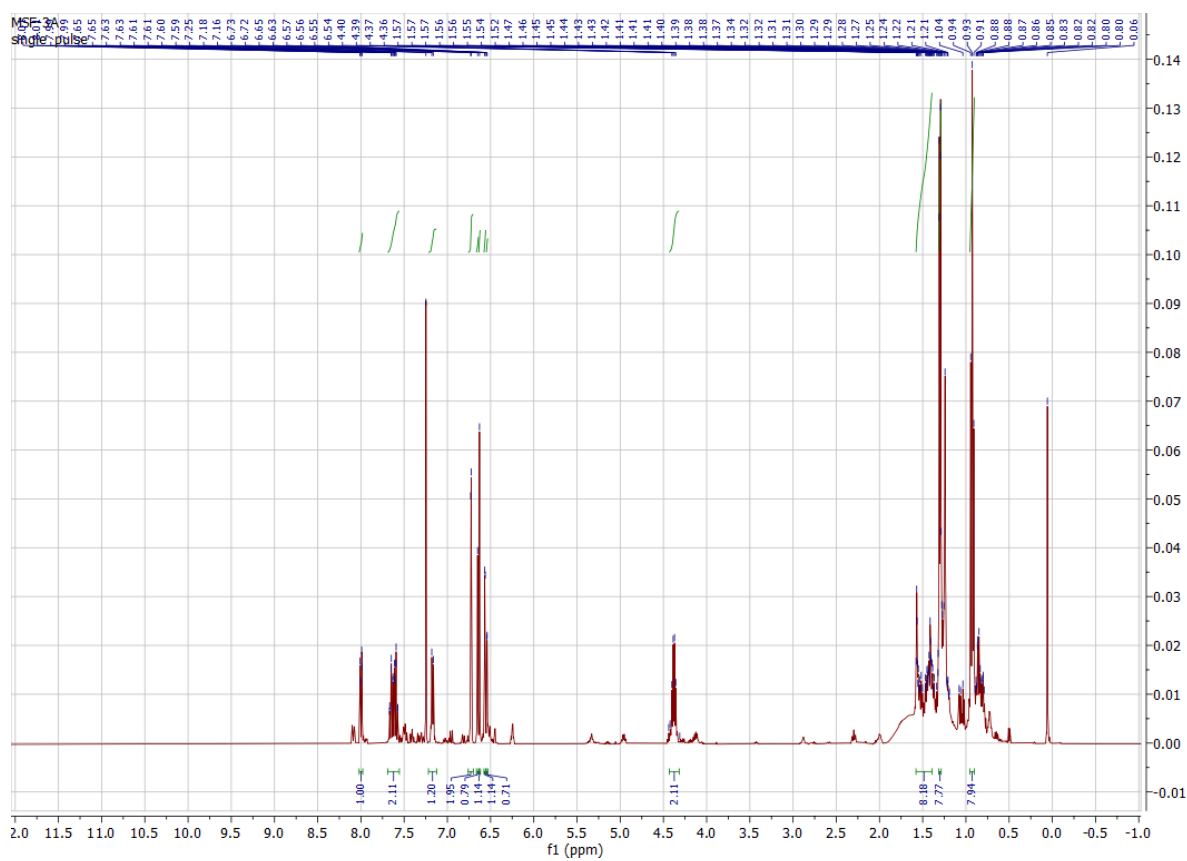


Figure S33. ^1H -NMR (600 MHz, chloroform- d) spectrum of product **5A**.

