

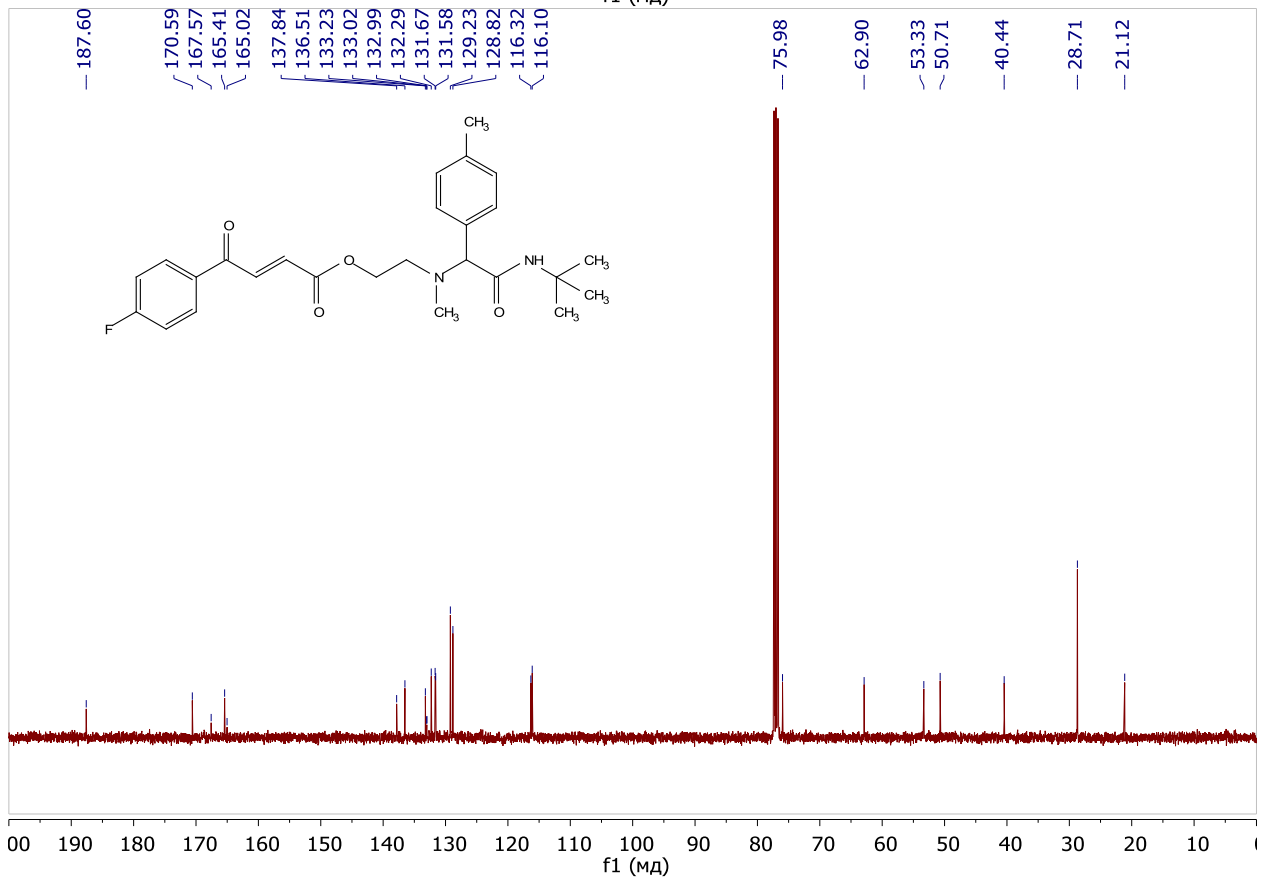
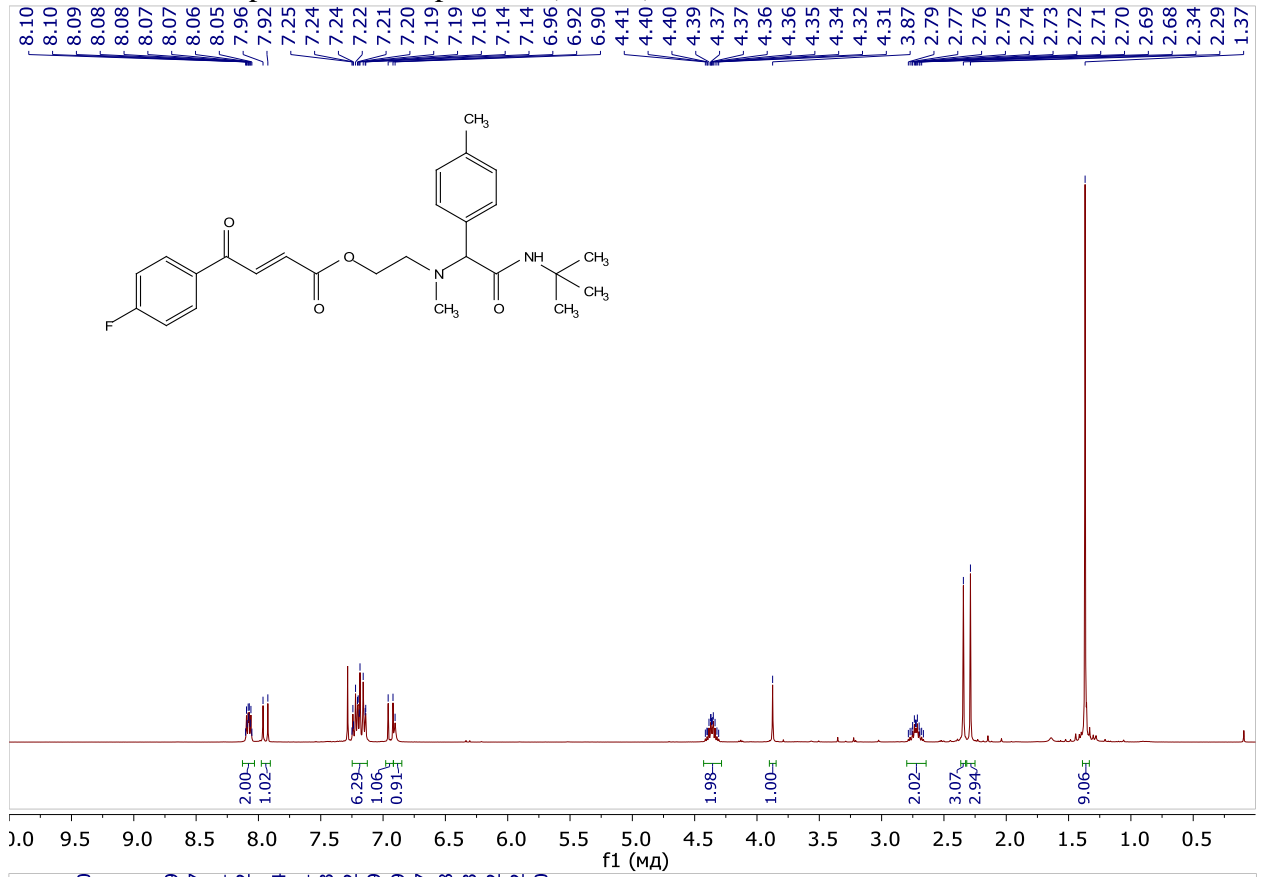
Further exploration of DVD-445 as