Electronic Supplementary Information (ESI)

Proton transfer fluorescent secondary amines. Synthesis, photophysics, theoretical calculation and preparation of photoactive phosphatidylcholine-based liposomes

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Summary

^{1}H NMR data

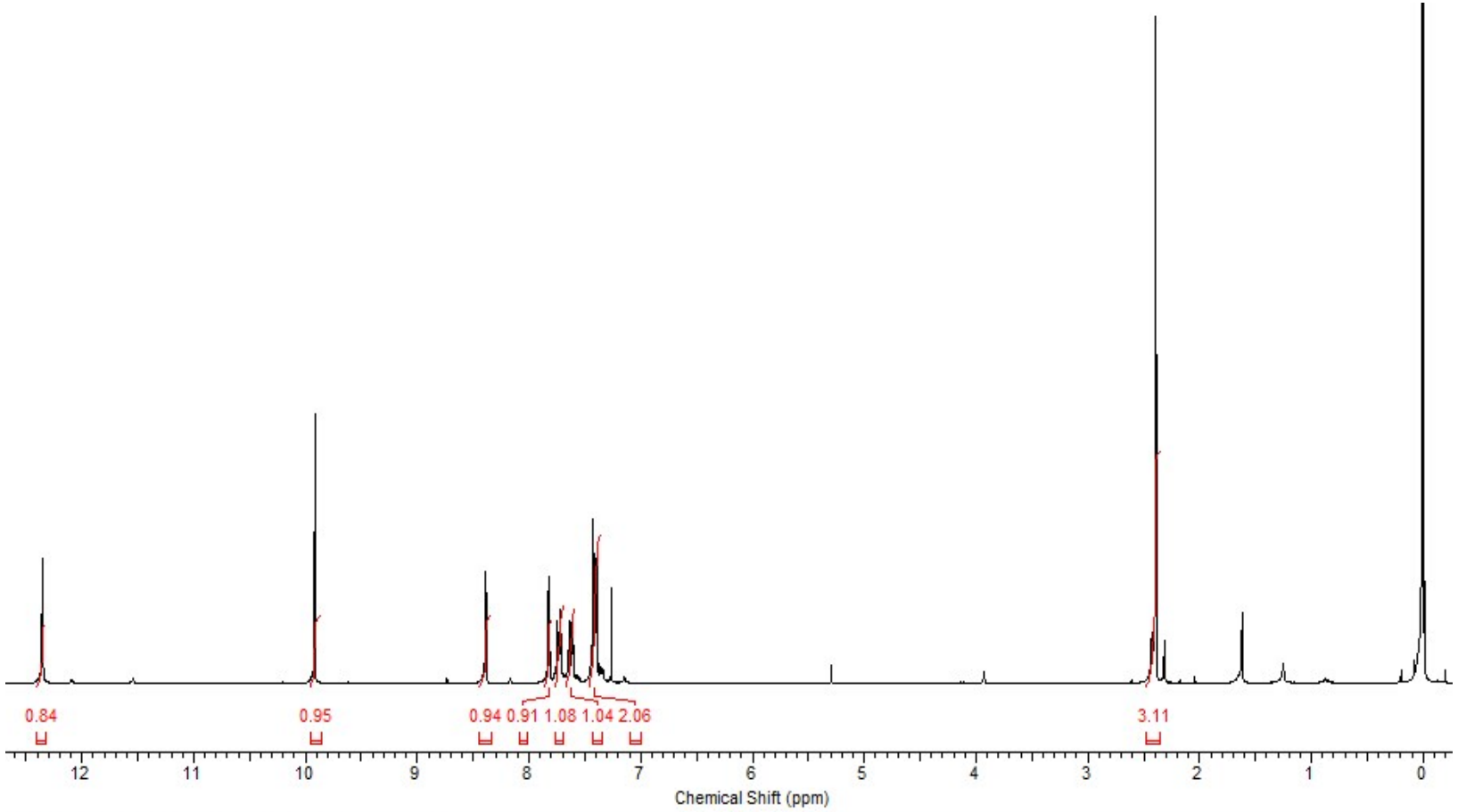


Figure ESI1. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **8**.

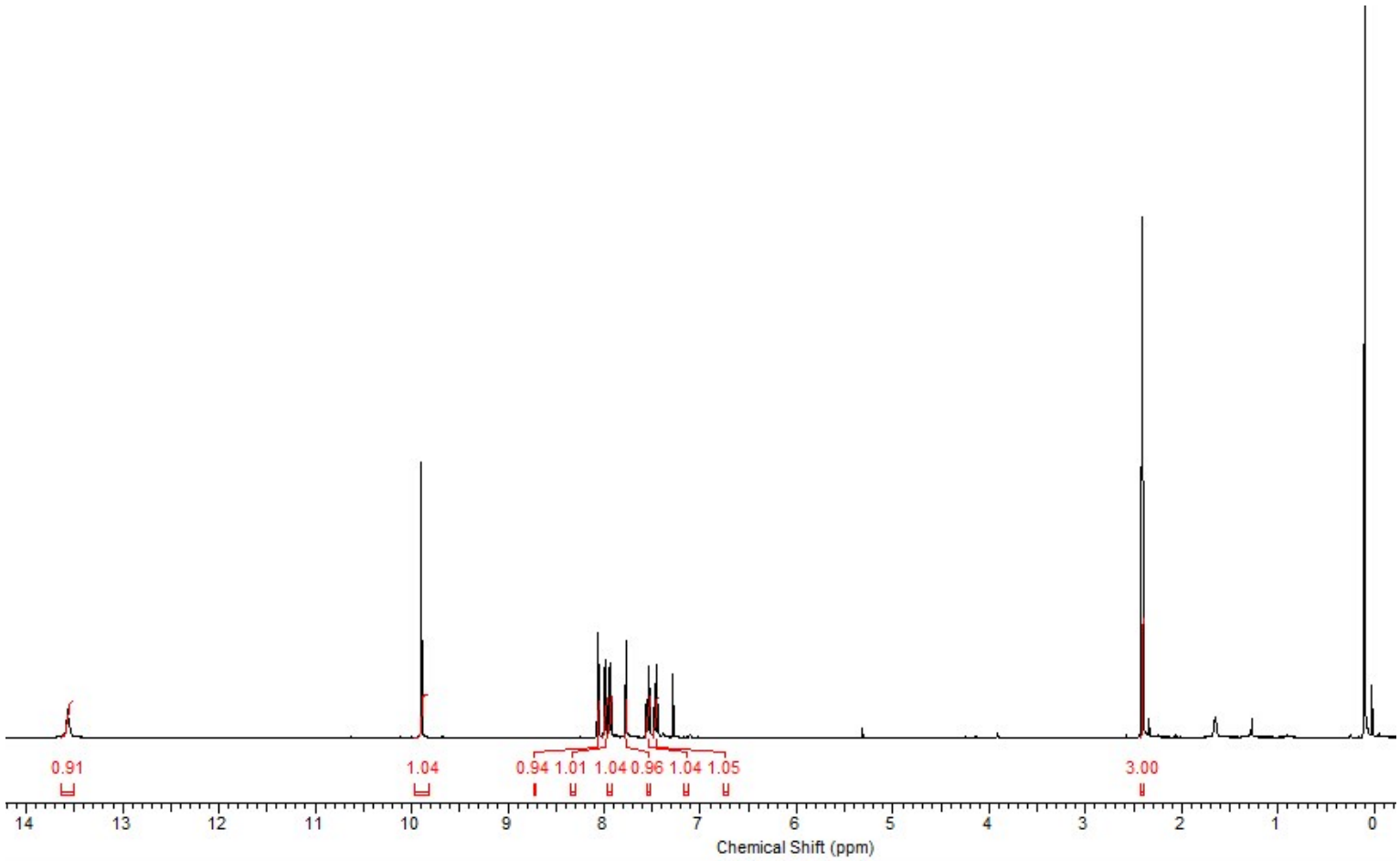


Figure ESI2. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **9**.

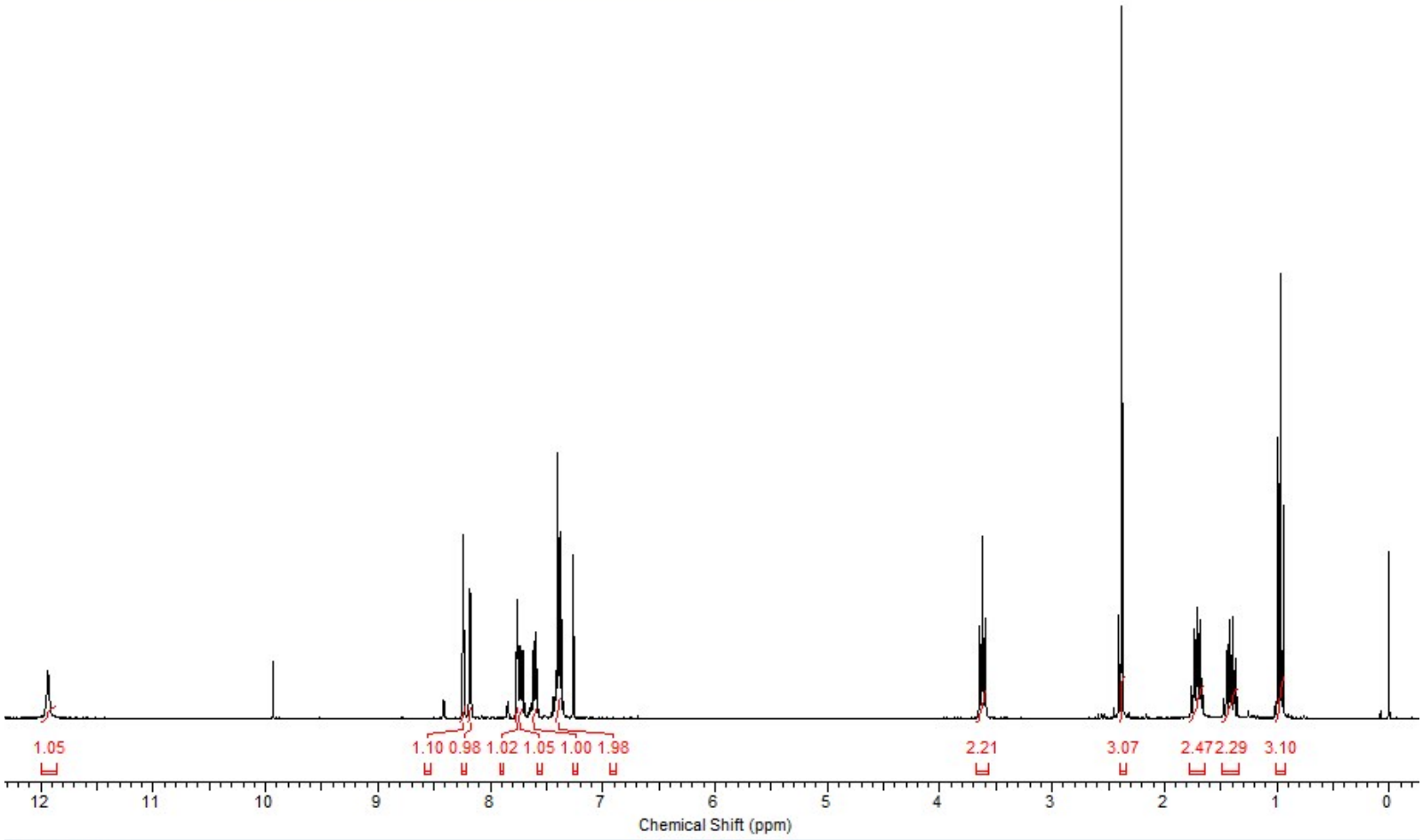


Figure ESI3. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **13**.

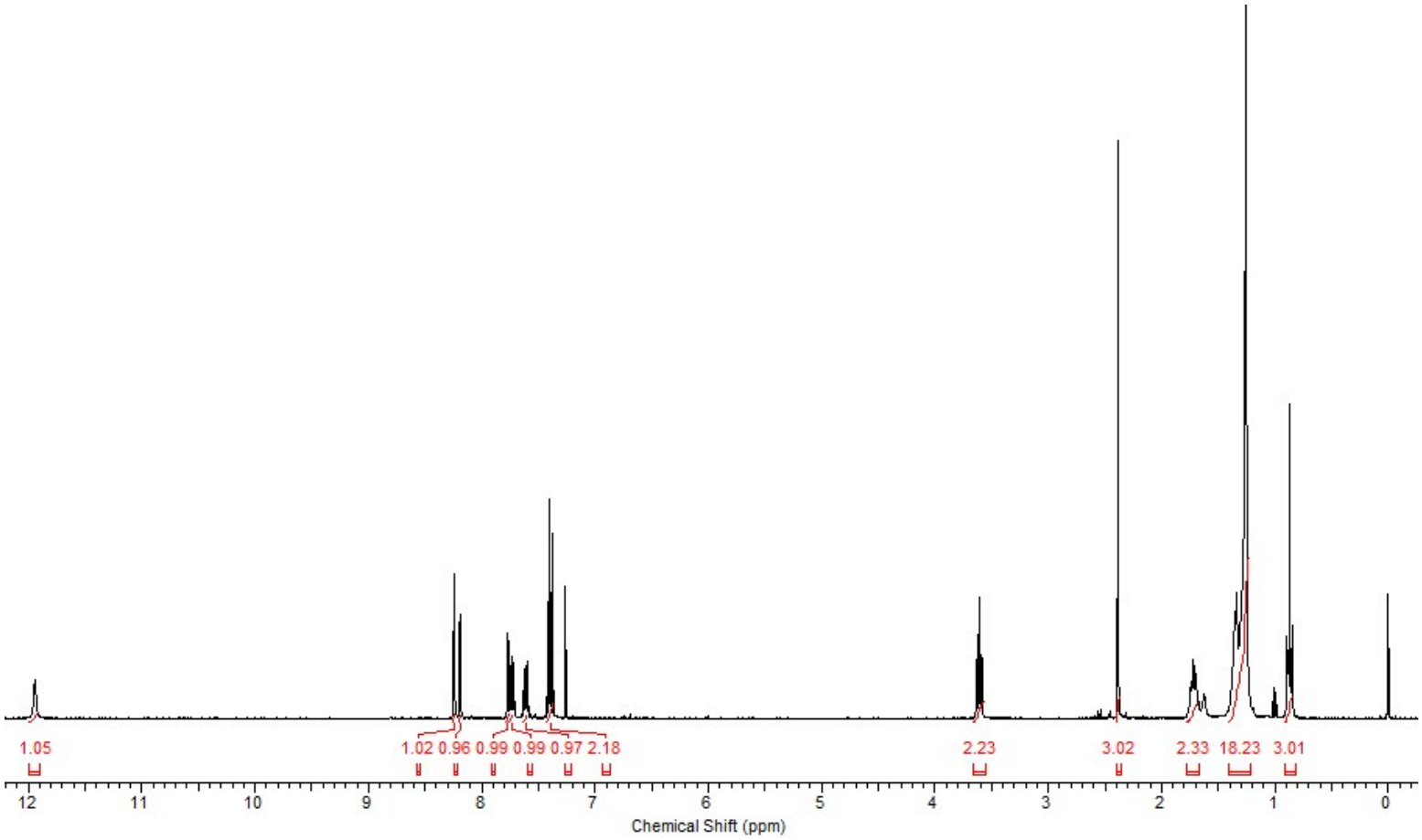


Figure ESI4. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **14**.

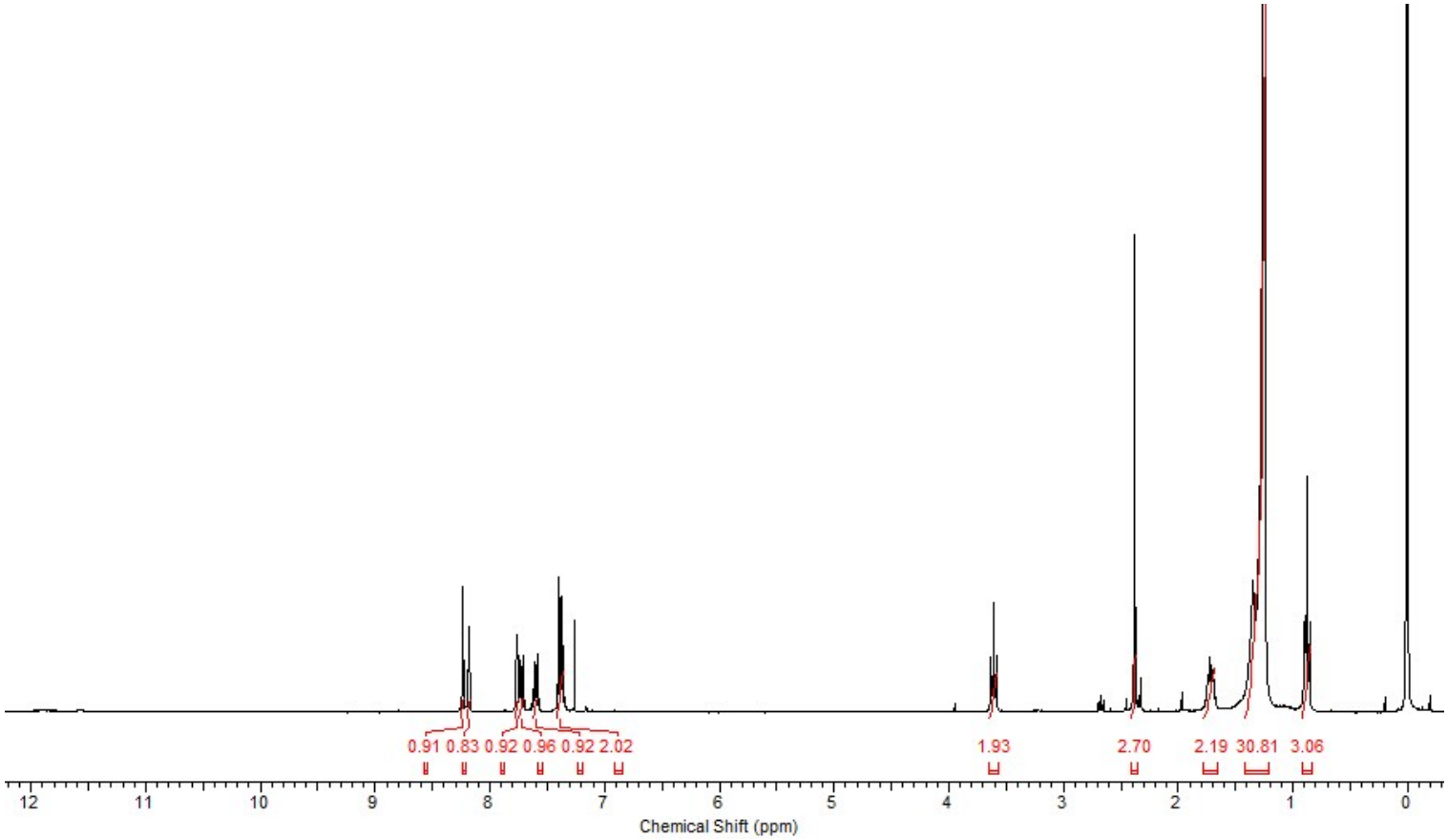


Figure ESI5. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **15**.

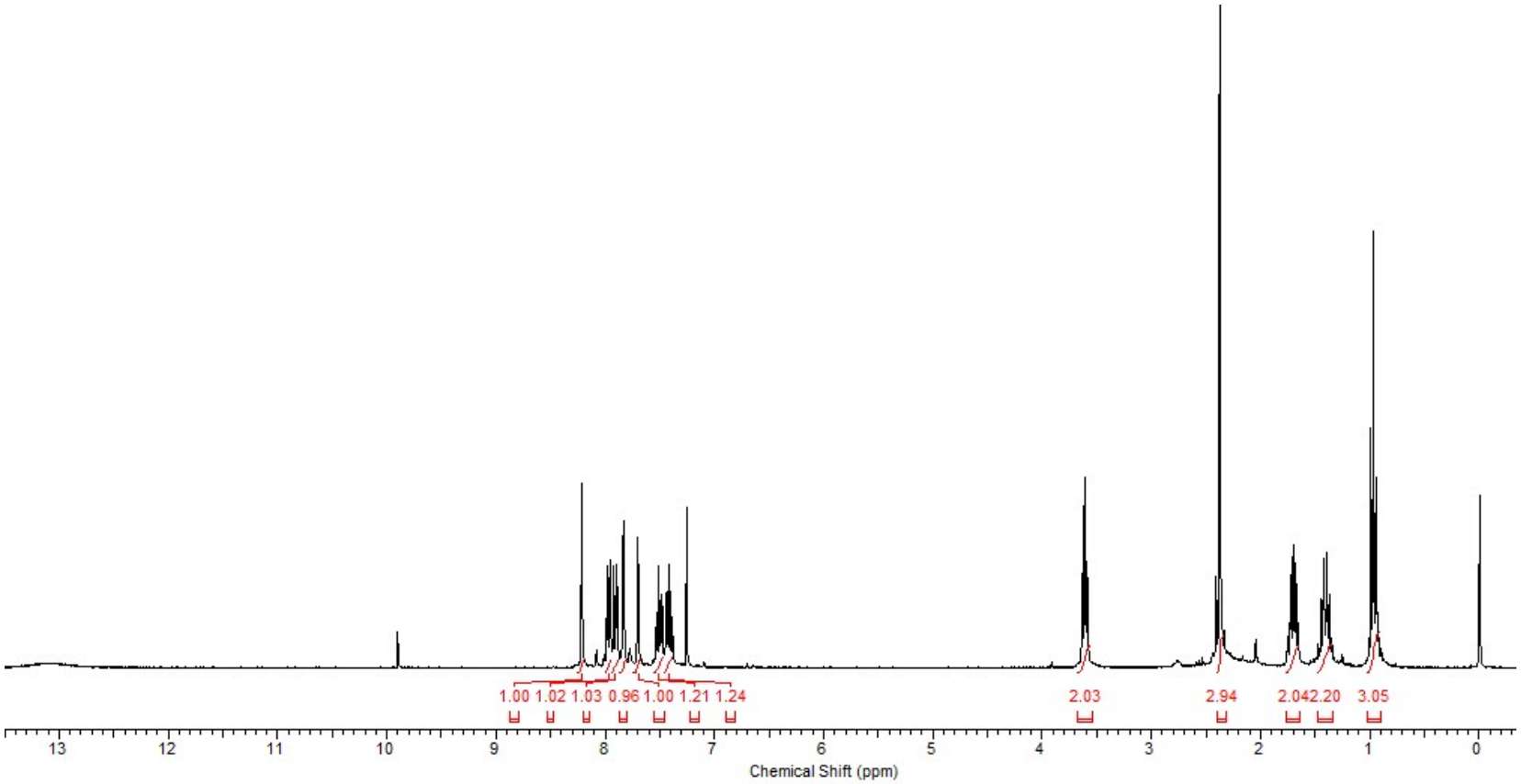


Figure ESI6. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **16**.