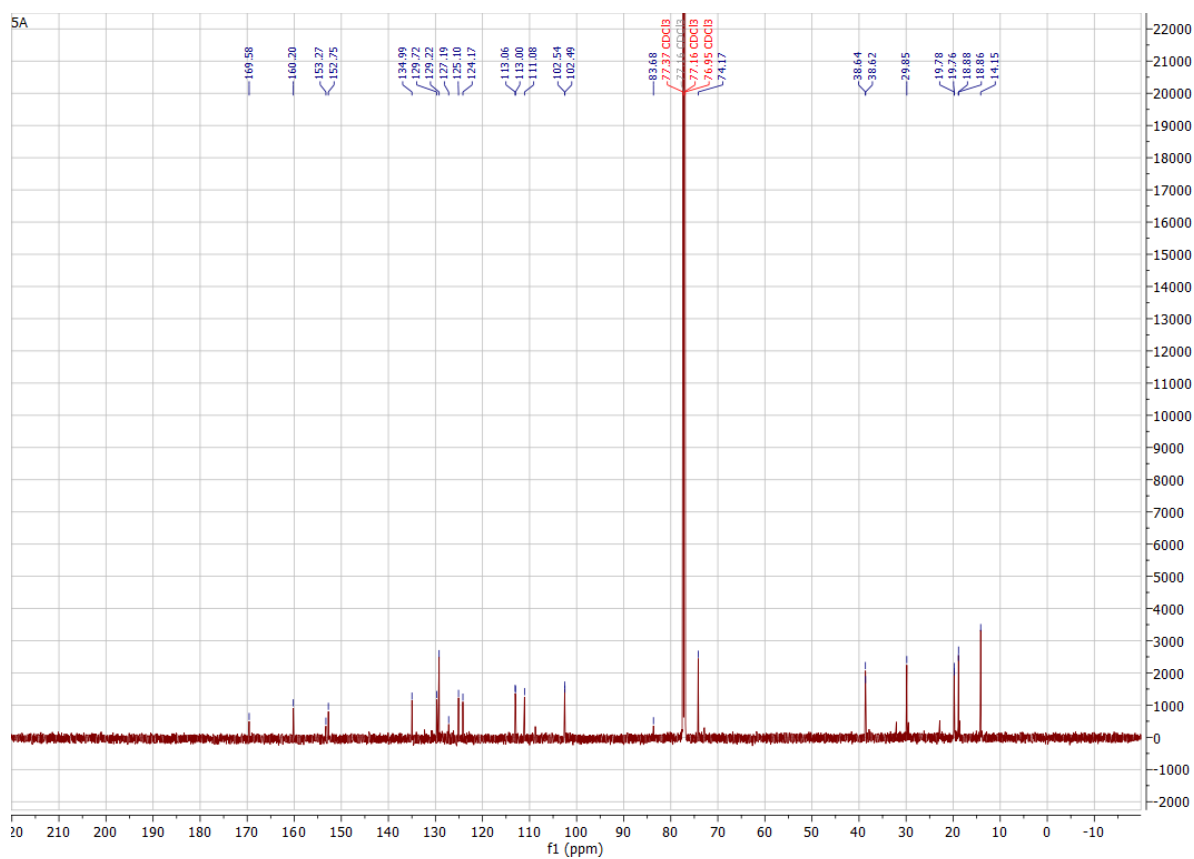


Figure S34. ^{13}C -NMR (151 MHz, chloroform-*d*) spectrum of product 5A.