a lead thioredoxin reductase (TrxR) inhibitor for cancer therapy: optimization of potency and evaluation of anticancer potential

Mirna Jovanović, Daniil Zhukovsky, Ana Podolski-Renić, Raivis Žalubovskis, Dmitry Dar'in, Vladimir Sharoyko, Tatiana Tennikova, Milica Pešić* and Mikhail Krasavin*

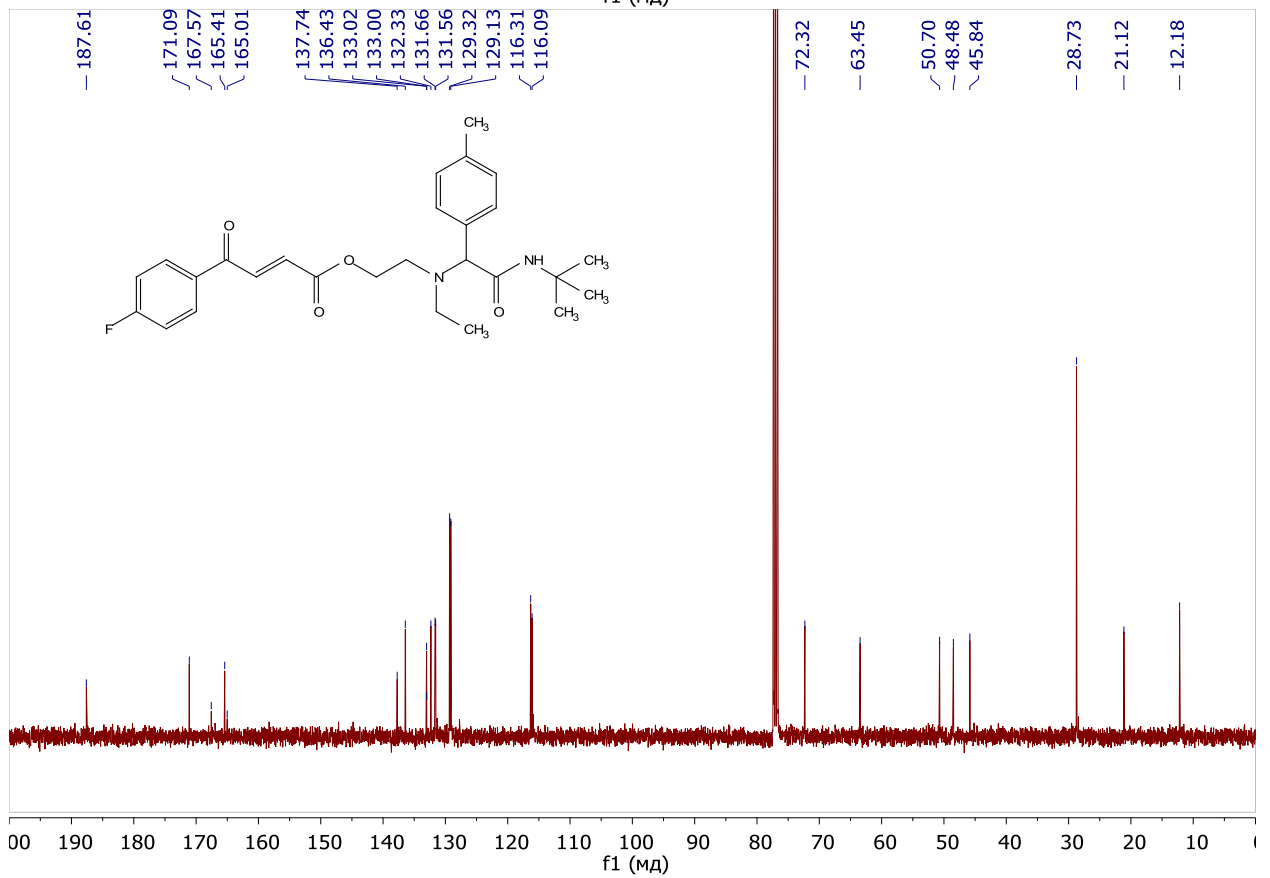