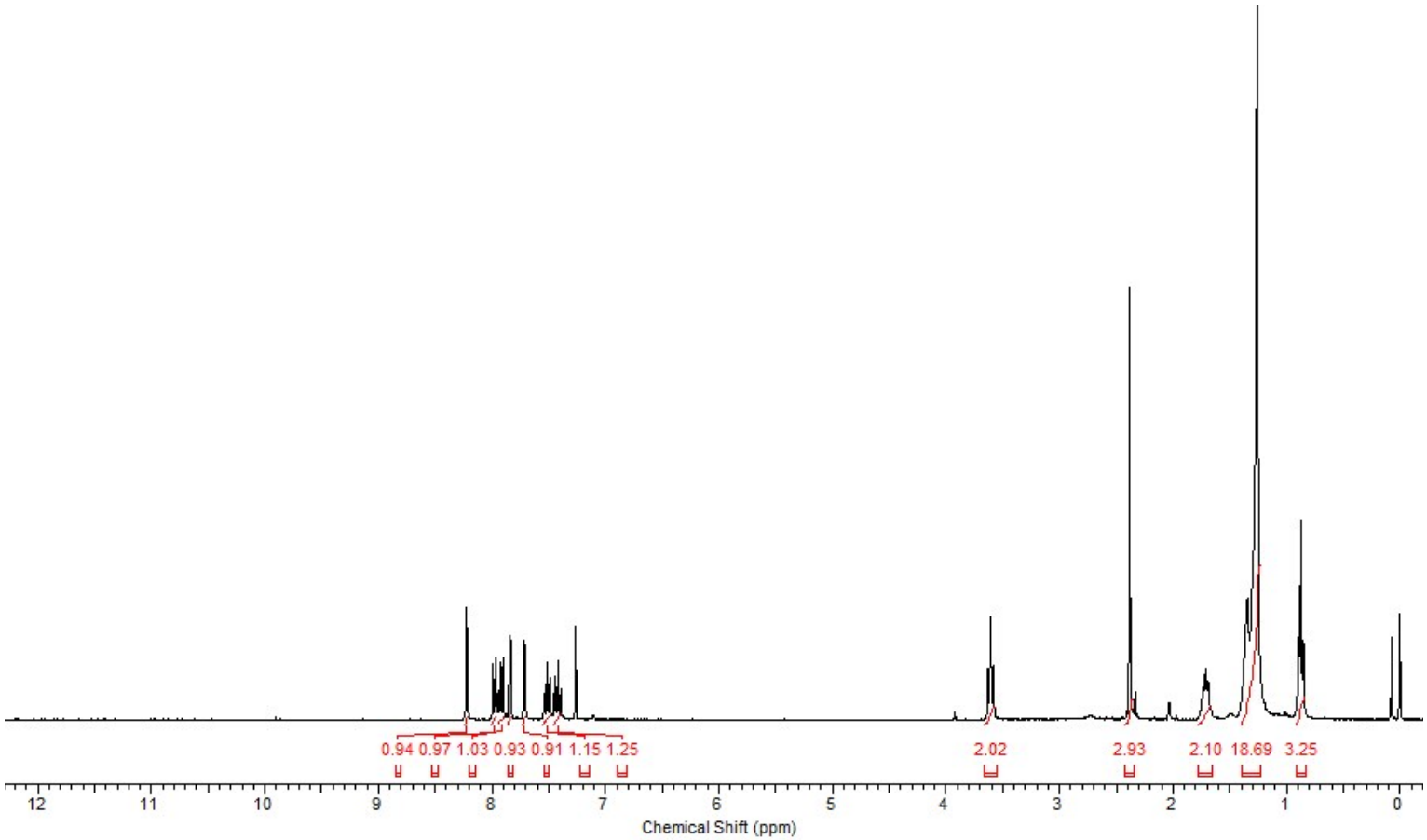


Figure ESI7. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **17**.

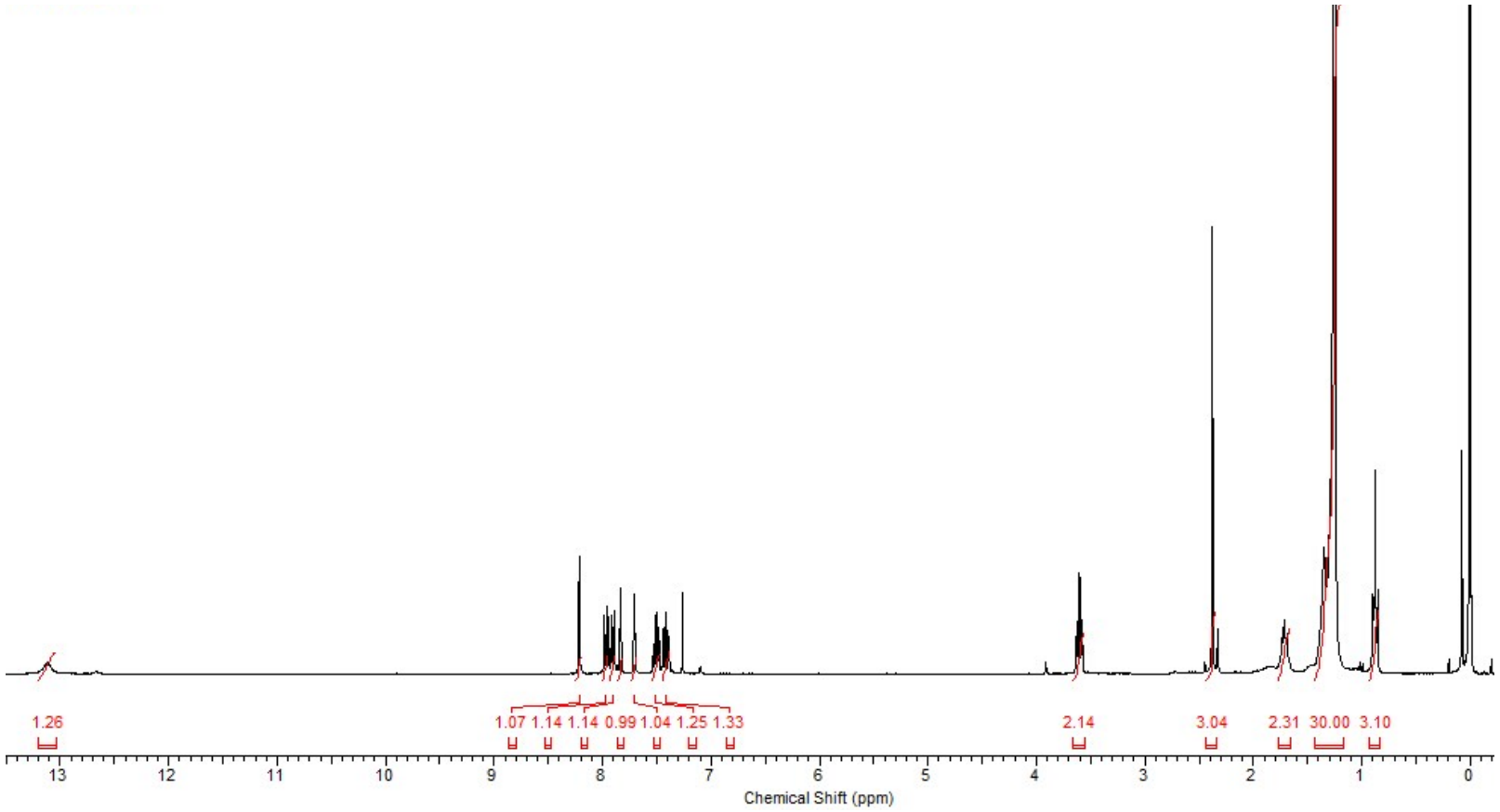


Figure ESI8. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **18**.

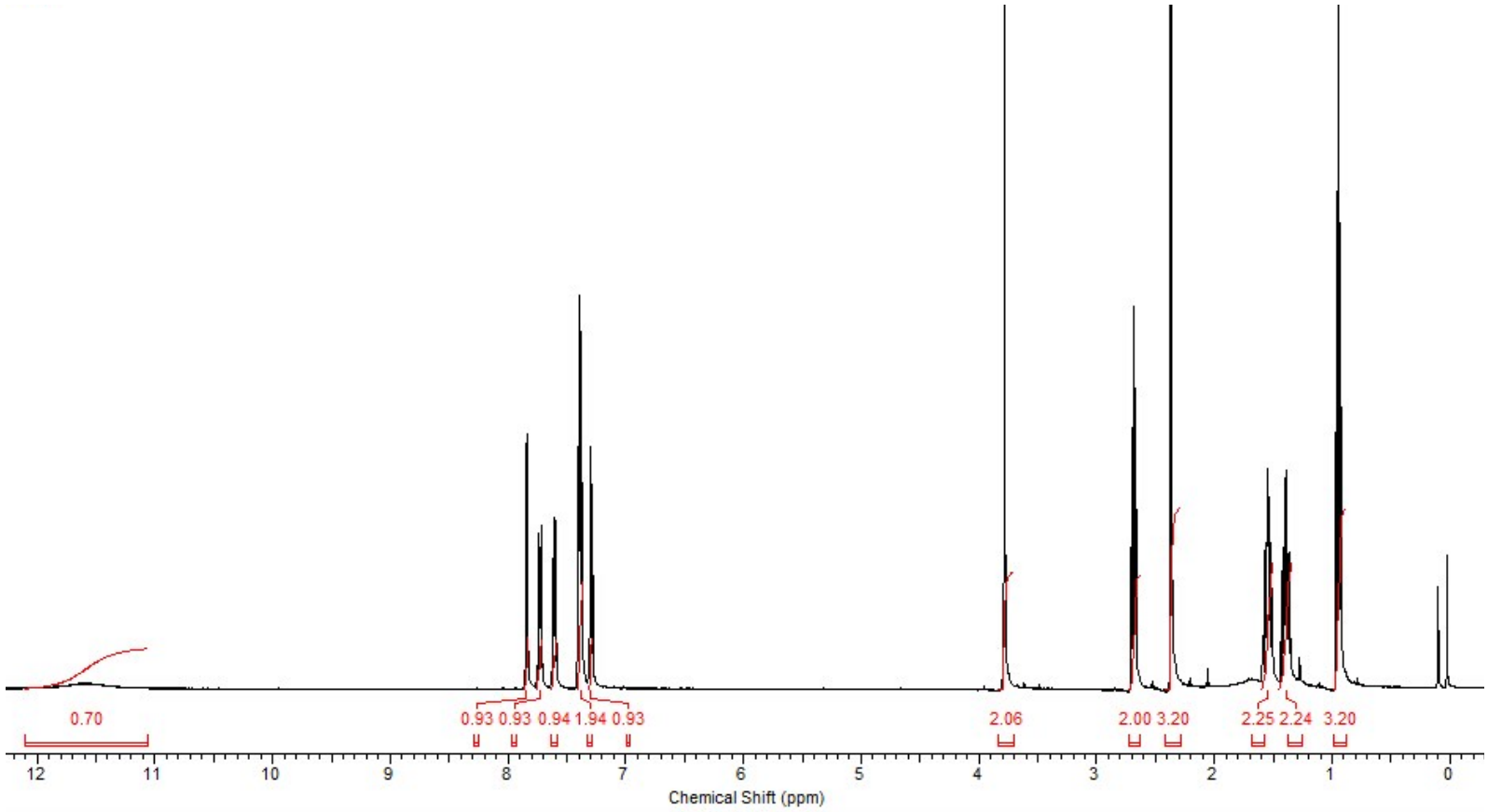


Figure ESI9. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **19**.

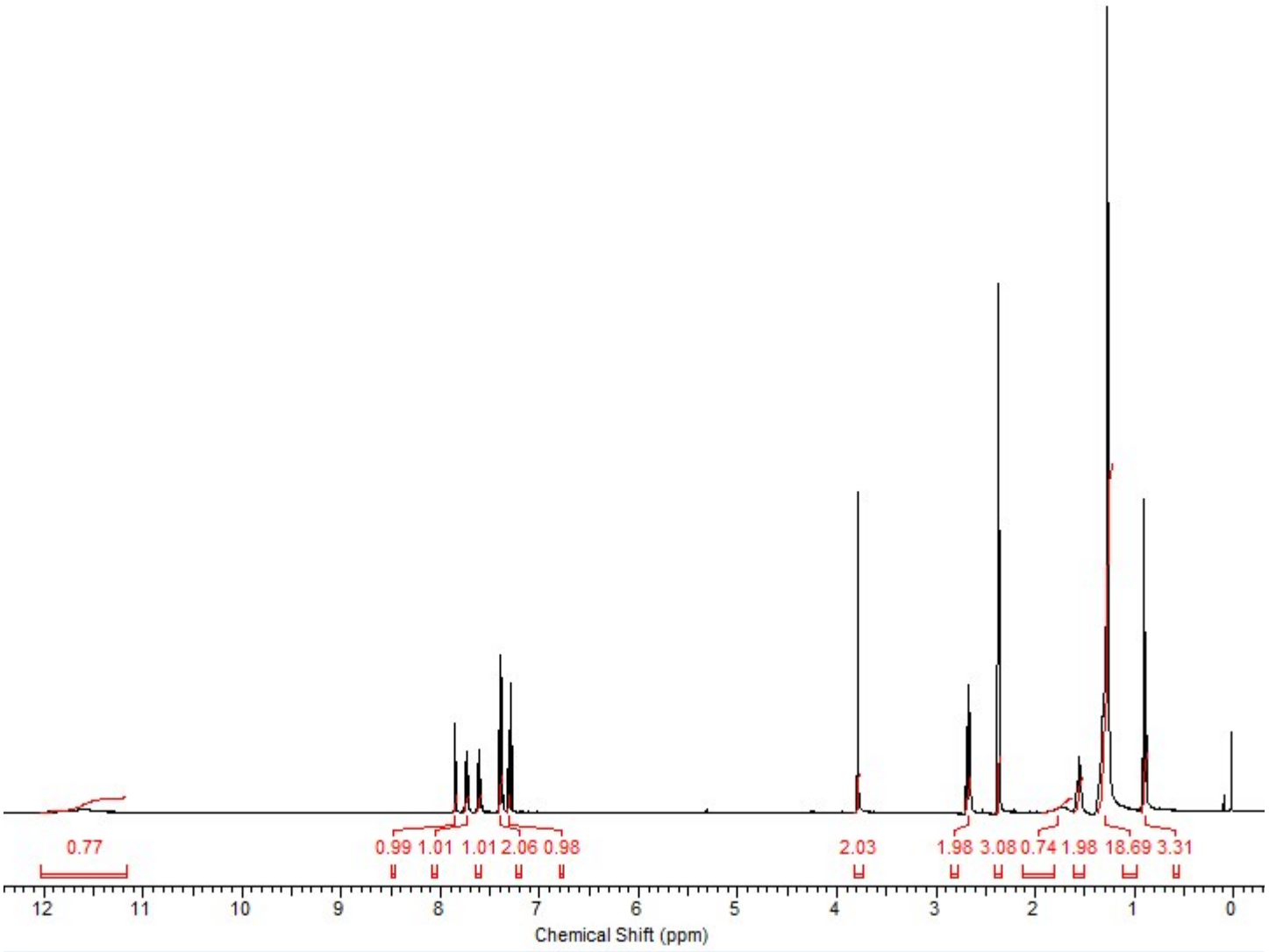


Figure ESI10. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **20**.

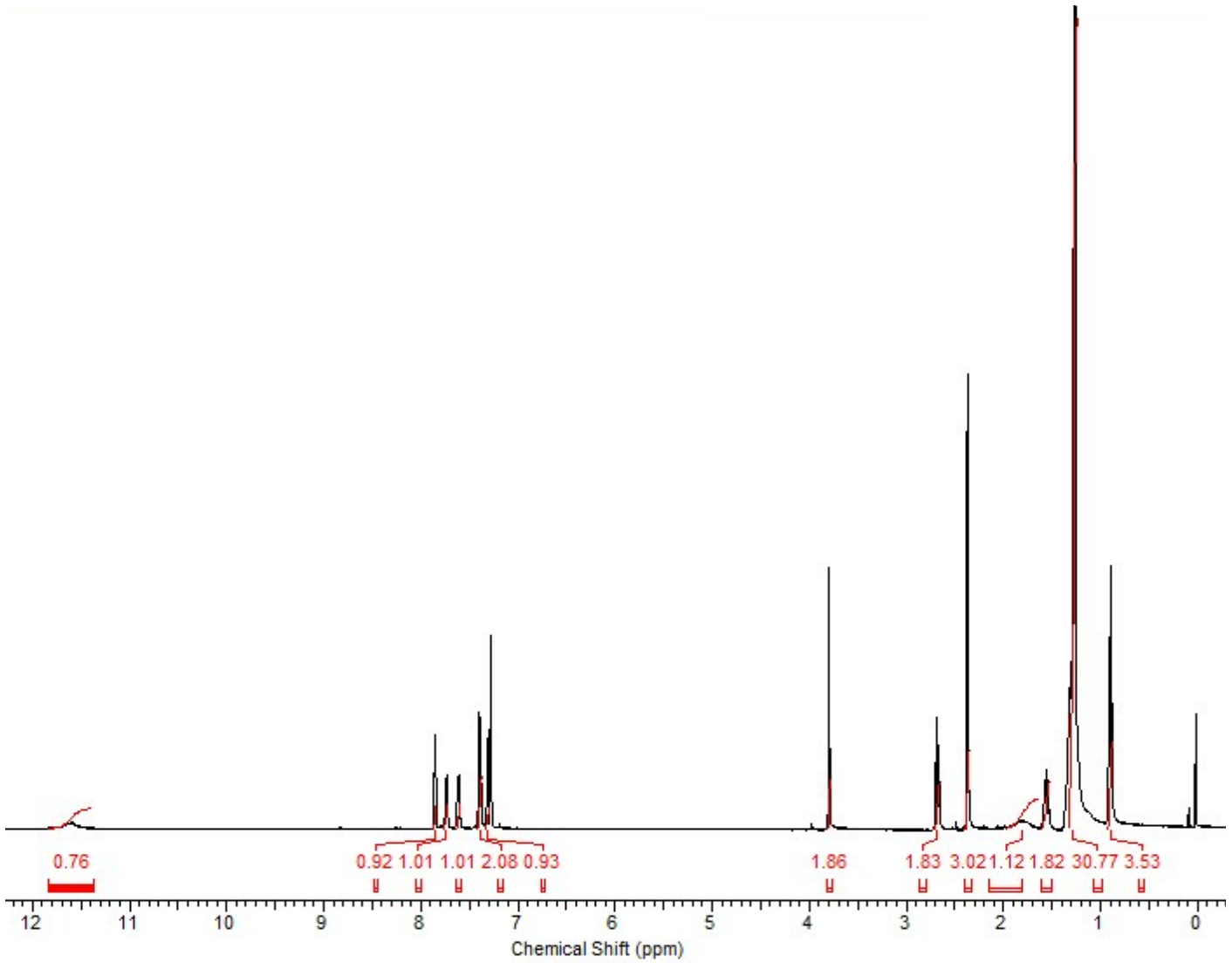


Figure ESI11. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **21**.