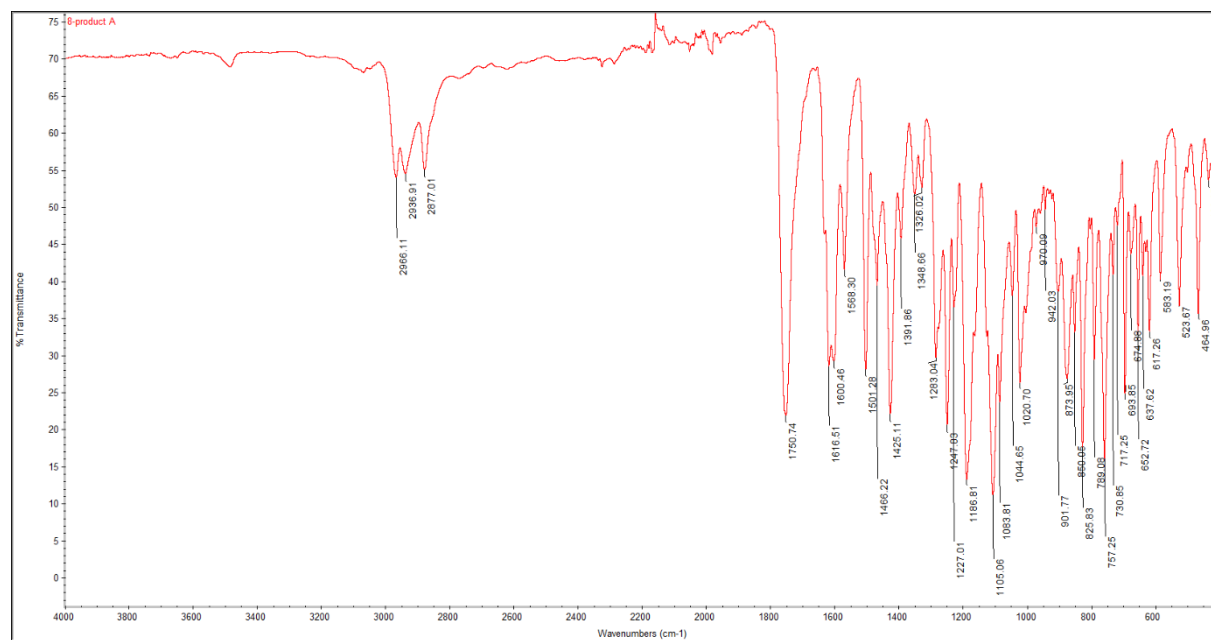


Figure S35. FTIR-ATR spectrum of product 5A.

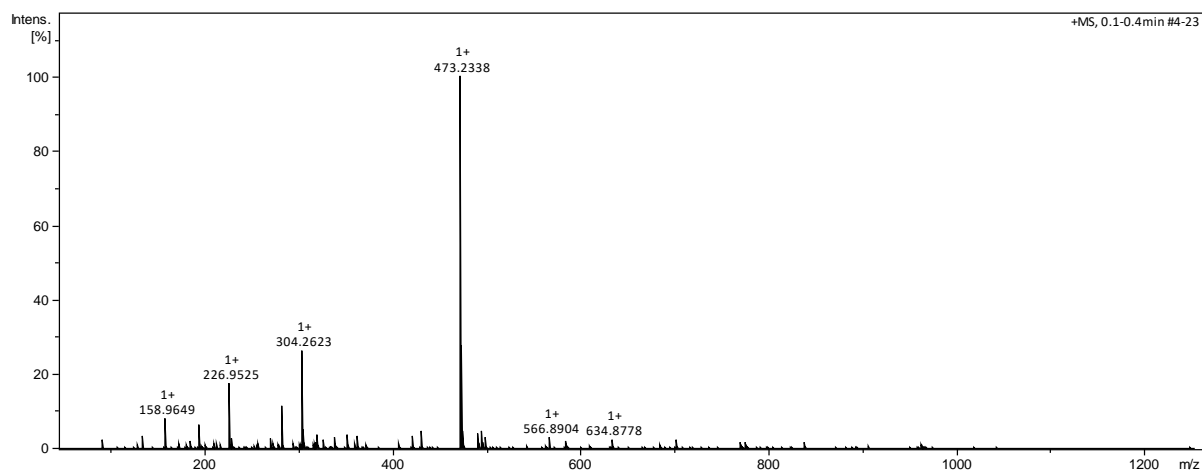


Figure S36. HR ESI-MS spectrum of product 5A.