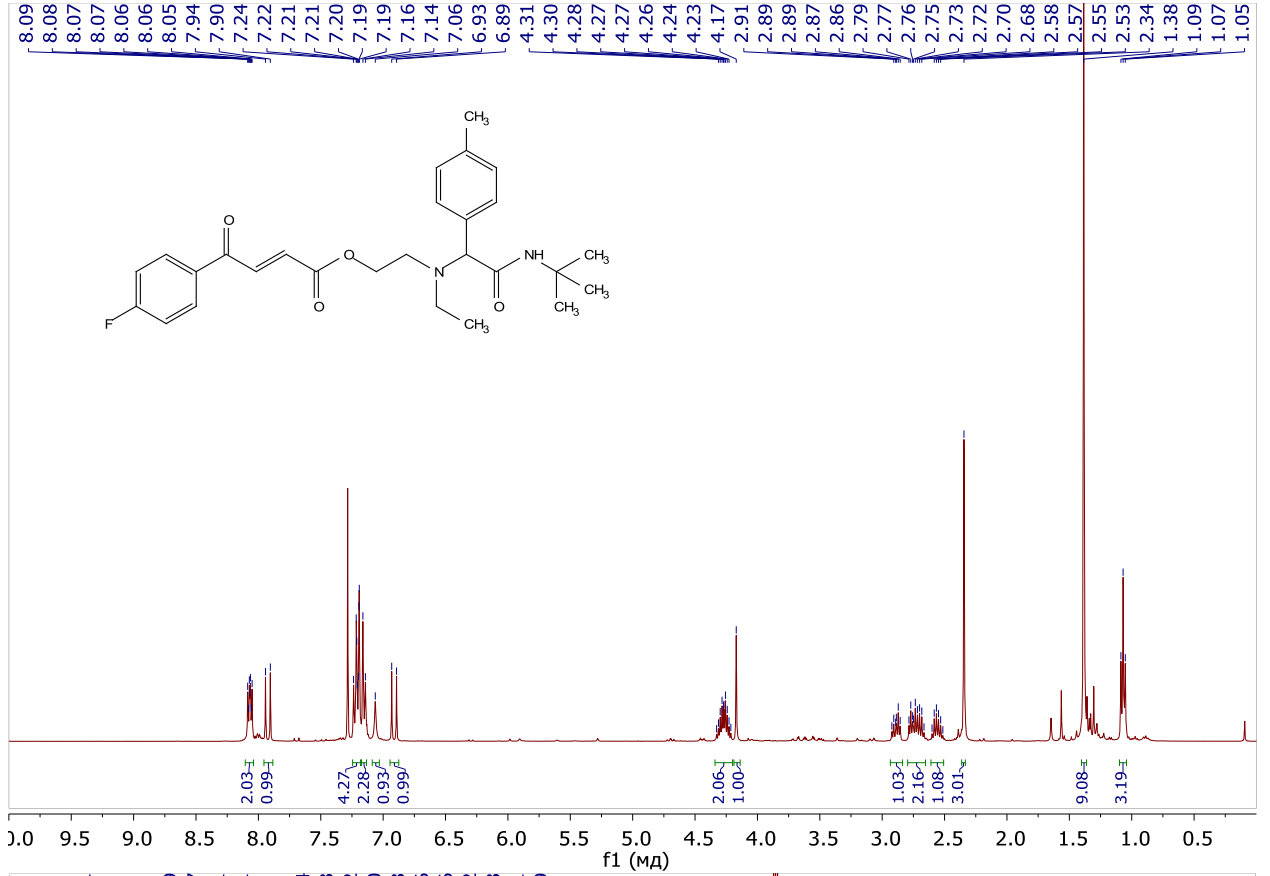
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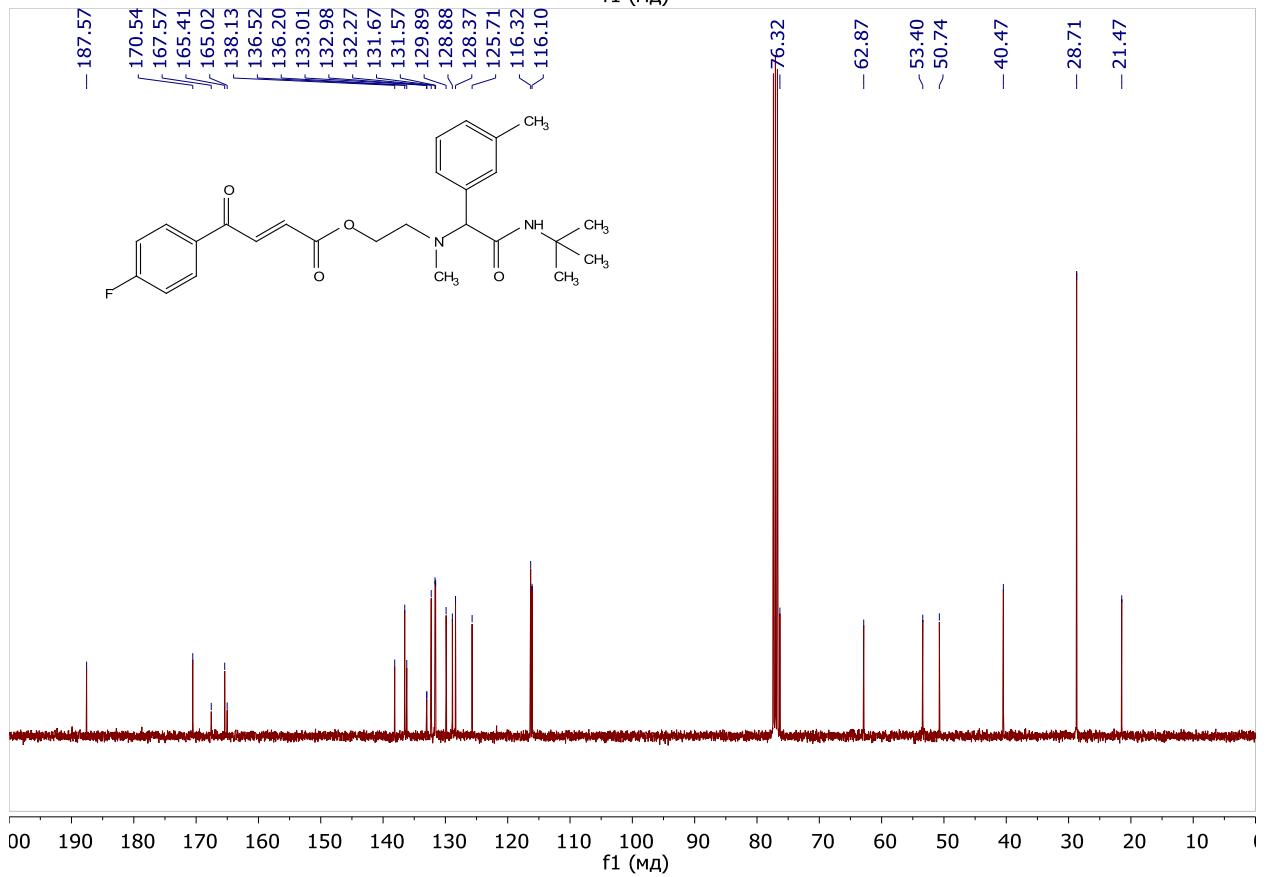