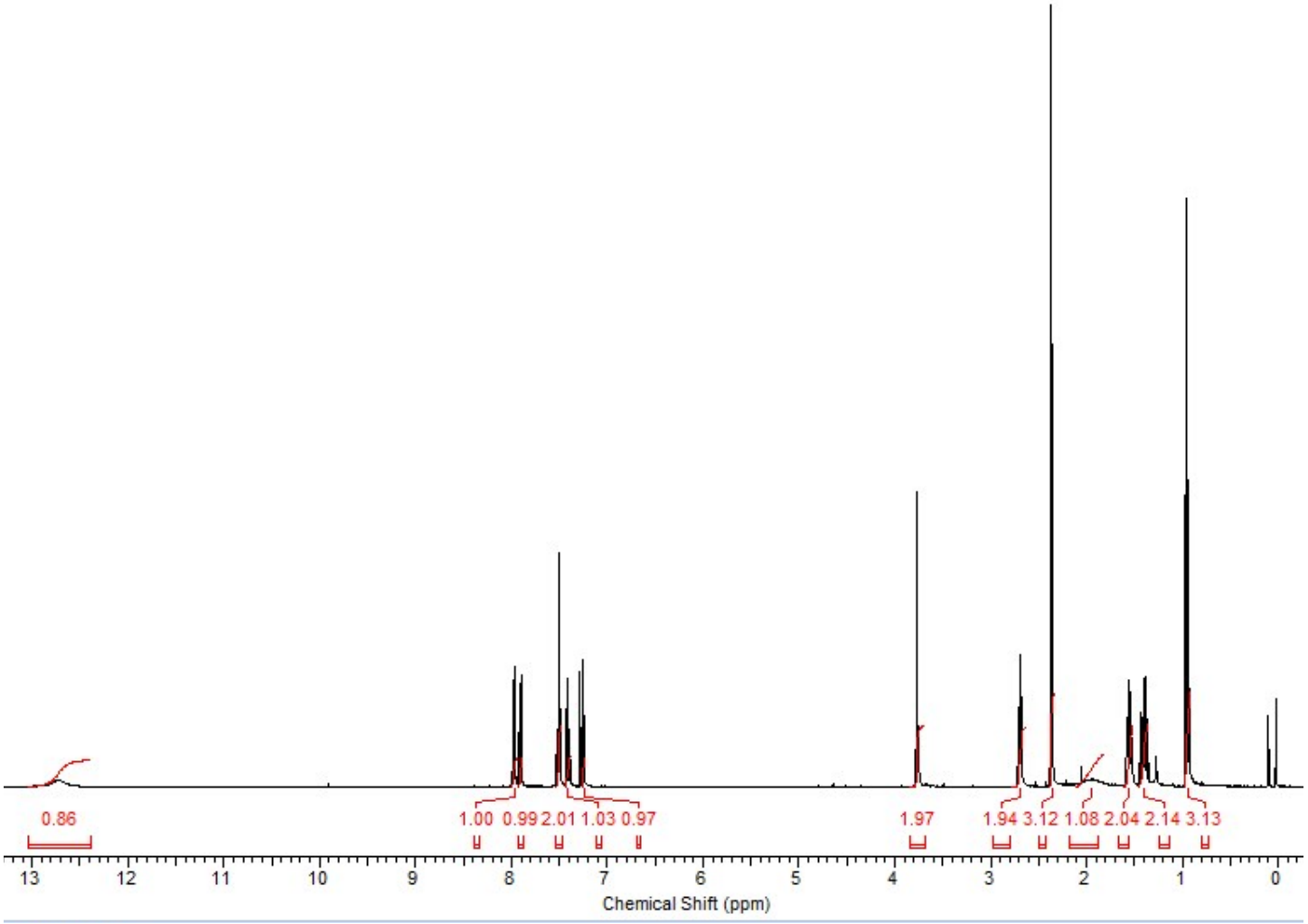


Figure ESI12. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **22**.

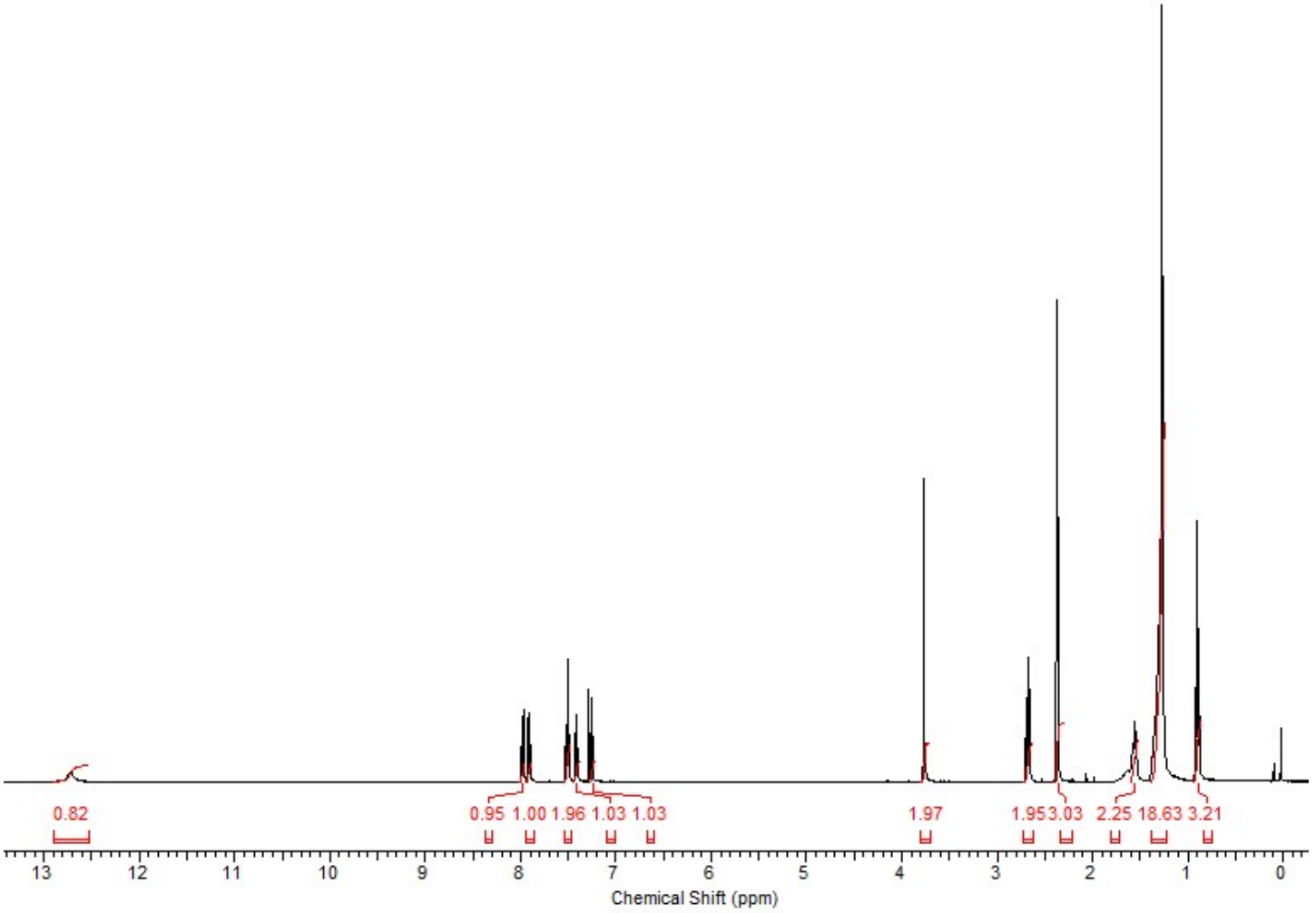


Figure ESI13. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **23**.

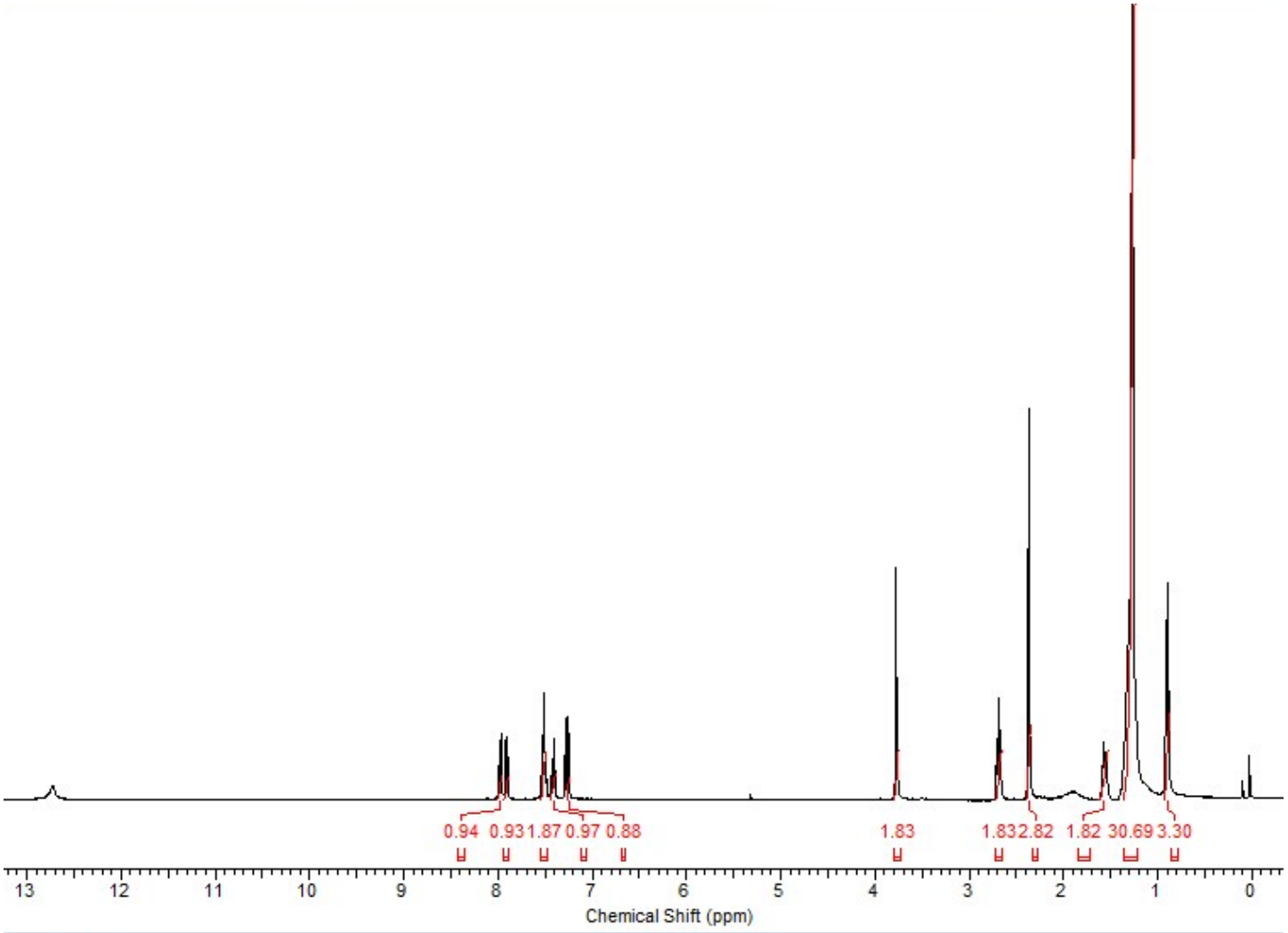


Figure ESI14. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **24**.

^{13}C NMR data

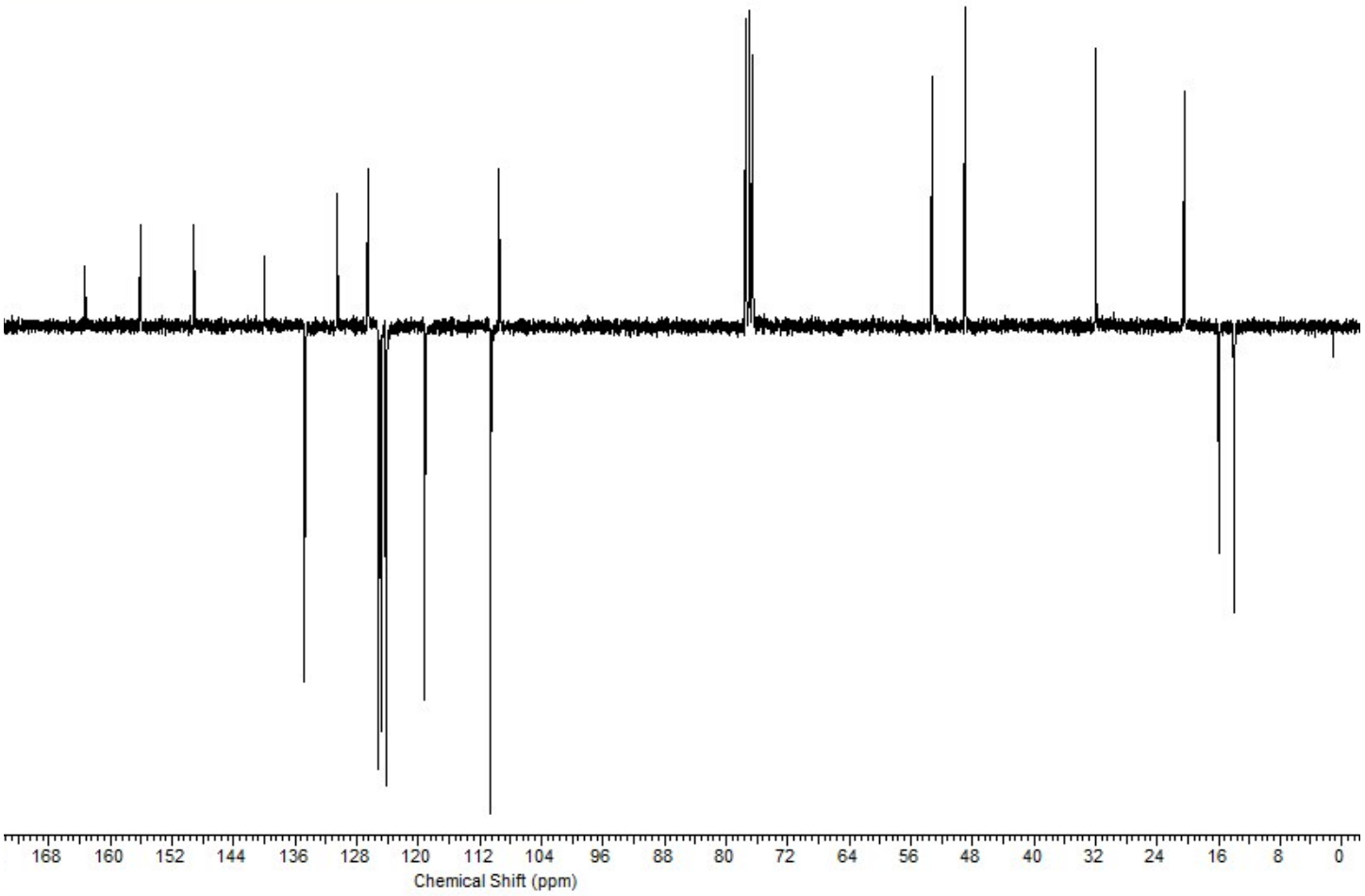


Figure ESI15. ^{13}C NMR spectrum (75,4 MHz, $CDCl_3$) of compound **19**.

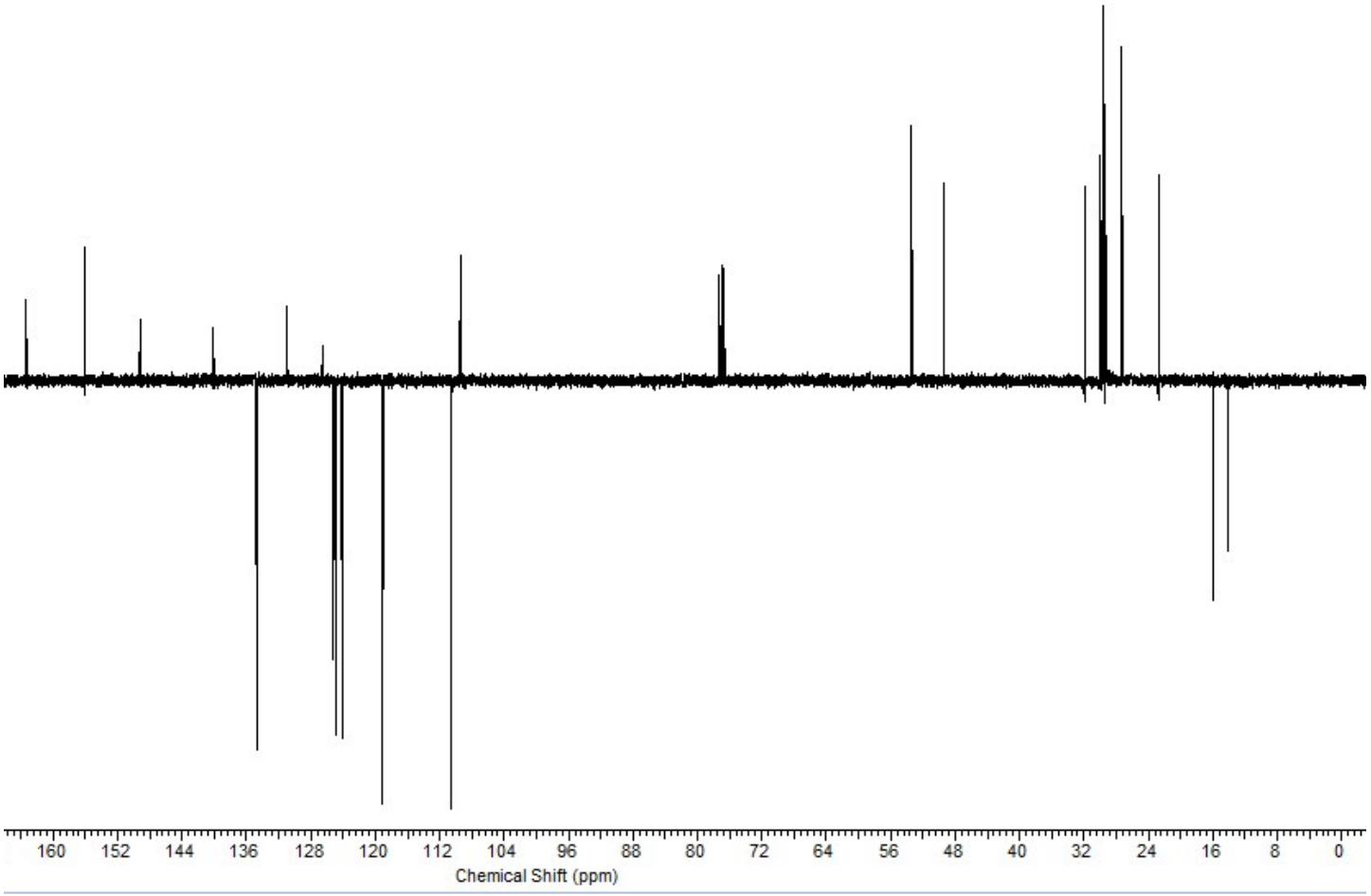


Figure ESI16. ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$) of compound **20**.

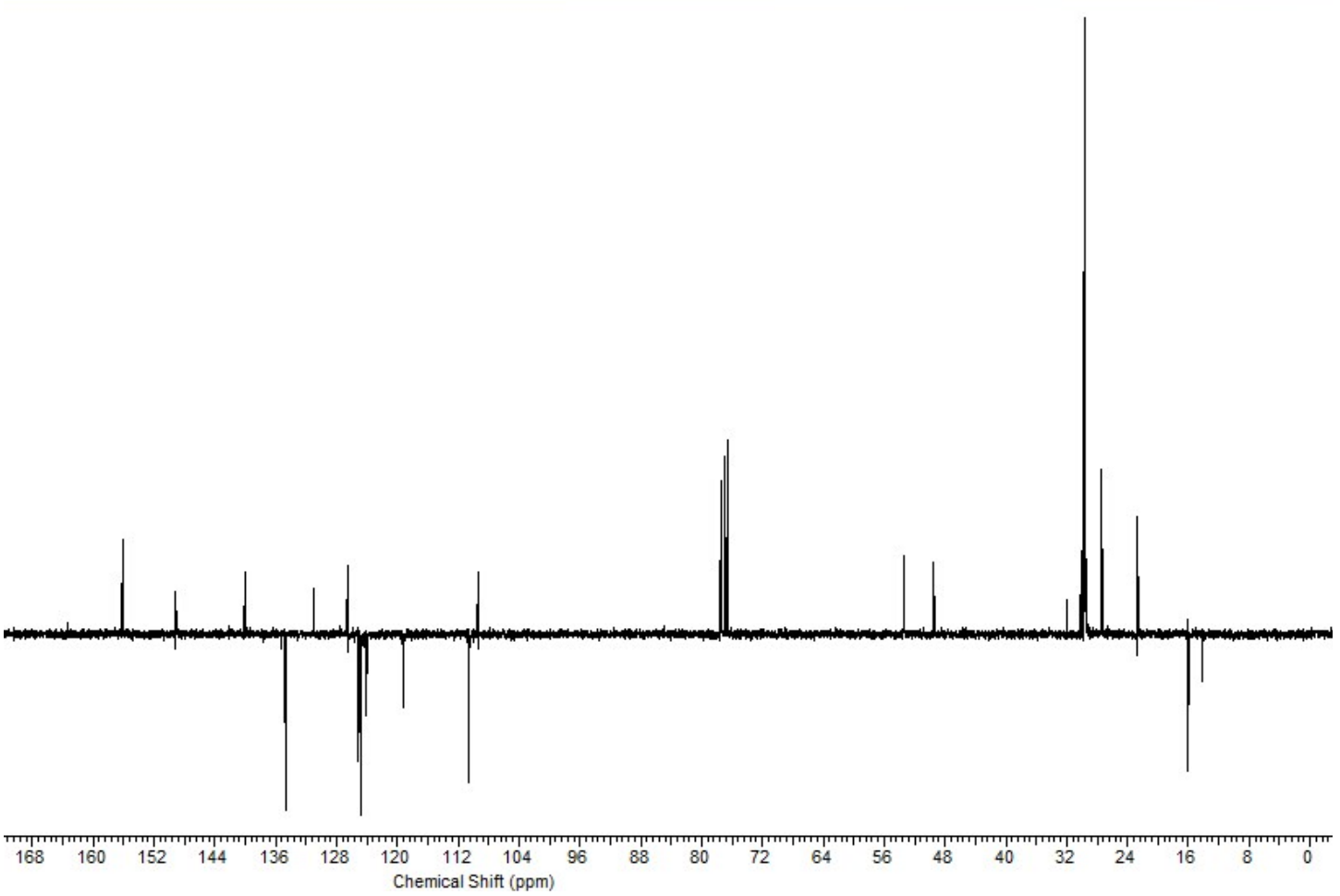


Figure ESI17. ^{13}C NMR spectrum (75.4 MHz, $CDCl_3$) of compound **21**.