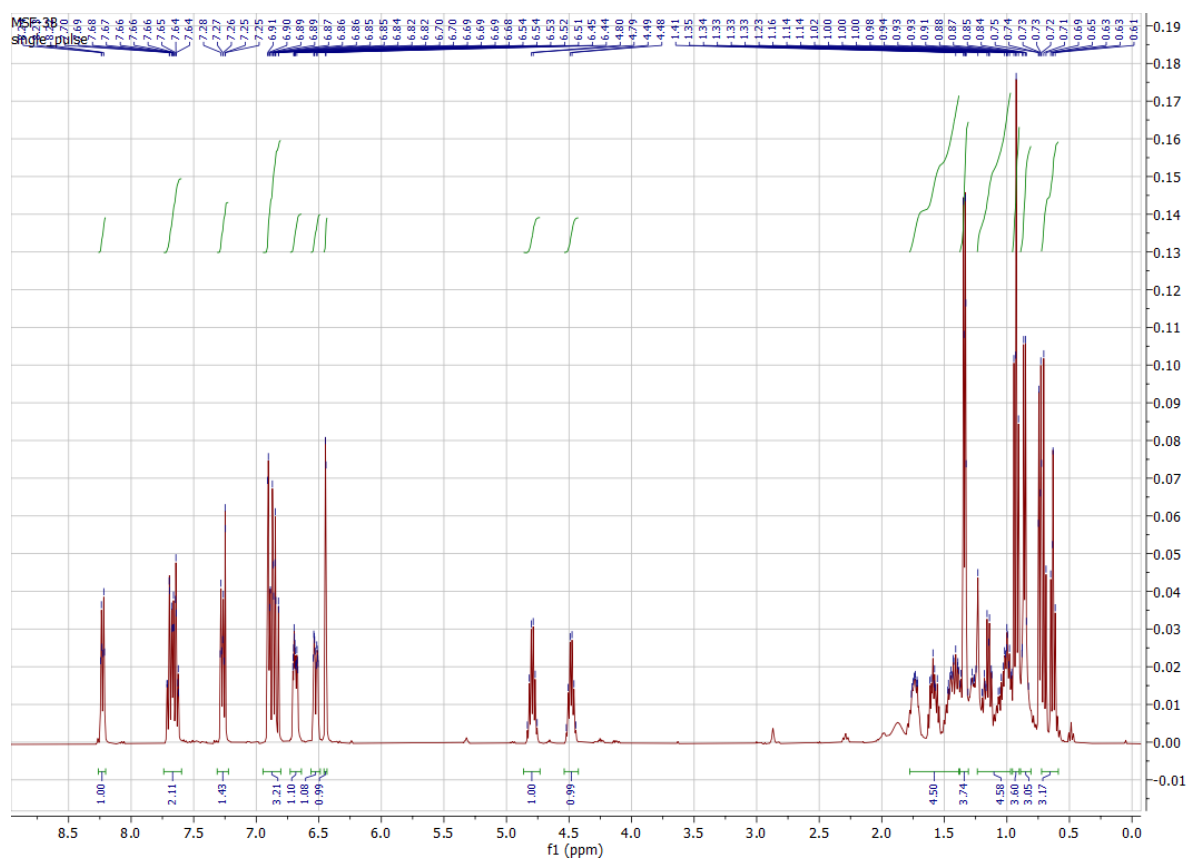


Figure S37. ¹H-NMR (600 MHz, chloroform-*d*) spectrum of product 5B.