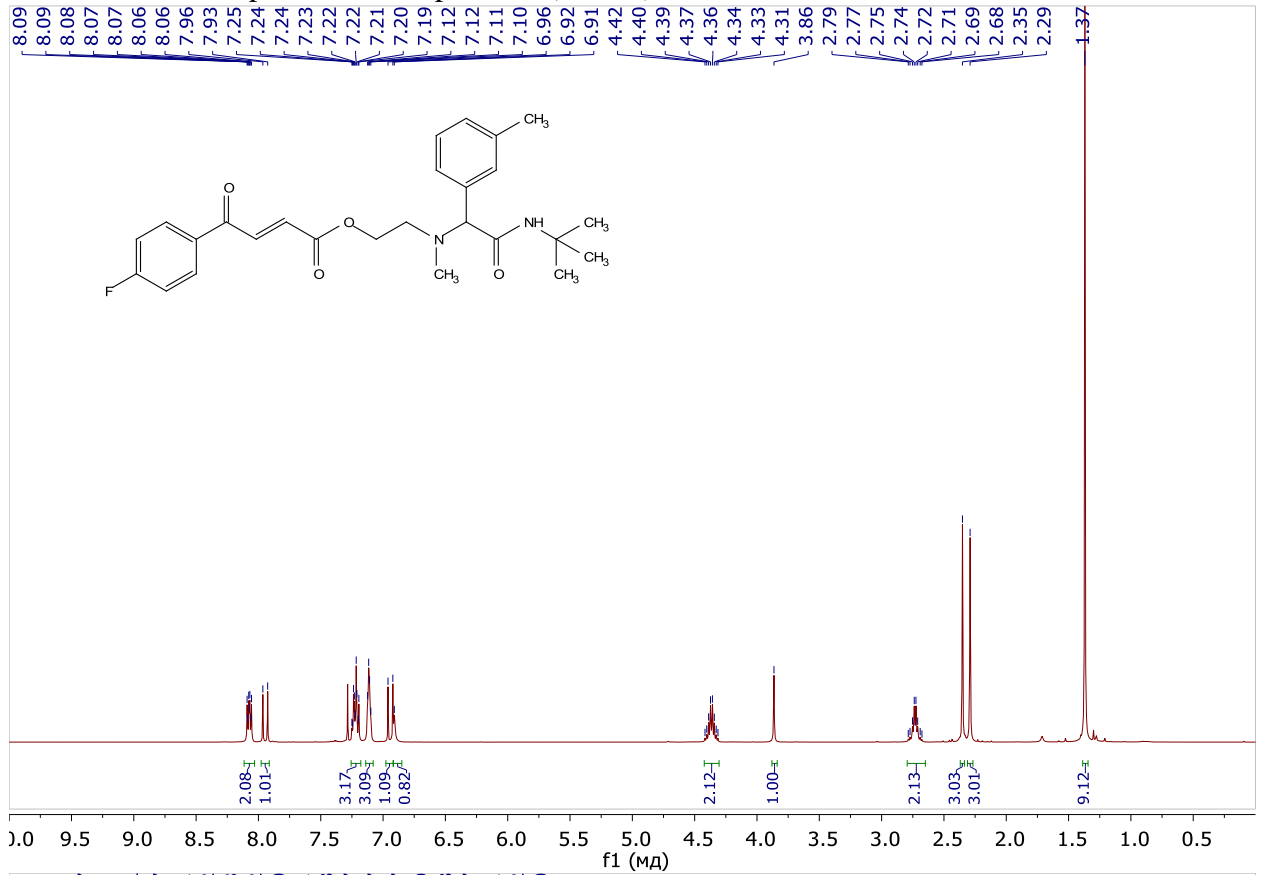
¹H and ¹³C NMR spectra for compound 1 (CDCl₃)



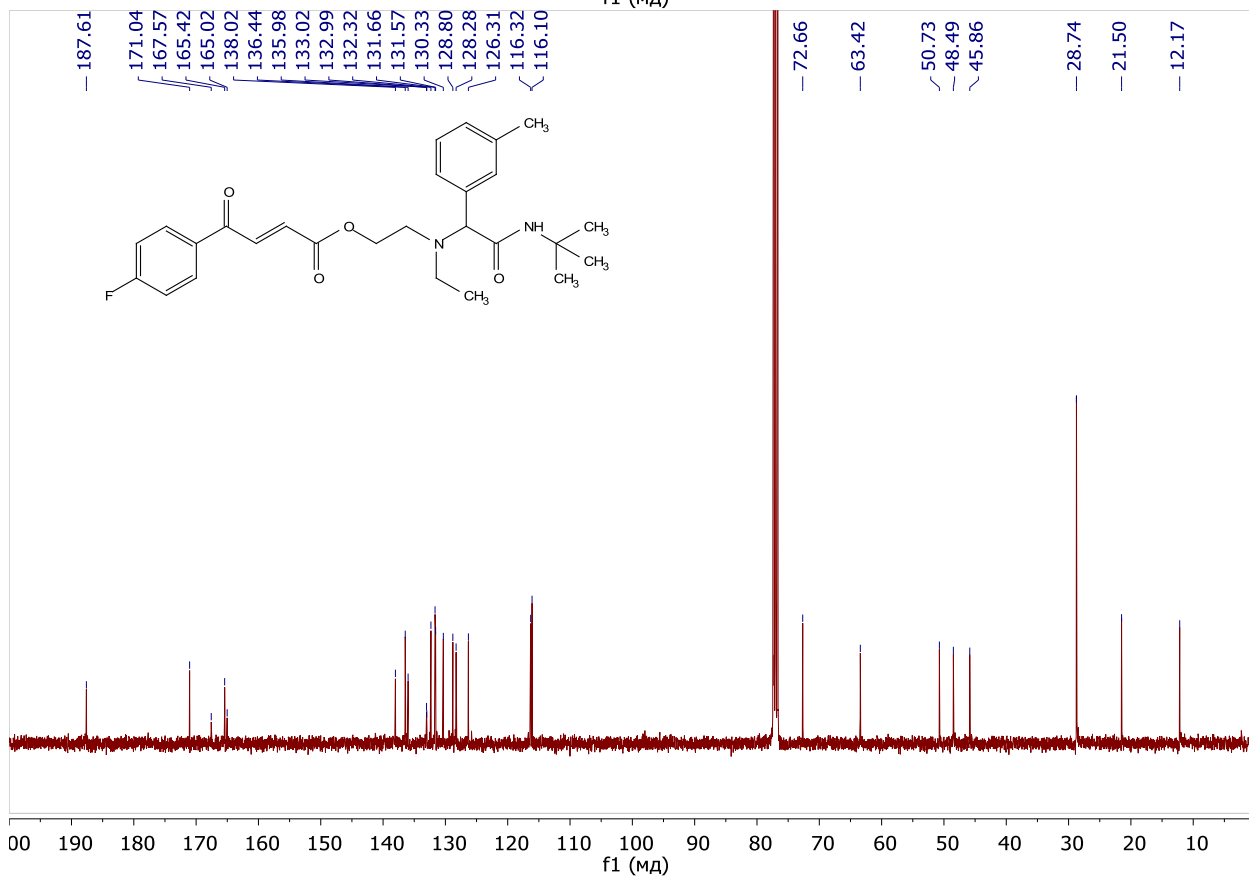