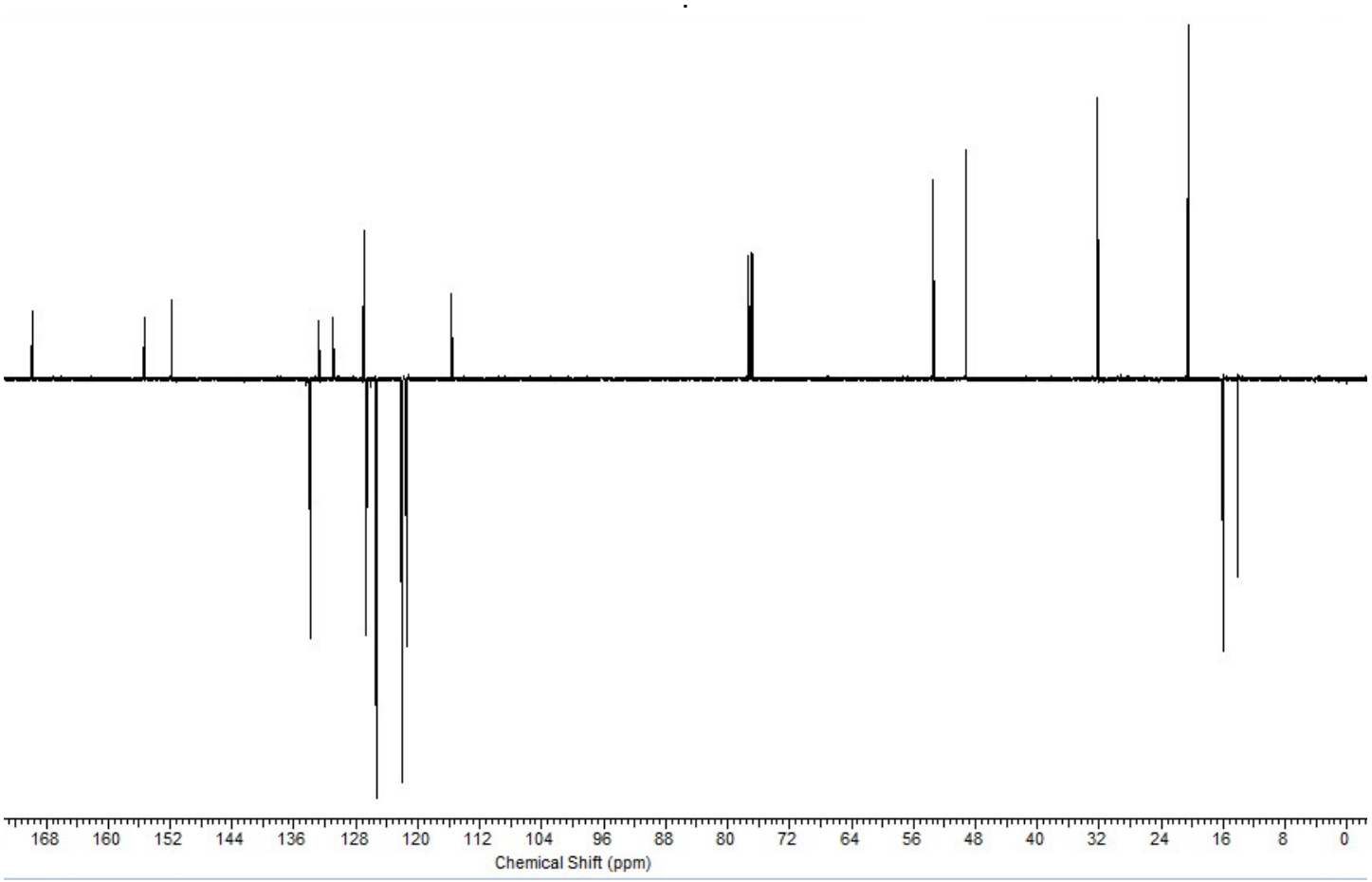


Figure ESI18. ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$) of compound **22**.

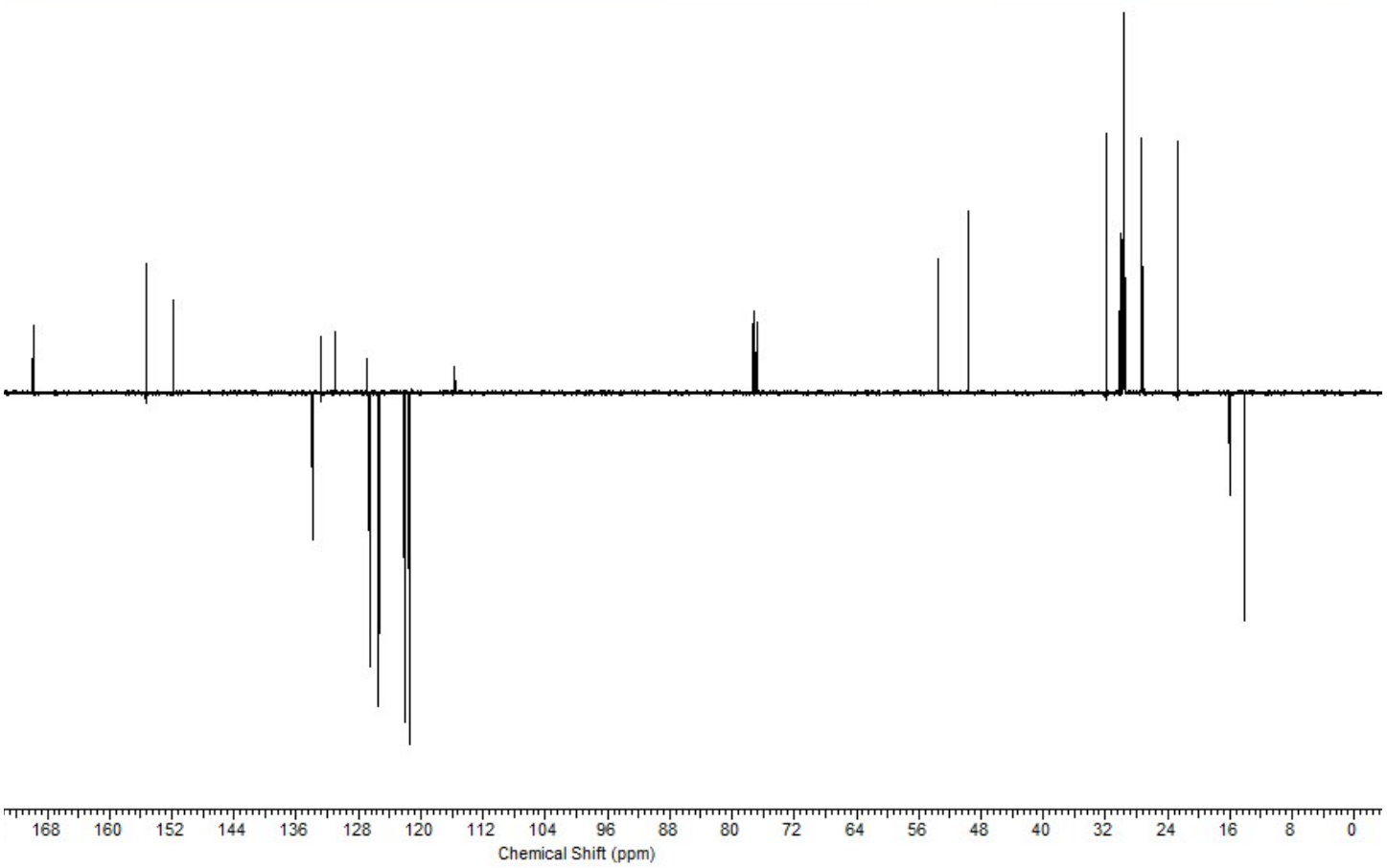


Figure ESI19. ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$) of compound **23**.

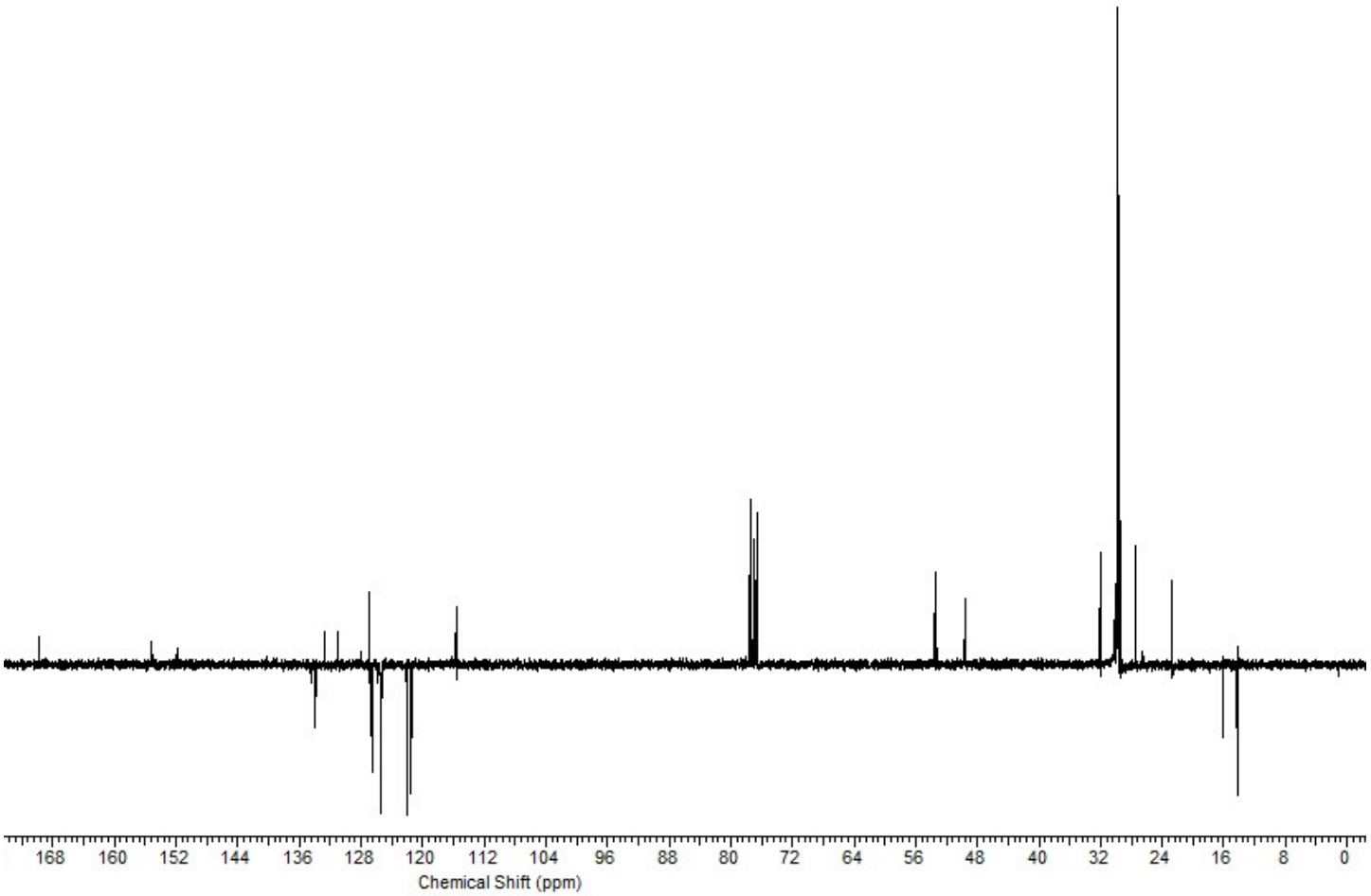


Figure ESI20. ^{13}C NMR spectrum (75.4 MHz, $CDCl_3$) of compound **24**.

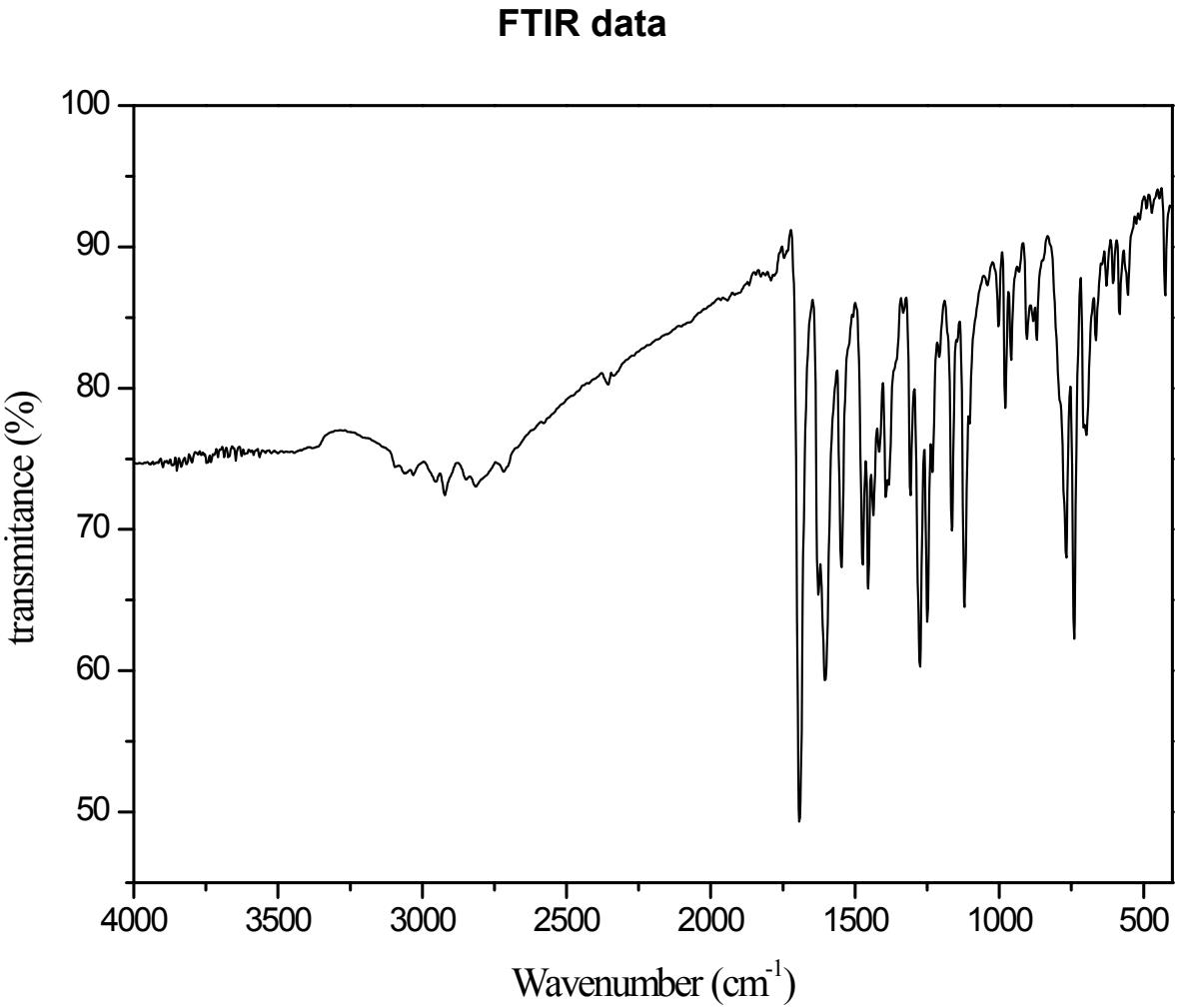


Figure ESI21. FTIR spectra of **8**.

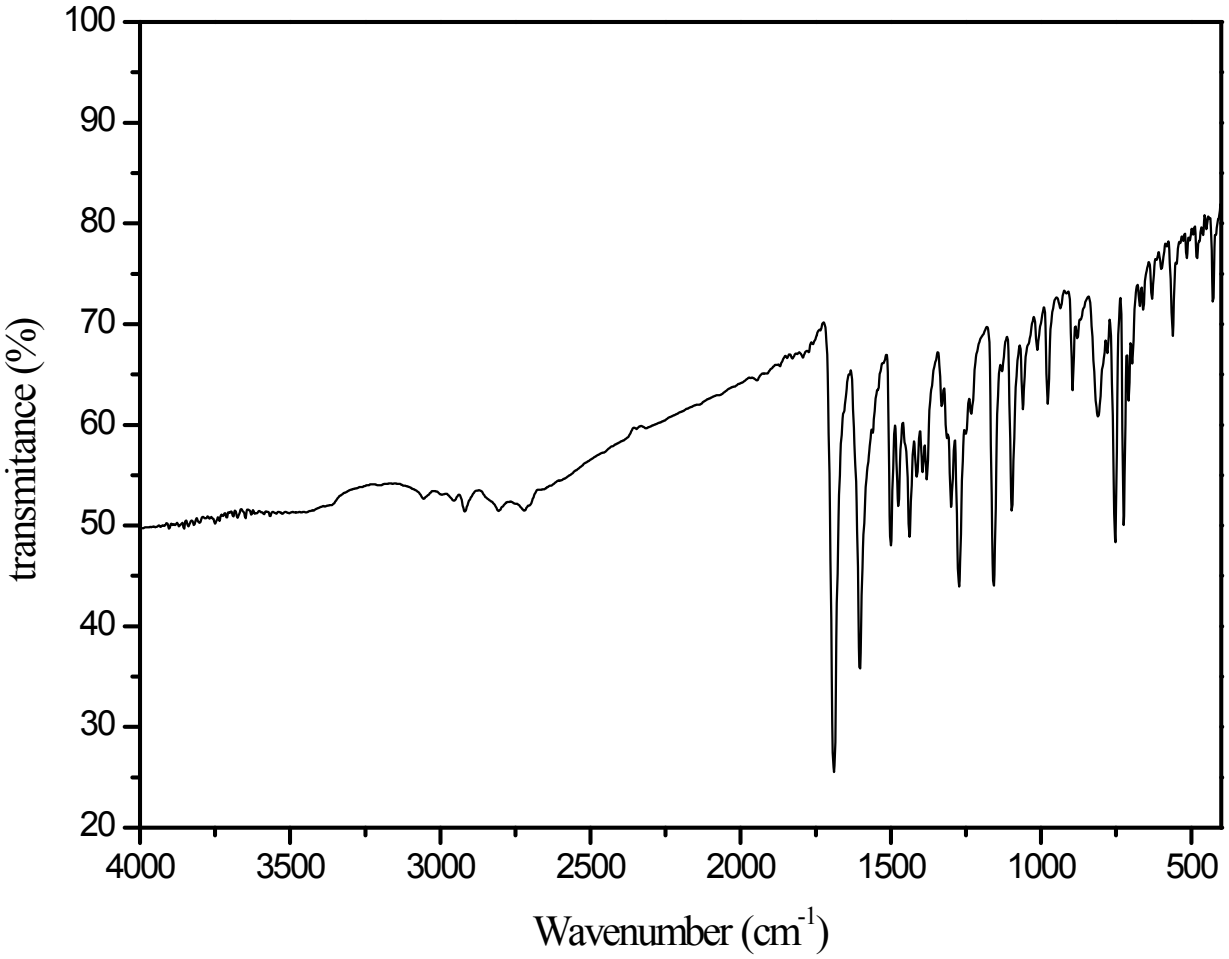


Figure ESI22. FTIR spectra of **9**.