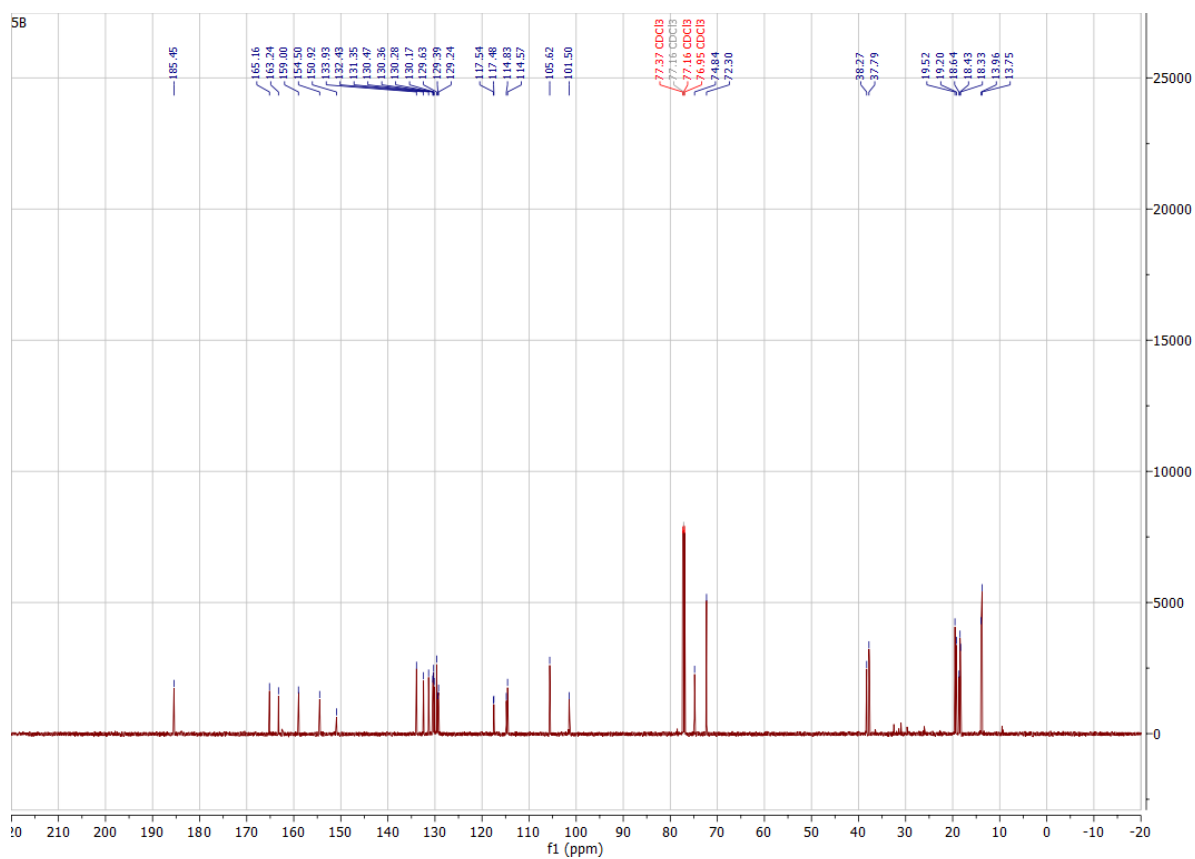


Figure S38. ^{13}C -NMR (151 MHz, chloroform-*d*) spectrum of product **5B**.