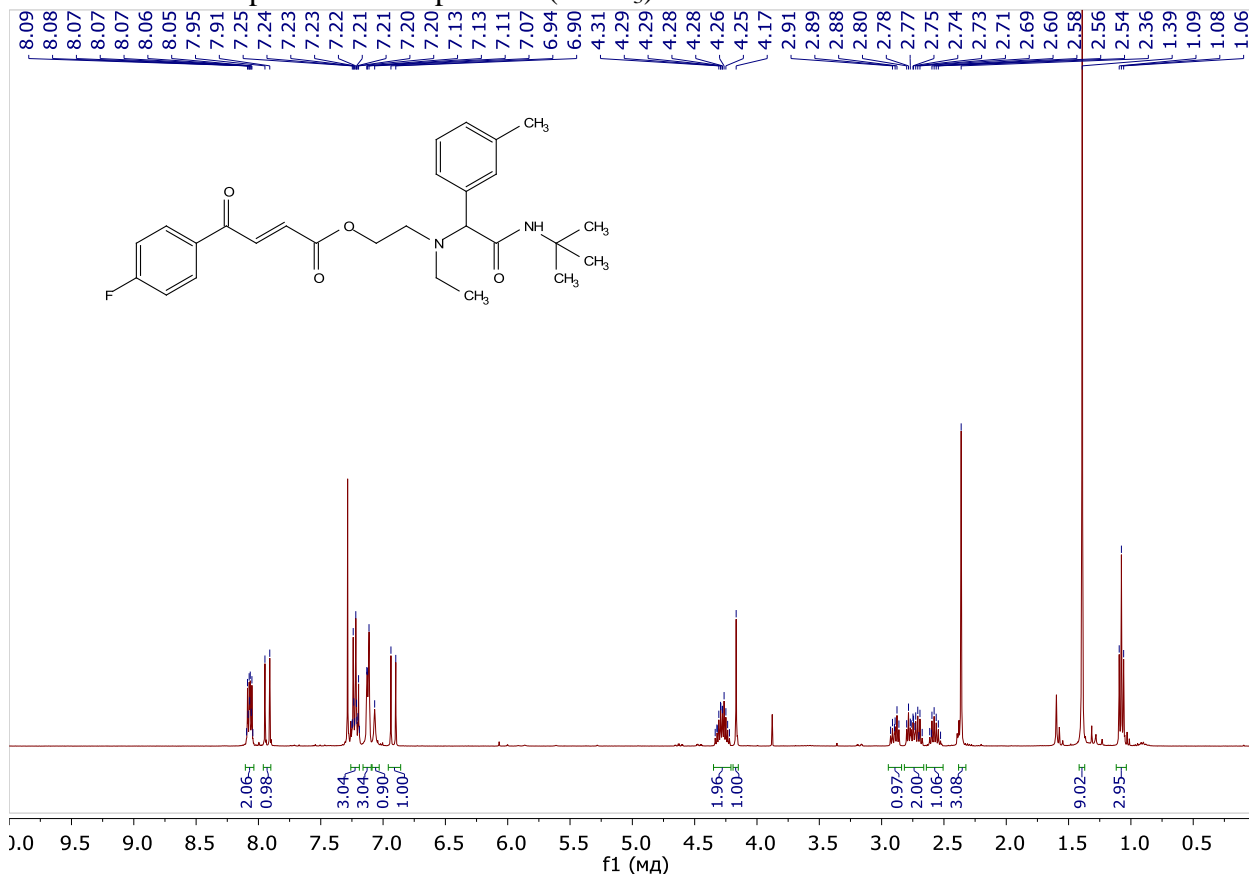
¹H and ¹³C NMR spectra for compound 2 (CDCl₃)