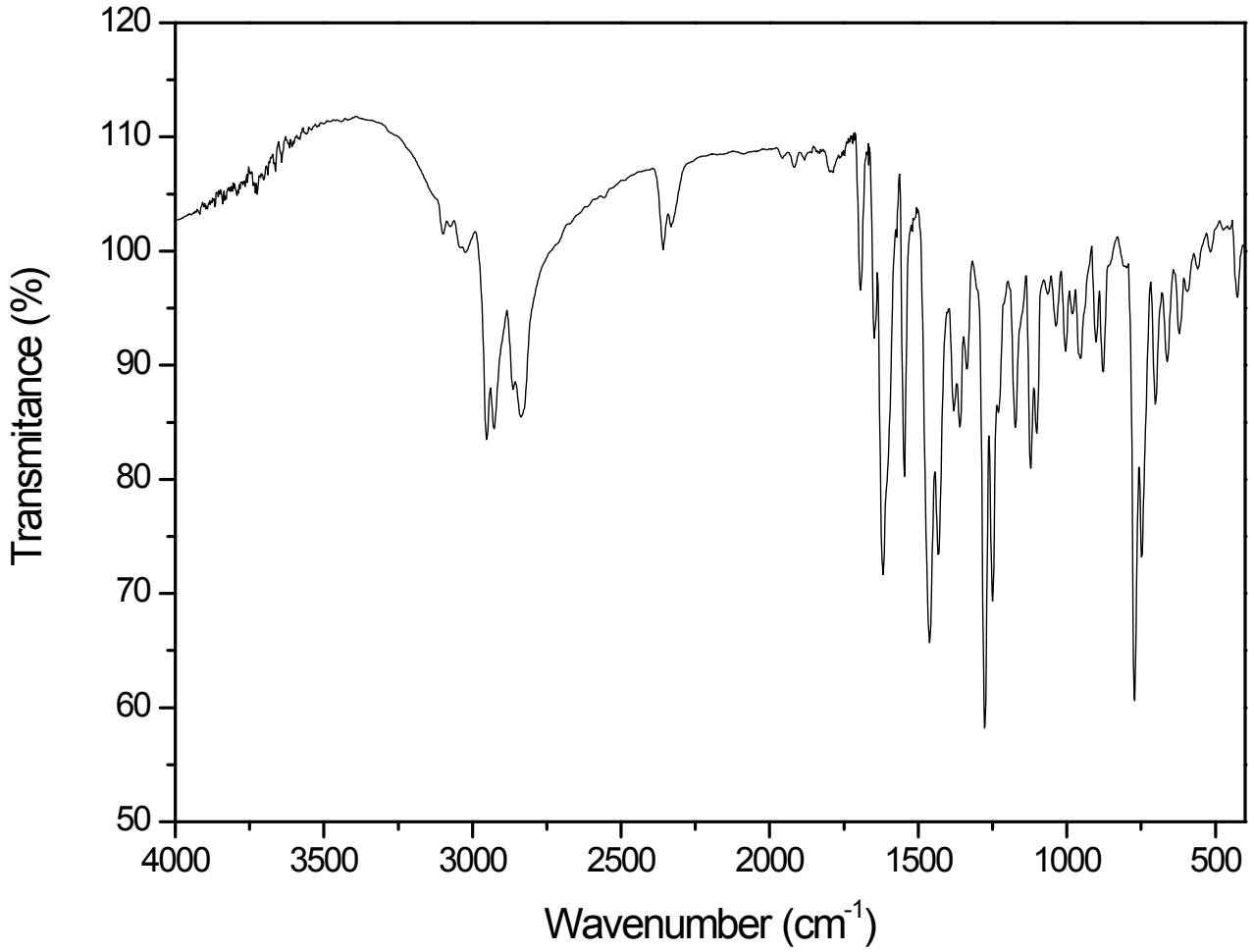


Figure ESI23. FTIR spectra of **13**.

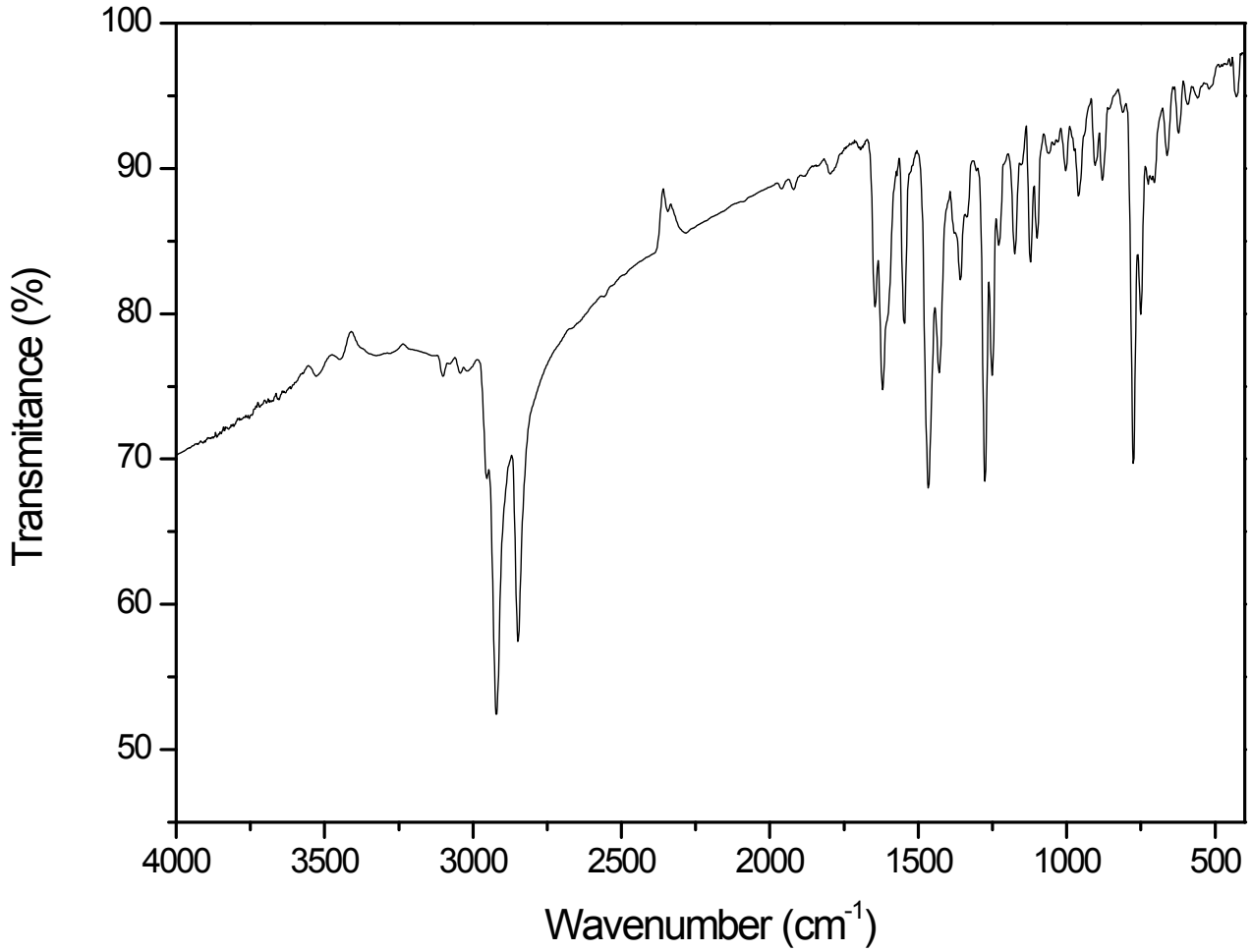


Figure ESI24. FTIR spectra of **14**.

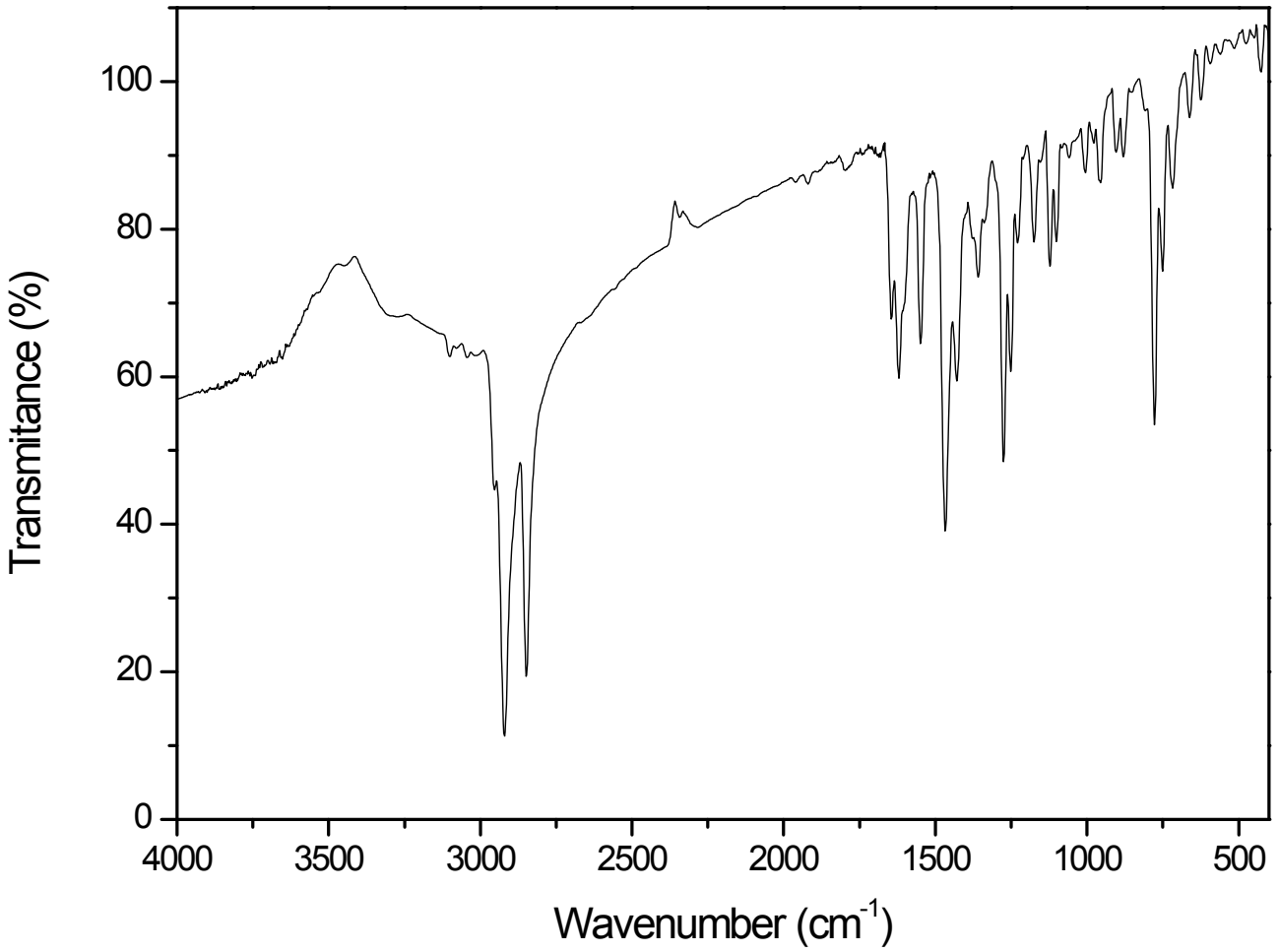


Figure ESI25. FTIR spectra of **15**.

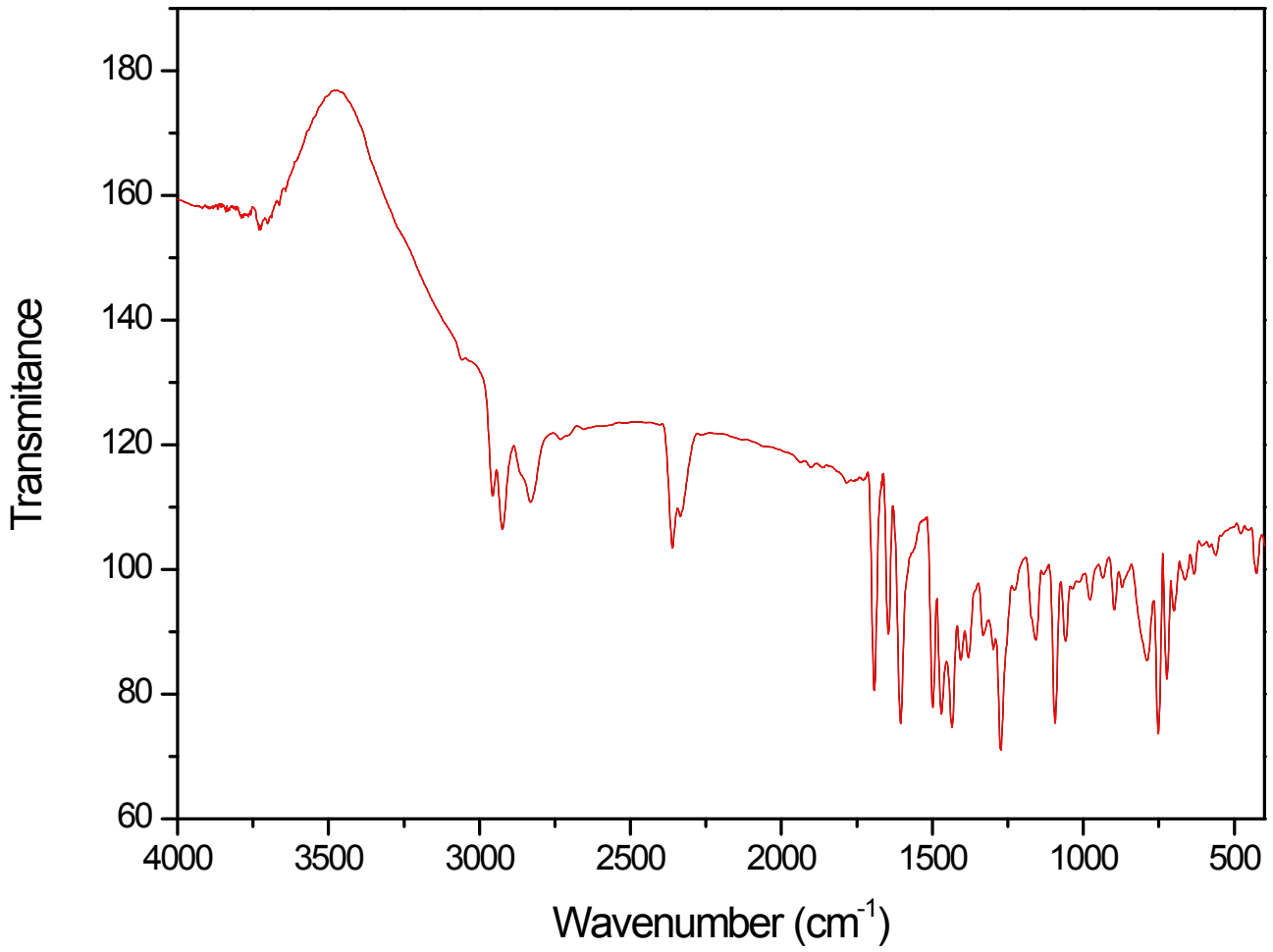


Figure ESI26. FTIR spectra of **16**.

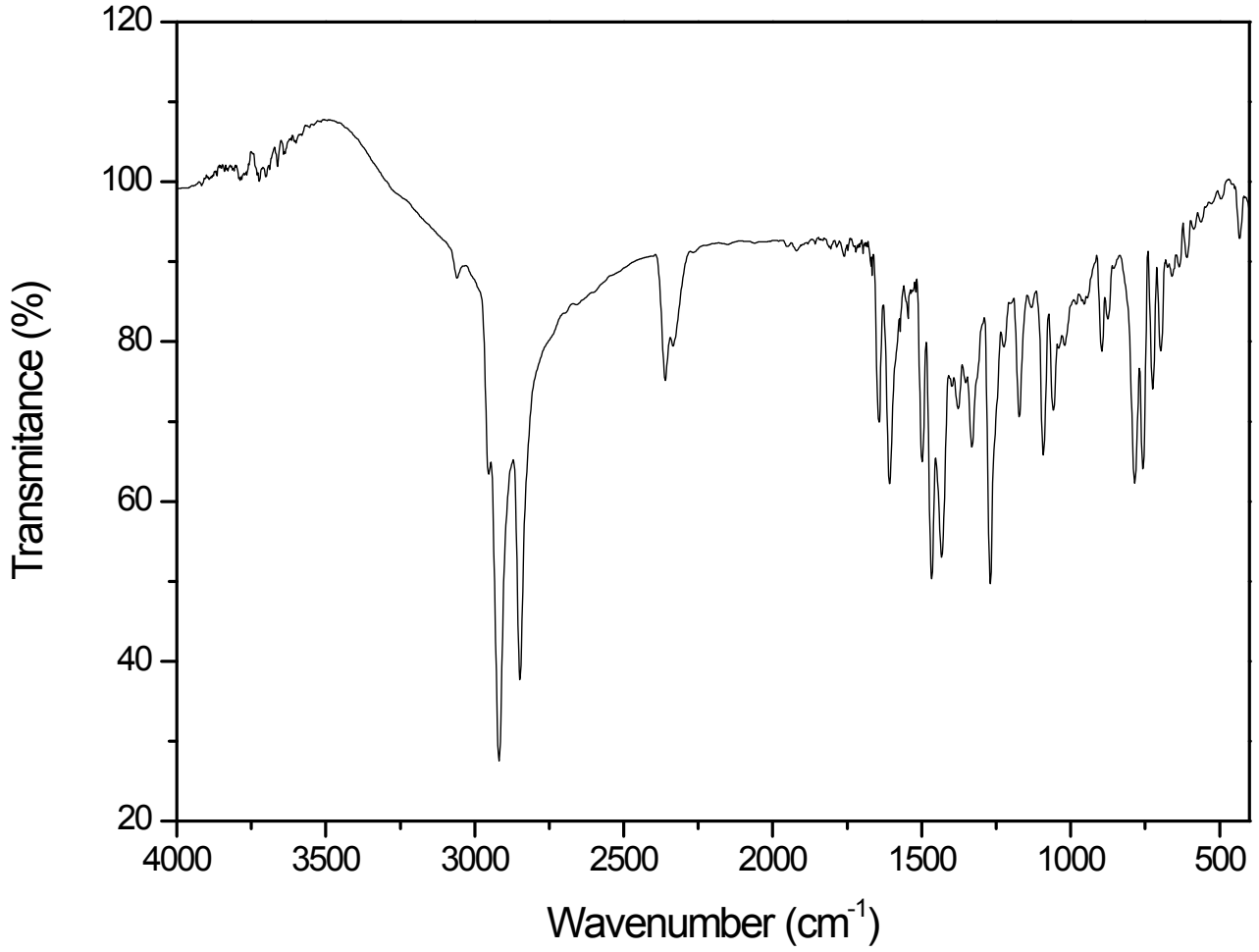


Figure ESI27. FTIR spectra of **17**.

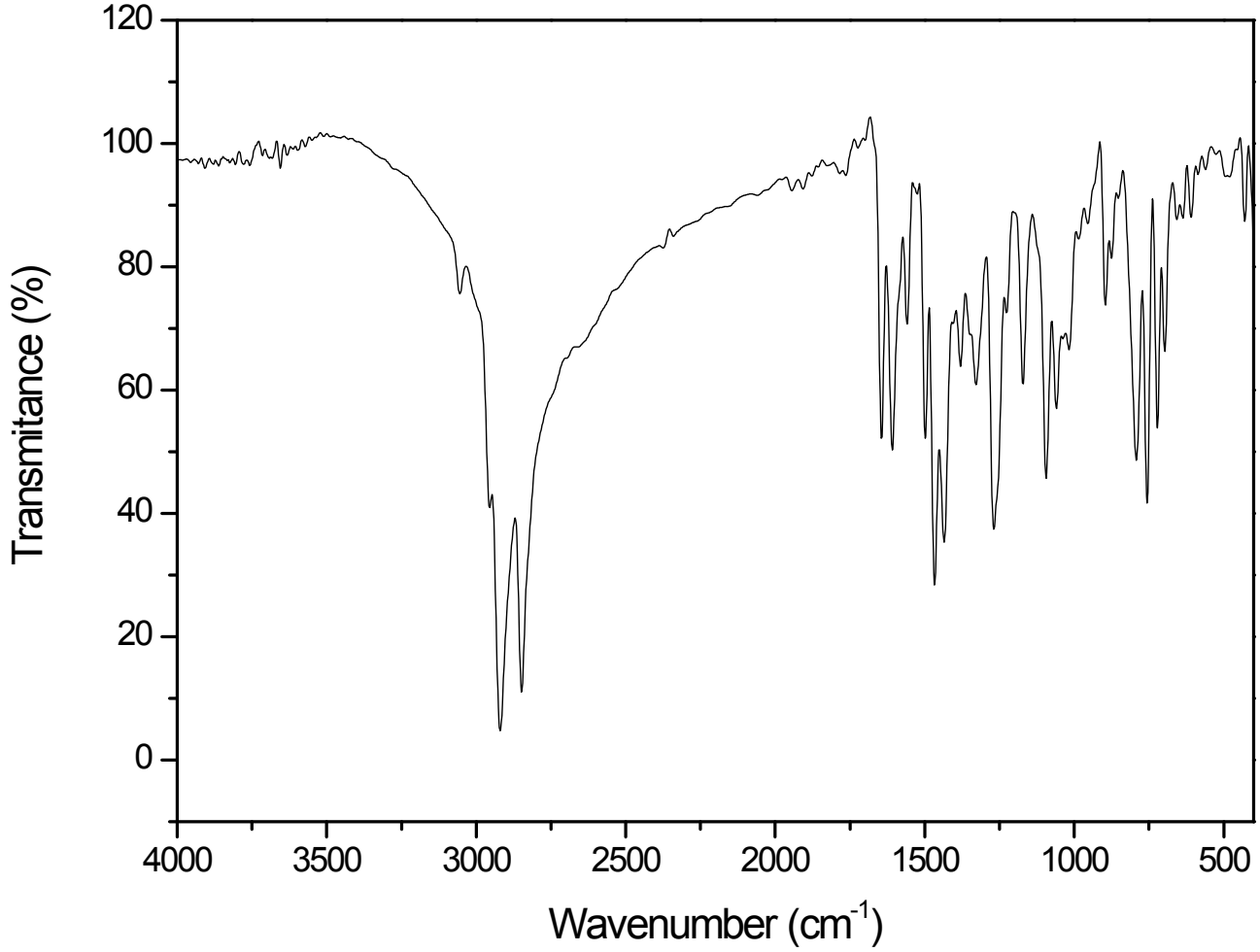


Figure ESI28. FTIR spectra of **18**.