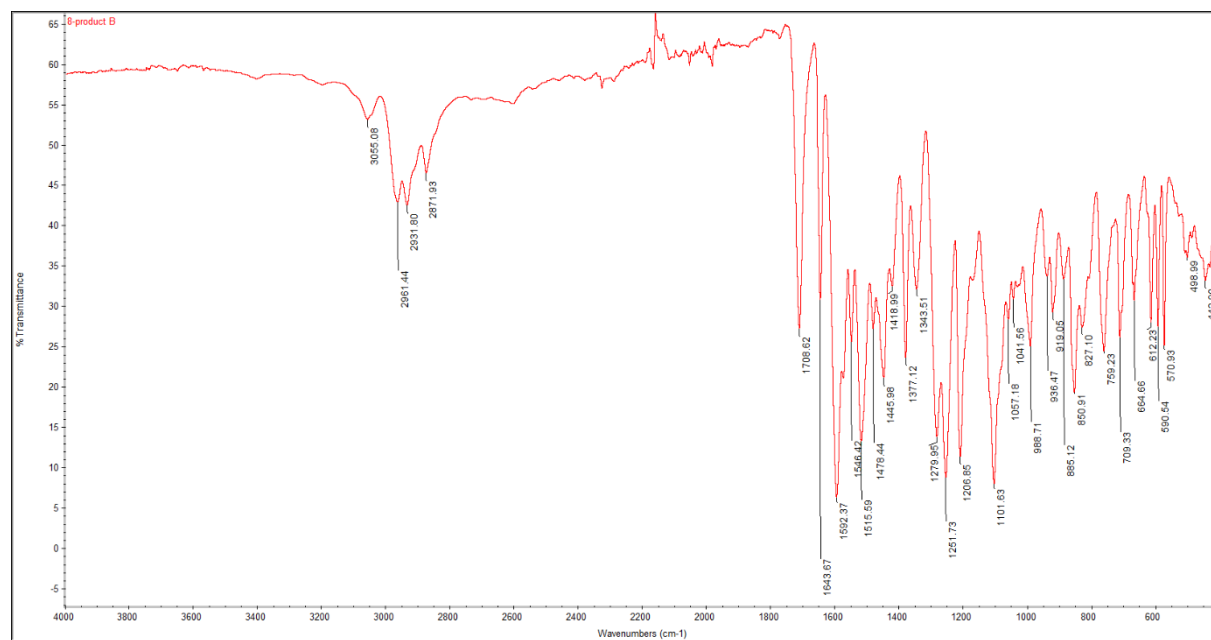


Figure S39. FTIR-ATR spectrum of product **5B**.

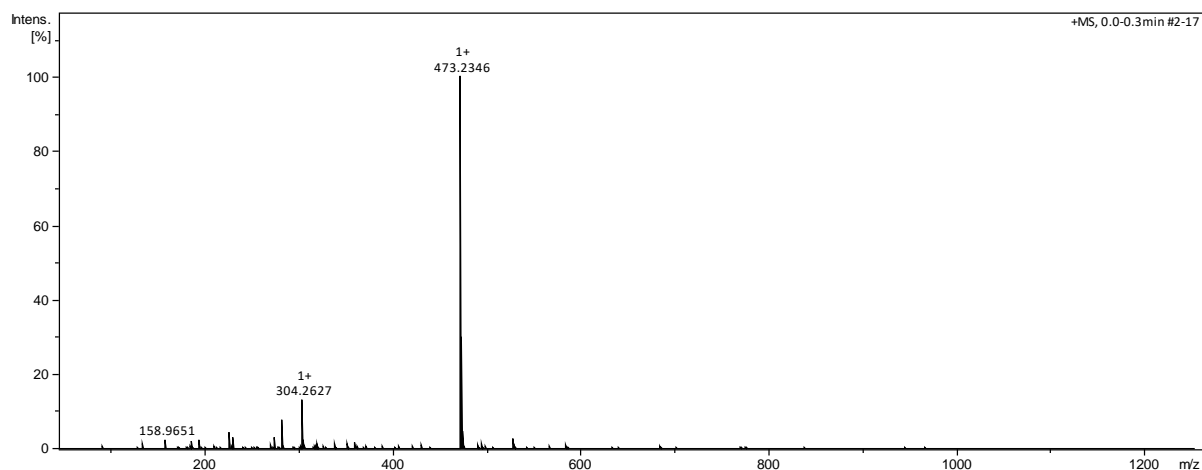


Figure S40. HR ESI-MS spectrum of product **5B**.

S2. Spectroscopic properties

Table S1. Summary of spectroscopic properties measured for all compounds.

Compound	λ_{abs} (nm)	λ_{em} (nm)	τ (ns)	QY (%)
1A	445	464	4.5	20.94
2A	445	465	5.9	12.12
3A	445	462	5.6	26.83
4A	445	464	5.3	32.3
5A	442	465	5.5	29.55
1B	452 / 475	517	3.3	28.90
2B	453 / 475	515	3.2	32.14
3B	455	518	3.3	24.15
4B	455	520 / 556	3.1	36.56
5B	454 / 480	518	3.2	27.65
Parent dye – cationic form	437	475	3.5–4.4	90-100
Parent dye – neutral form	453; 474	517	2.97	29