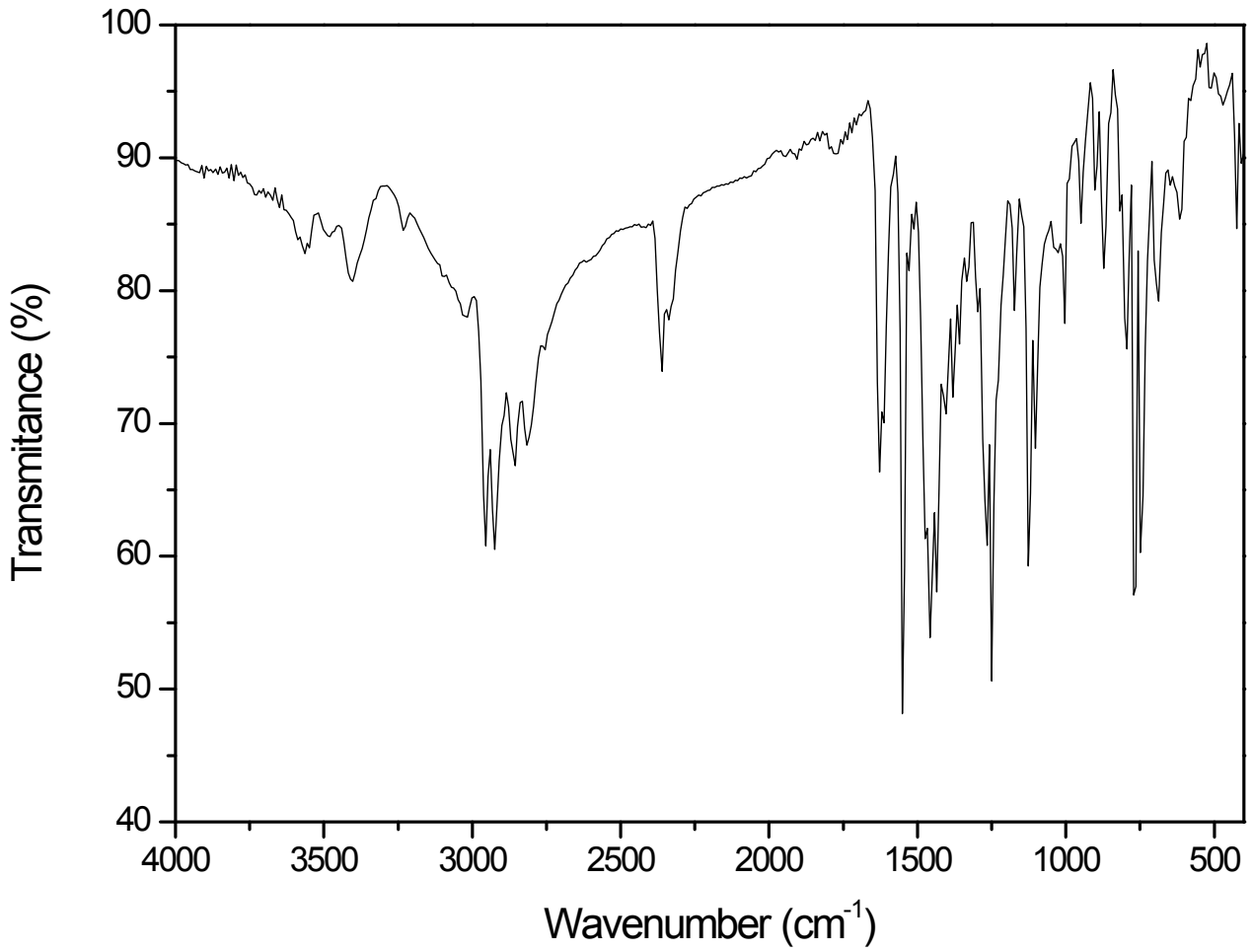


Figure ESI29. FTIR spectra of **19**.

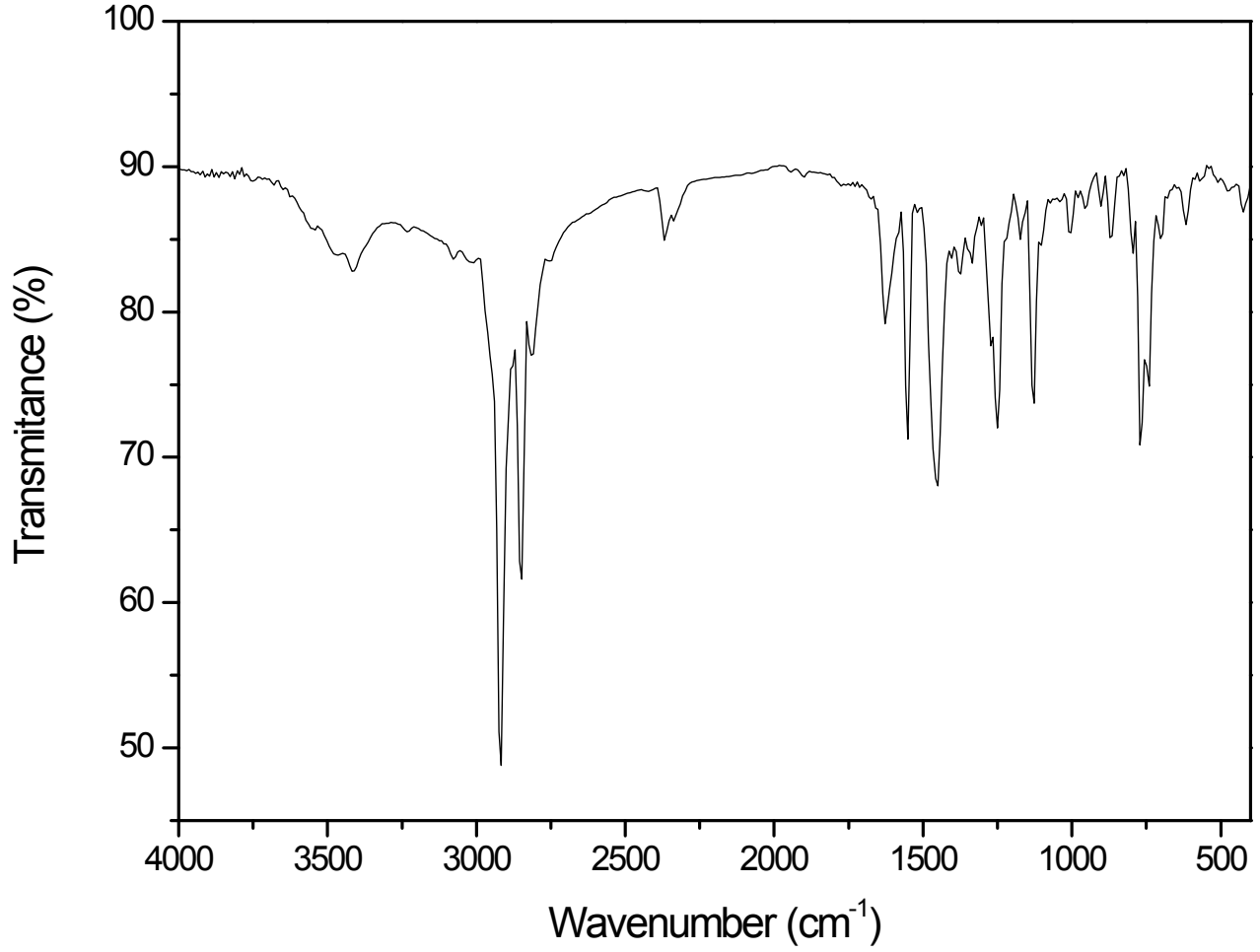


Figure ESI30. FTIR spectra of **20**.

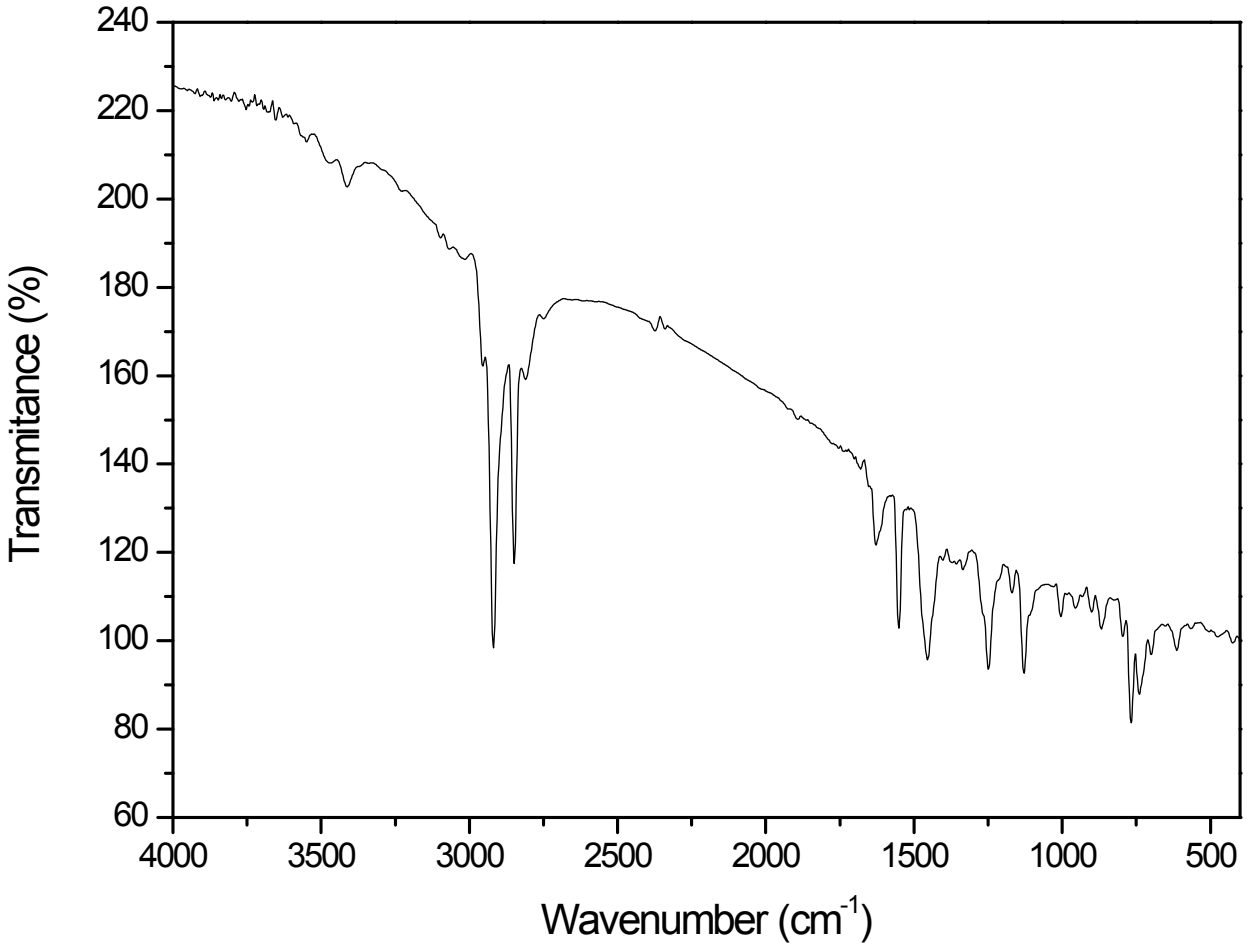


Figure ESI31. FTIR spectra of **21**.

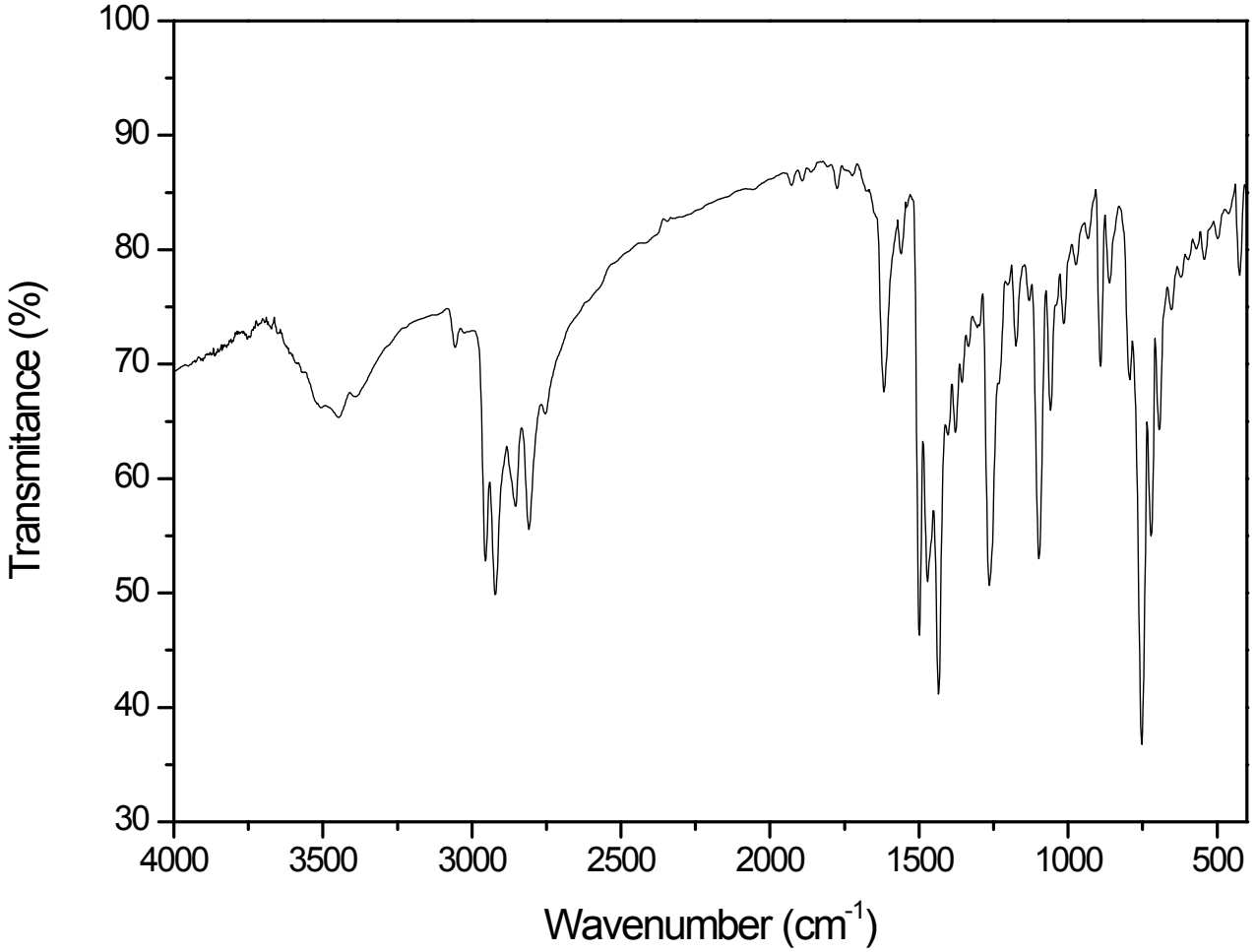


Figure ESI32. FTIR spectra of **22**.

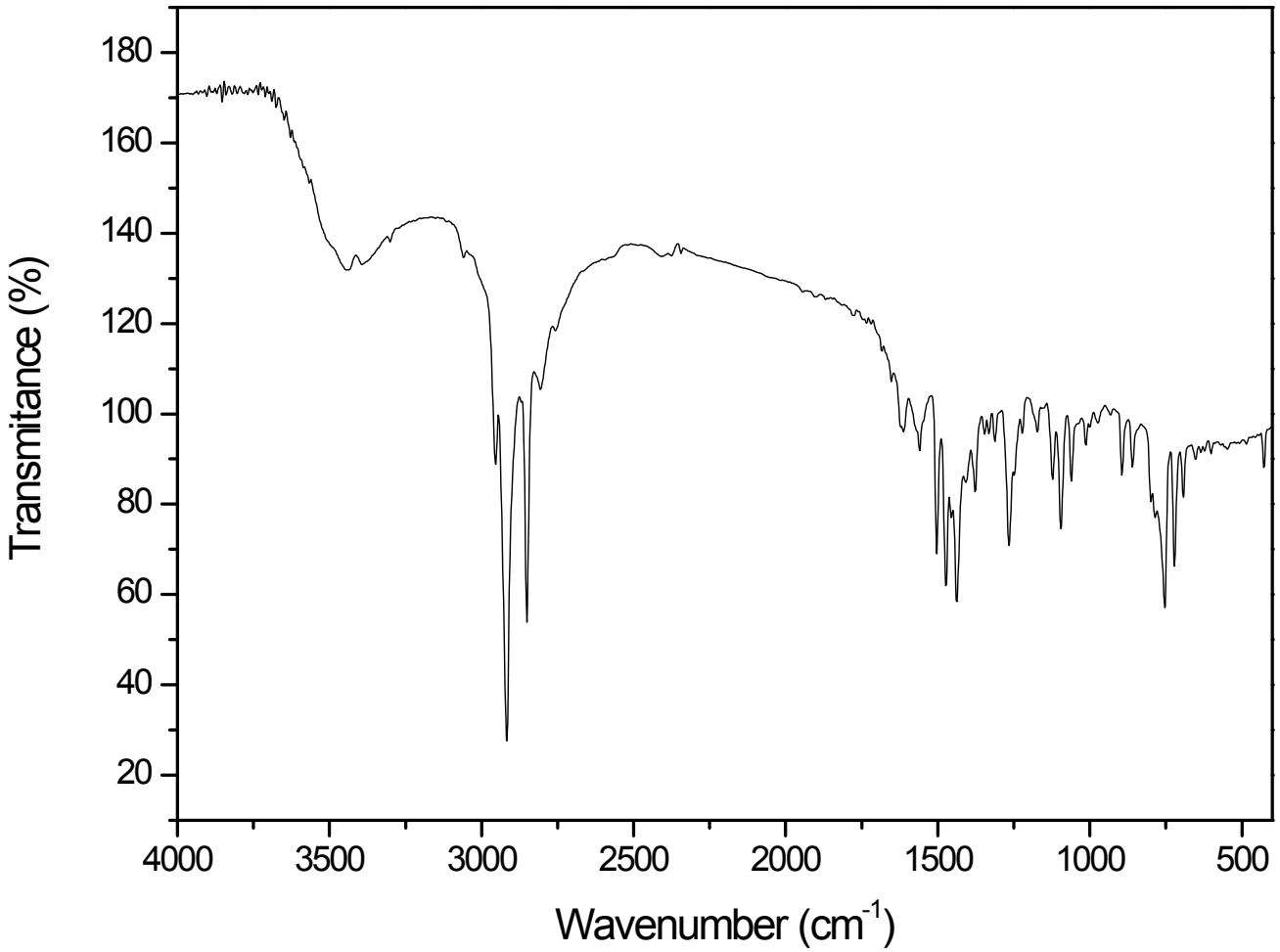


Figure ESI33. FTIR spectra of **23**.

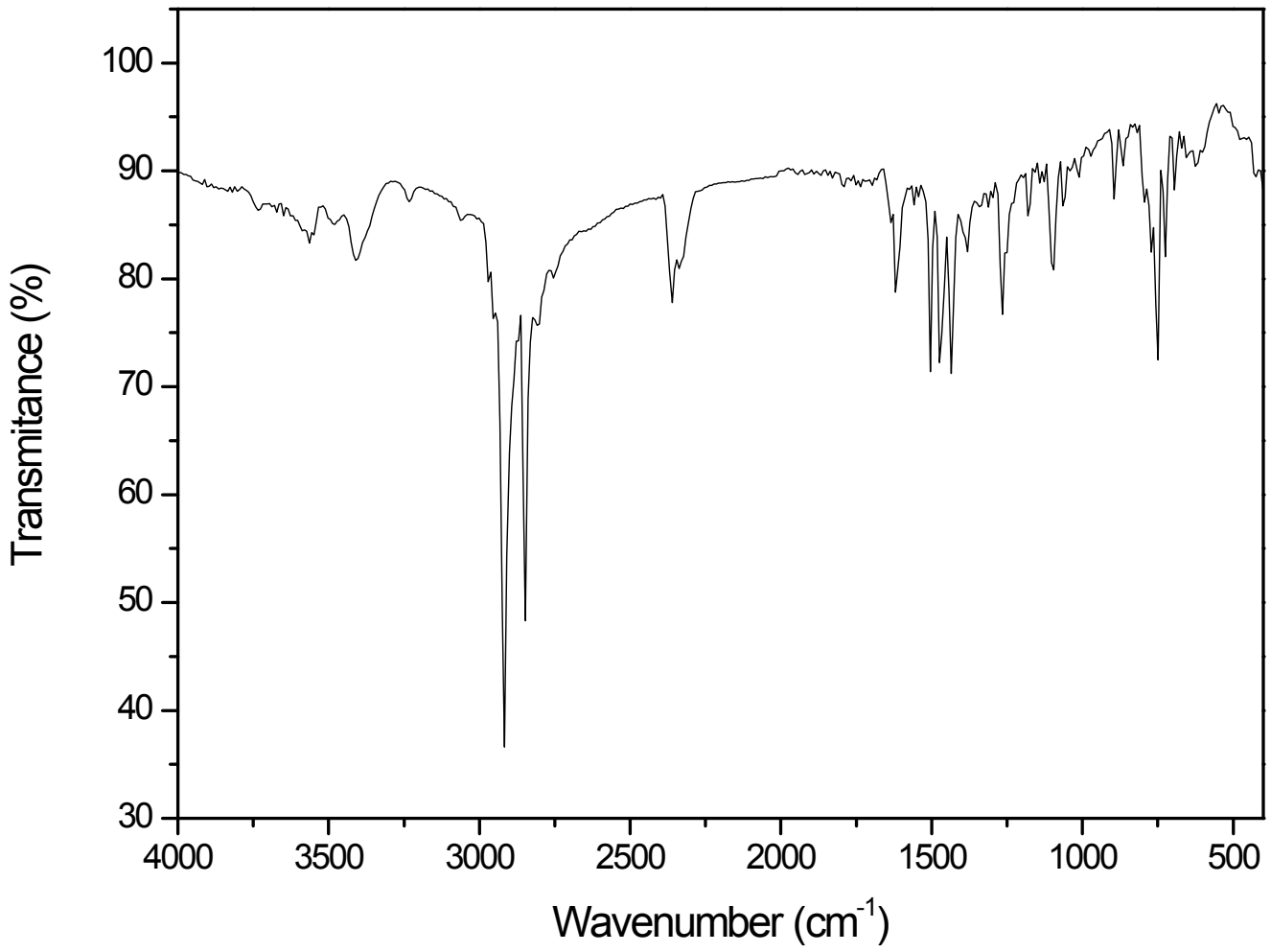
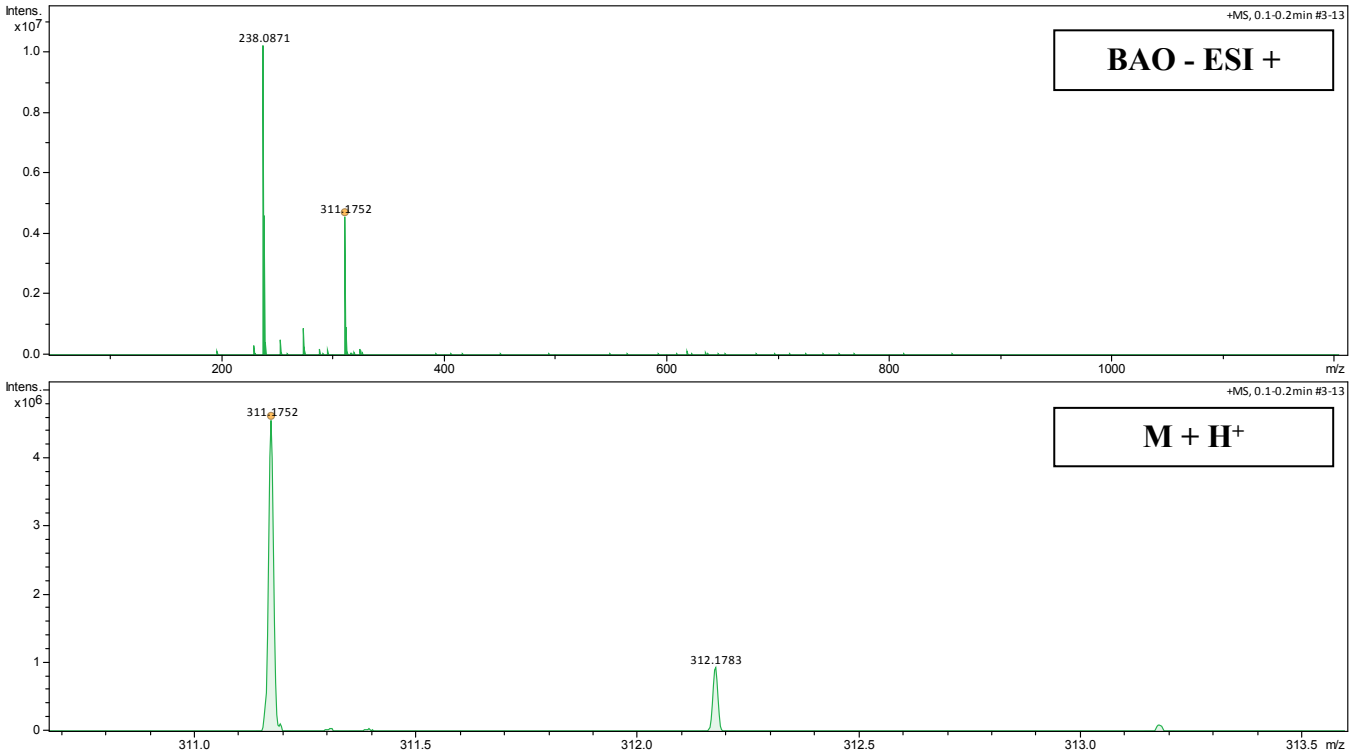


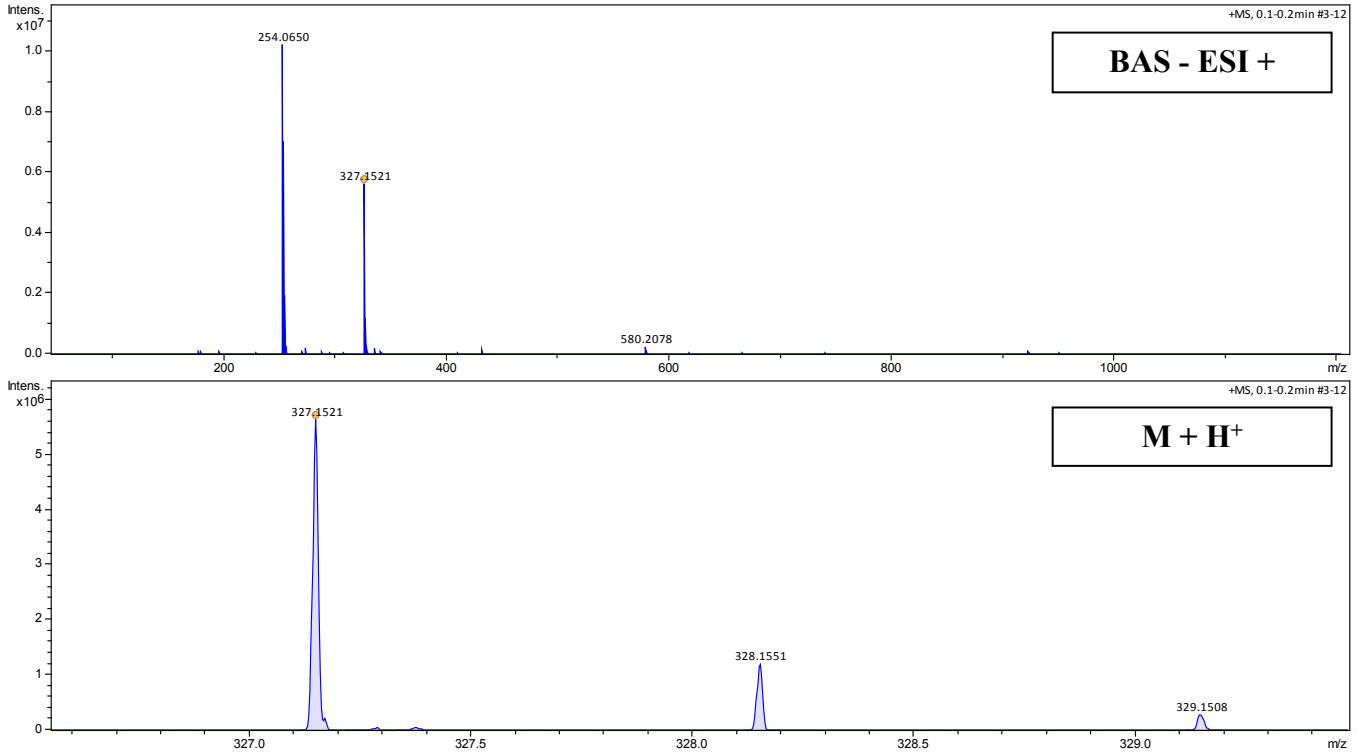
Figure ESI34. FTIR spectra of **24**.

HRMS data



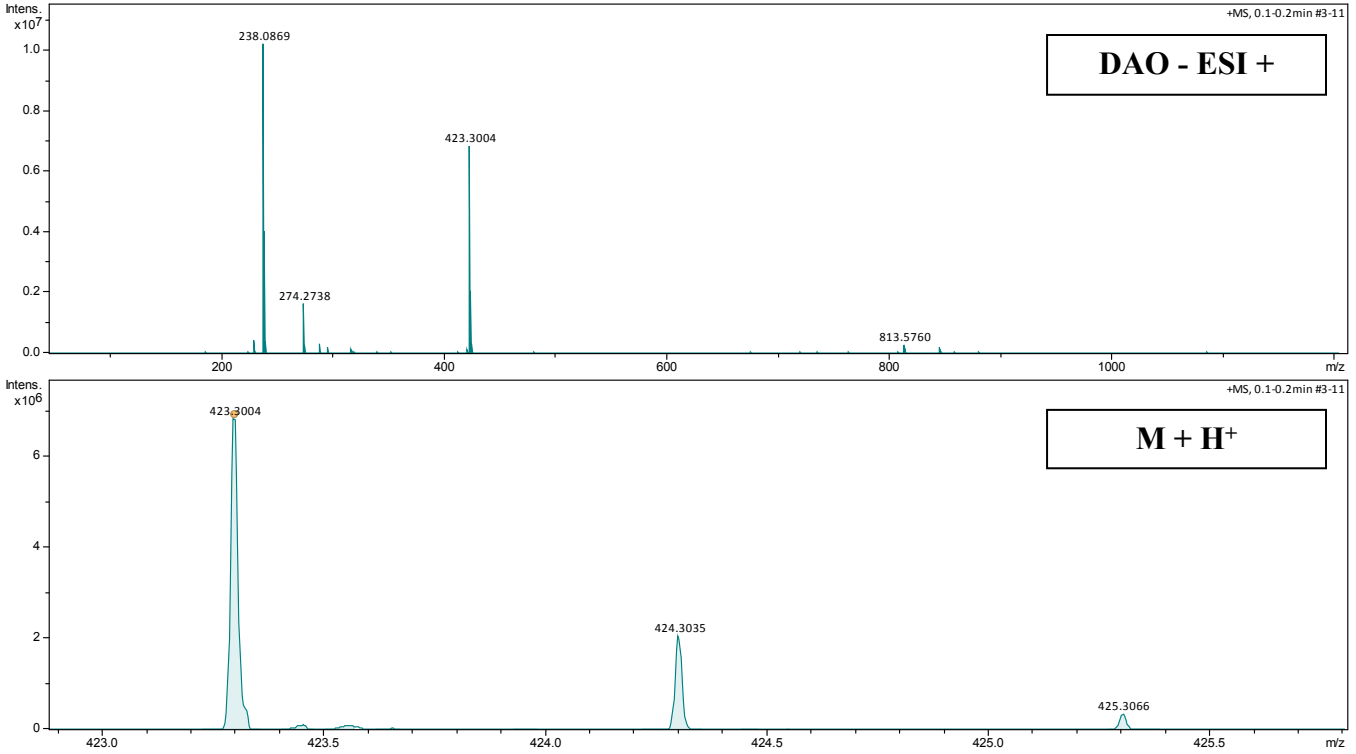
Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
311.1752	C19H23N2O2	311.1754	0.8	6.6	9.5	even	ok

Figure ESI35. HRMS data of **19**.



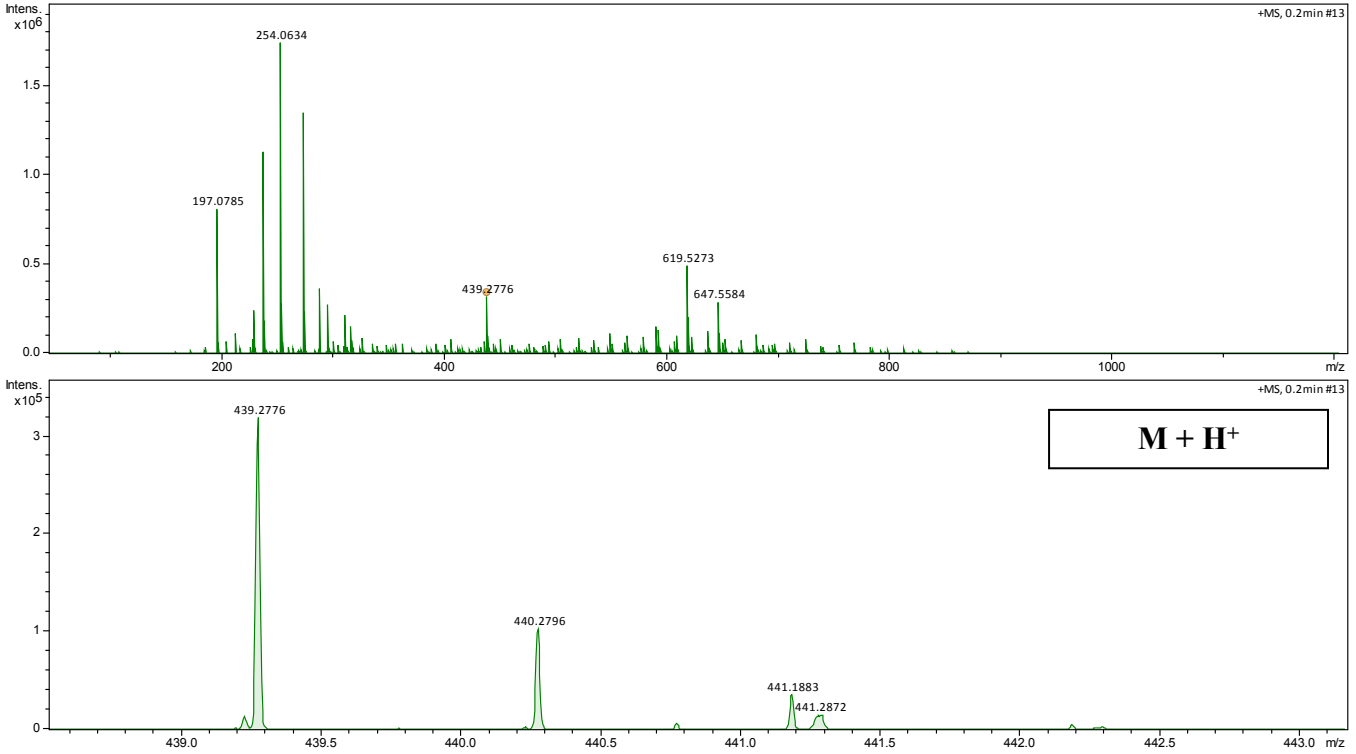
Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e^- Conf	N-Rule
327.1521	C19H23N2OS	327.1526	1.3	11.8	9.5	even	ok

Figure ESI36. HRMS data of **20**.



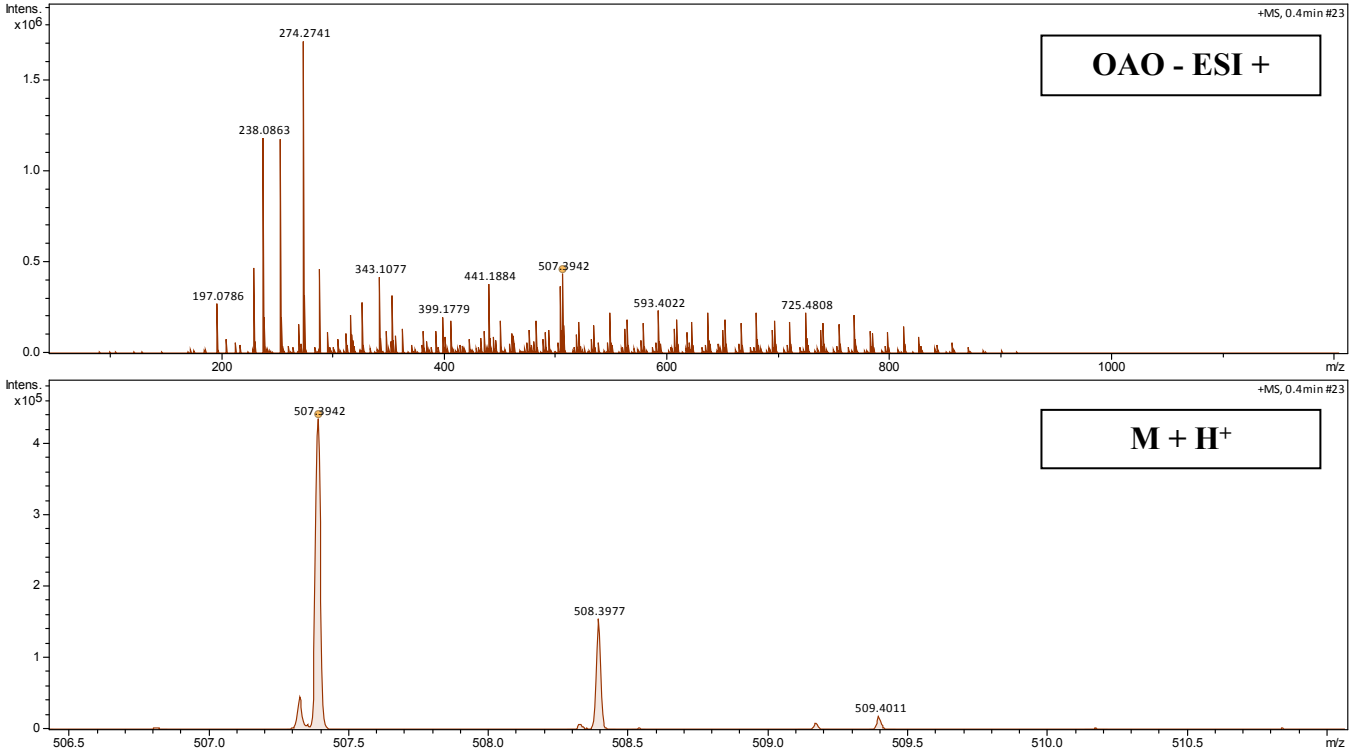
Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
423.3004	C27H39N2O2	423.3006	0.5	1.5	9.5	even	ok

Figure ESI37. HRMS data of **21**.



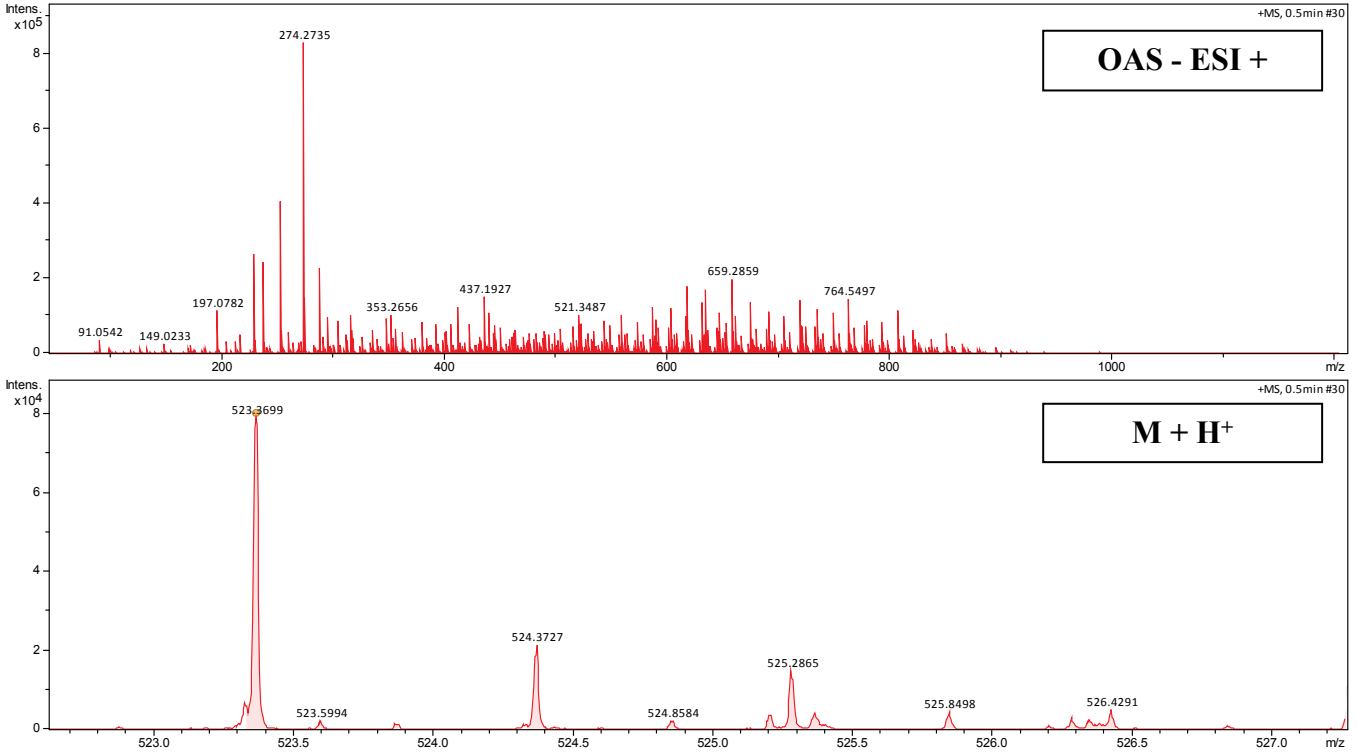
Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
439.2776	C27H39N2OS	439.2778	0.3	26.5	9.5	even	ok

Figure ESI38. HRMS data of **22**.



Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
507.3942	C33H51N2O2	507.3945	0.5	17.0	9.5	even	ok

Figure ESI39. HRMS data of **23**.



Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
523.3699	C33H51N2OS	523.3717	3.4	63.2	9.5	even	ok

Figure ESI40. HRMS data of **24**.

Additional Photophysical data

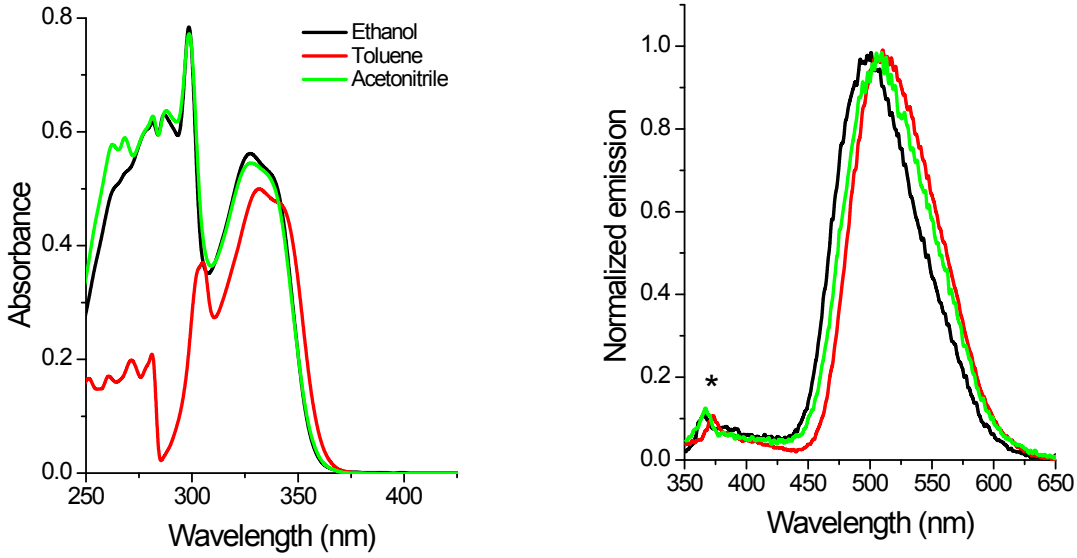


Figure ESI41. UV-Vis absorption (left) and normalized fluorescence emission (right) spectra of amine **19** (~10^{-5} M). (λ_{exc}=328 nm for ethanol and acetonitrile and λ_{exc}=332 nm for toluene). The asterisk indicates the Raman signal.

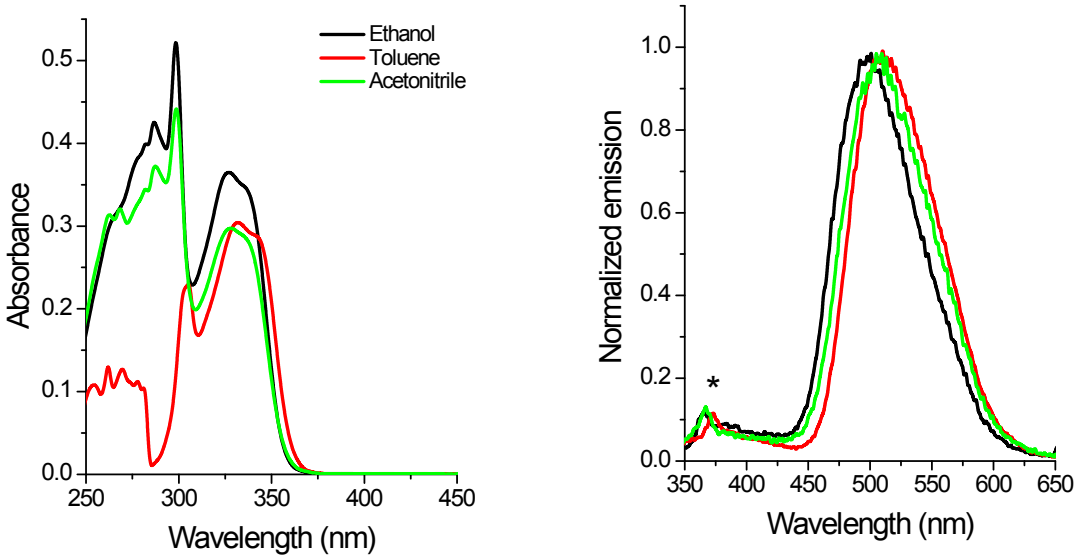


Figure ESI42. UV-Vis absorption (left) and normalized fluorescence emission (right) spectra of amine **20** (~10^{-5} M). (λ_{exc}=327 nm for ethanol, λ_{exc}=350 nm for acetonitrile and λ_{exc}=332 nm for toluene). The asterisk indicates the Raman signal.

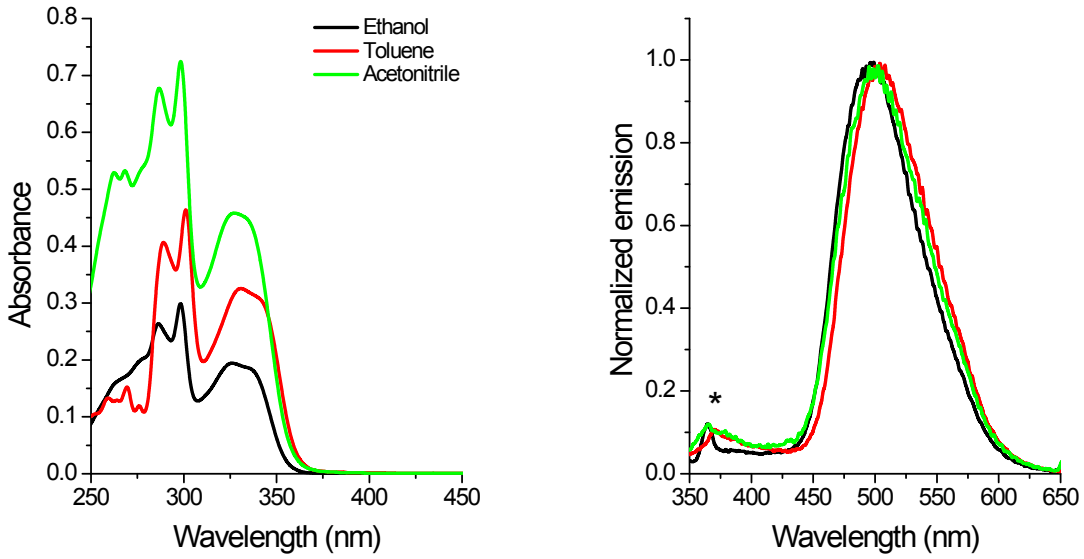


Figure ESI43. UV-Vis absorption (left) and normalized fluorescence emission (right) spectra of amine **21** (~10^{-5} M). (λ_{exc}=327 nm for ethanol and acetonitrile and λ_{exc}=332 nm for toluene). The asterisk indicates the Raman signal.

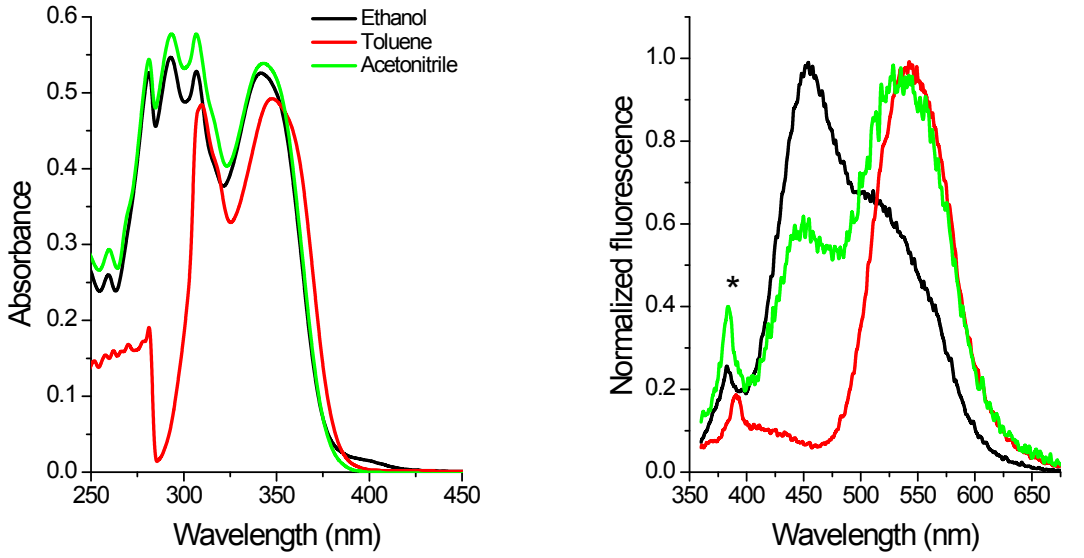


Figure ESI44. UV-Vis absorption (left) and normalized fluorescence emission (right) spectra of amine **22** (~10^{-5} M). (λ_{exc}=342 nm for ethanol, λ_{exc}=343 nm for acetonitrile and λ_{exc}=348 nm for toluene). The asterisk indicates the Raman signal.

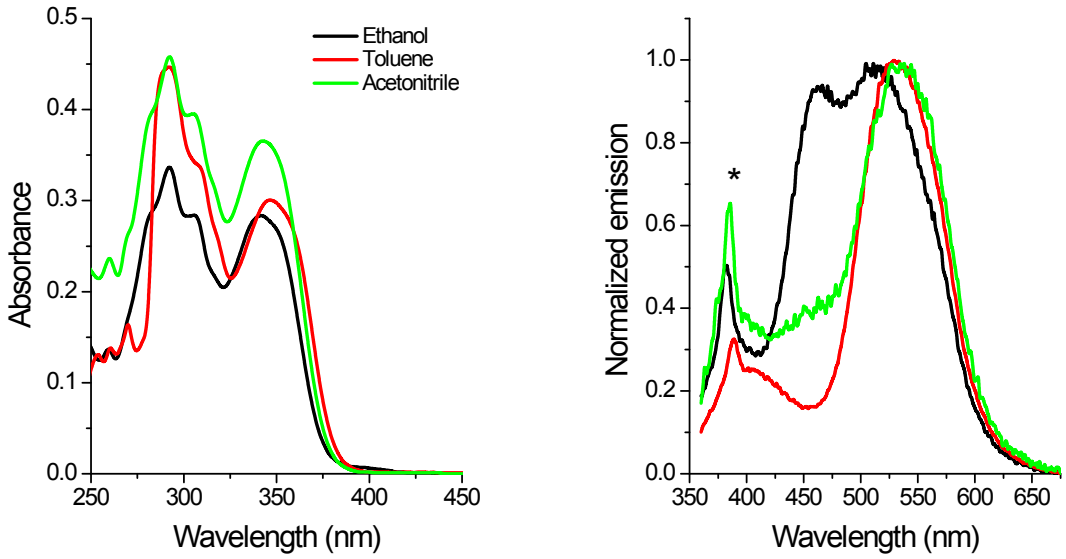


Figure ESI45. UV-Vis absorption (left) and normalized fluorescence emission (right) spectra of amine **22** (~10^{-5} M). (λ_{exc}=341 nm for ethanol, λ_{exc}=342 nm for acetonitrile and λ_{exc}=347 nm for toluene). The asterisk indicates the Raman signal.

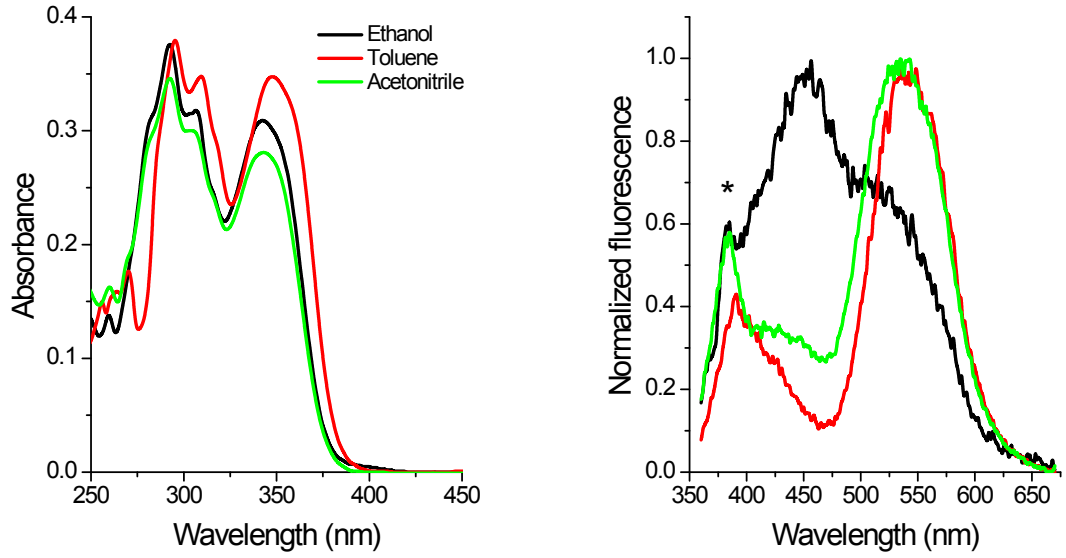


Figure ESI46. UV-Vis absorption (left) and normalized fluorescence emission (right) spectra of amine **24** (~10^{-5} M). (λ_{exc}=342 nm for ethanol and acetonitrile and λ_{exc}=348 nm for toluene). The asterisk indicates the Raman signal.

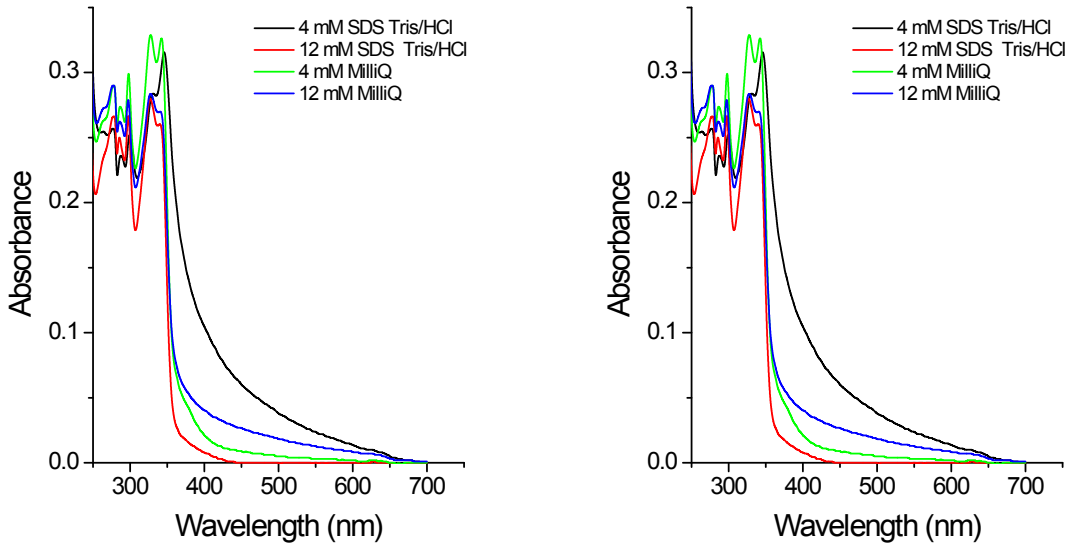


Figure ESI47. UV-Vis absorption spectra of compound **20** (left) and **23** (right) (~10^{-5} M) at different solutions of SDS in Tris/HCl (pH 9.0) and MilliQ Water below (4 mM) and above (12 mM) cmc.

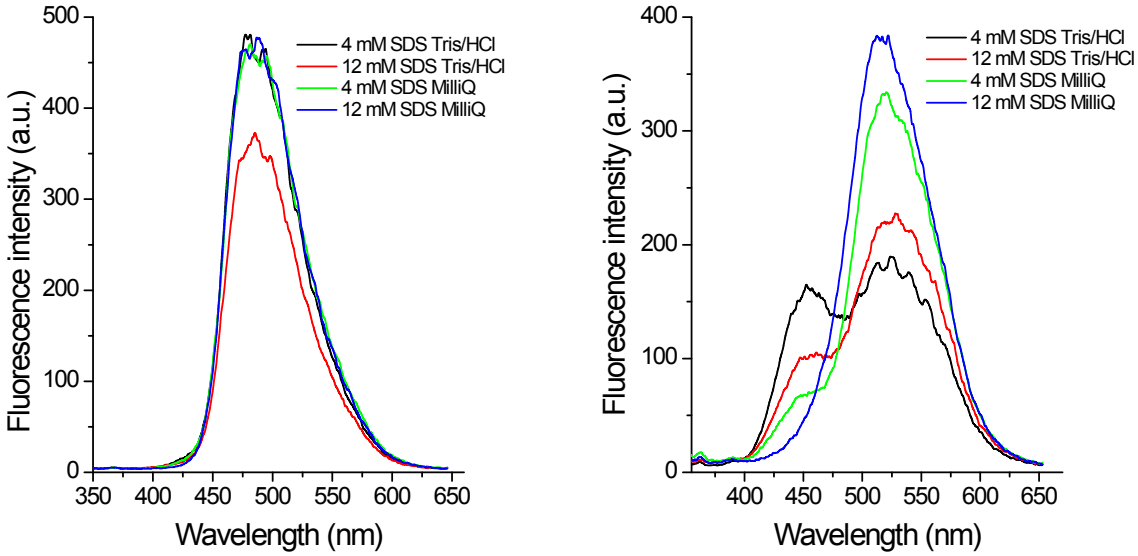


Figure ESI48. Normalized fluorescence emission spectra of compound **20** (left) and **23** (right) (~10^{-5} M) at different solutions of SDS in Tris/HCl (pH 9.0) and MilliQ Water below (4 mM) and above (12 mM) cmc.

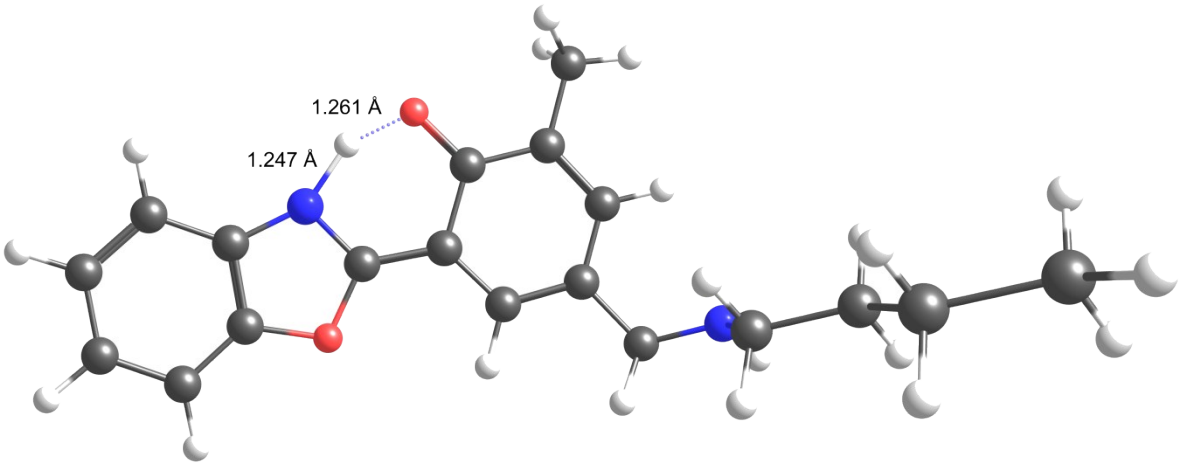


Figure ESI49. Geometry of the transition state of the proton transfer of molecule **19**.