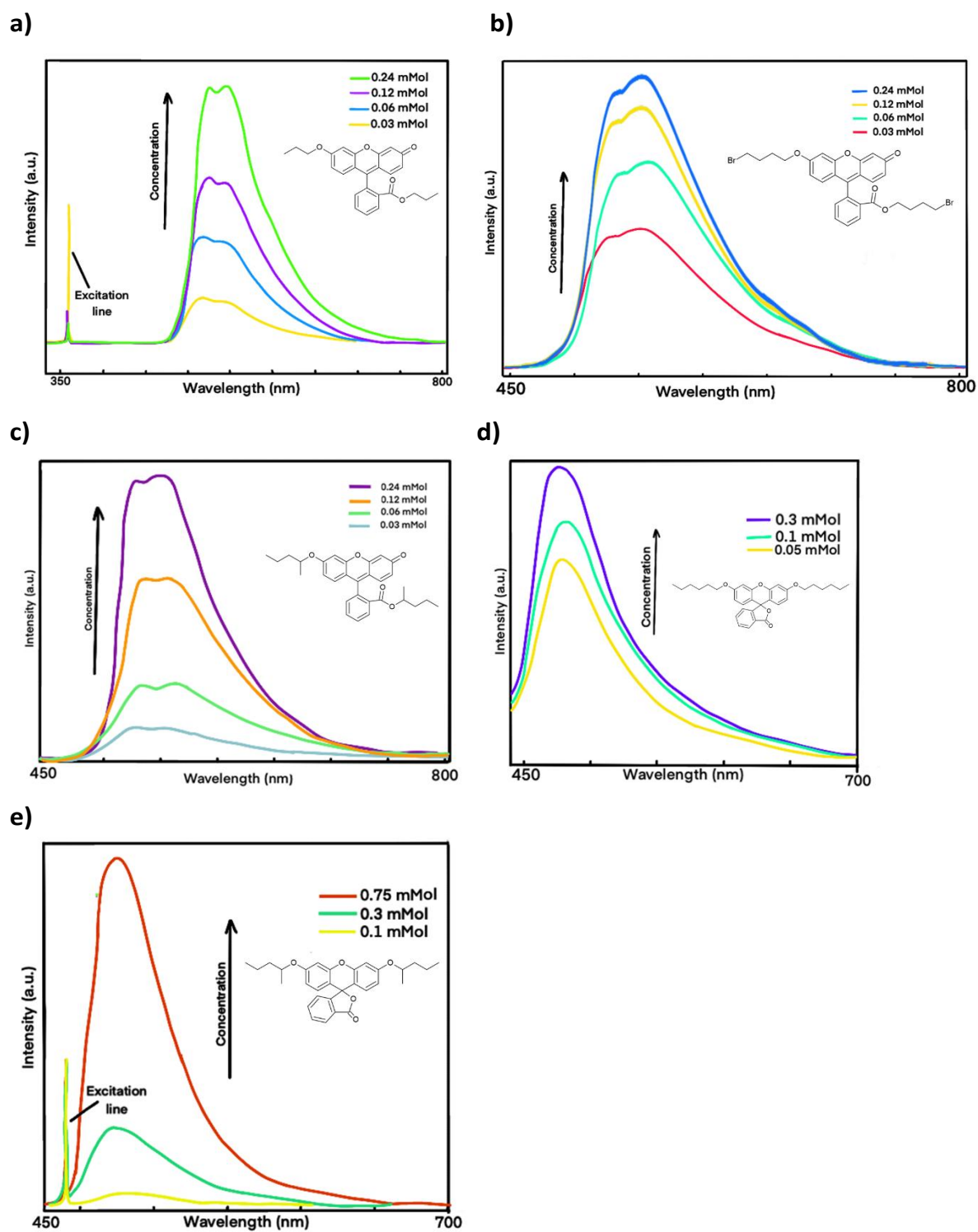


Figure S41. Emission spectra for different concentration measured for synthesized compounds (a) **1B**, (b) **2B**, (c) **5B**, (d) **3A**, (e) **5A**.