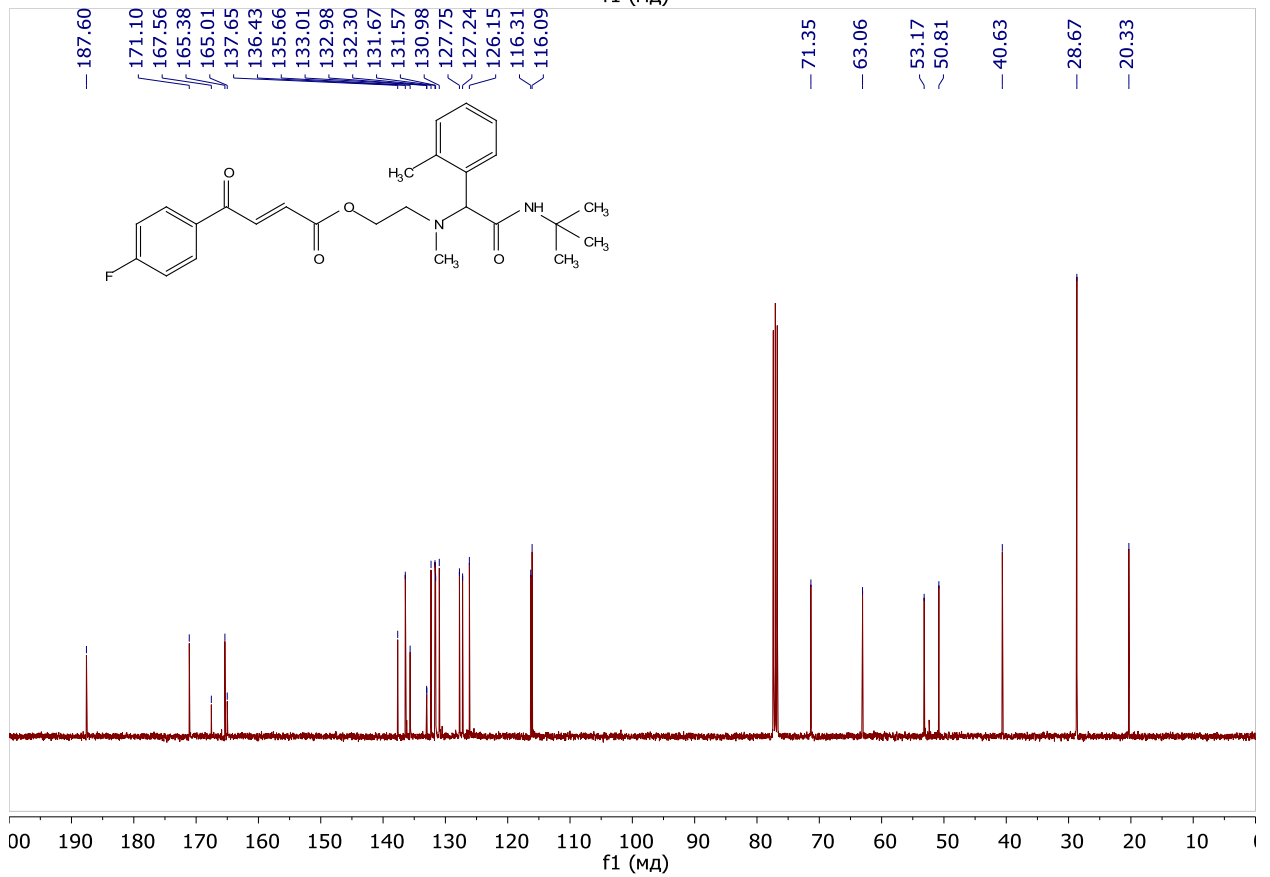
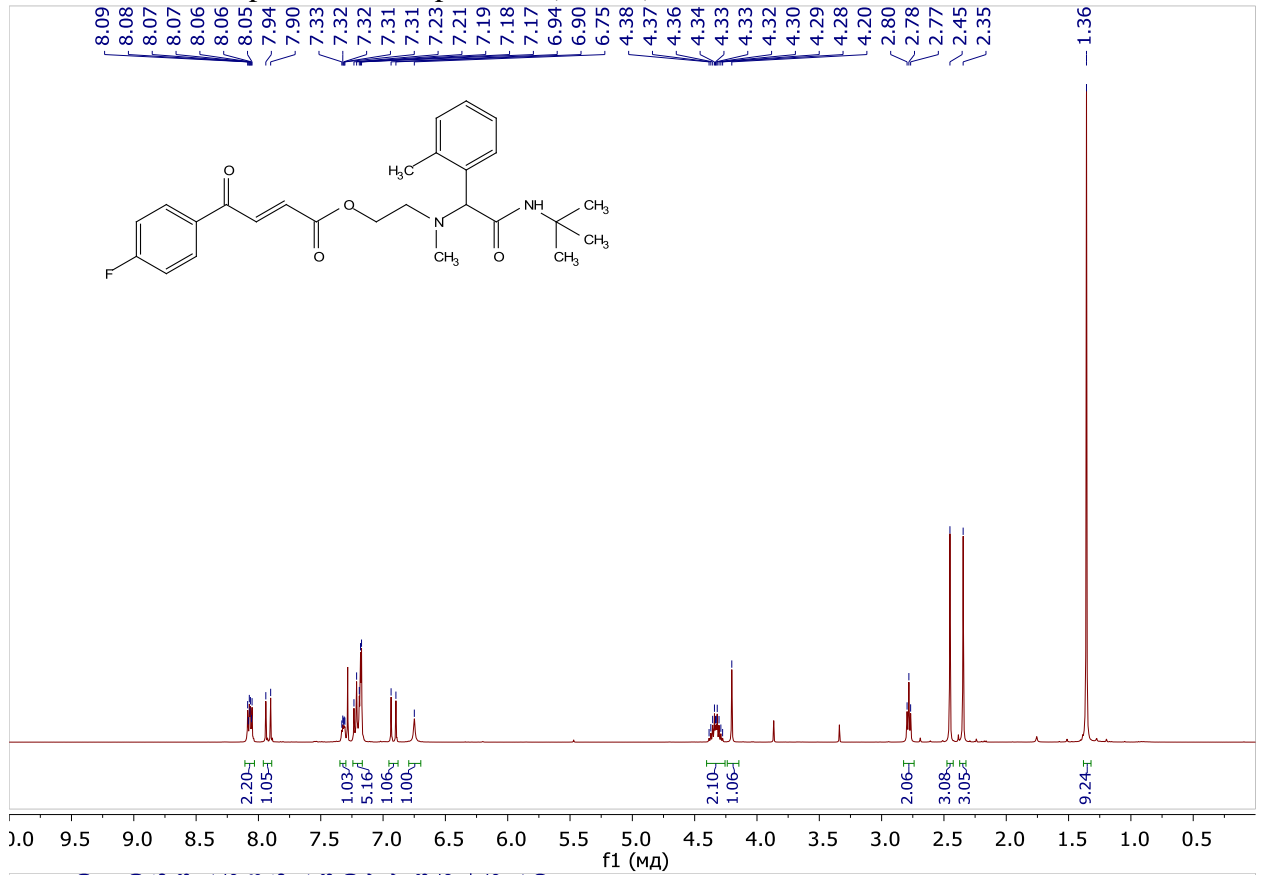
¹H and ¹³C NMR spectra for compound **3** (CDCl₃)



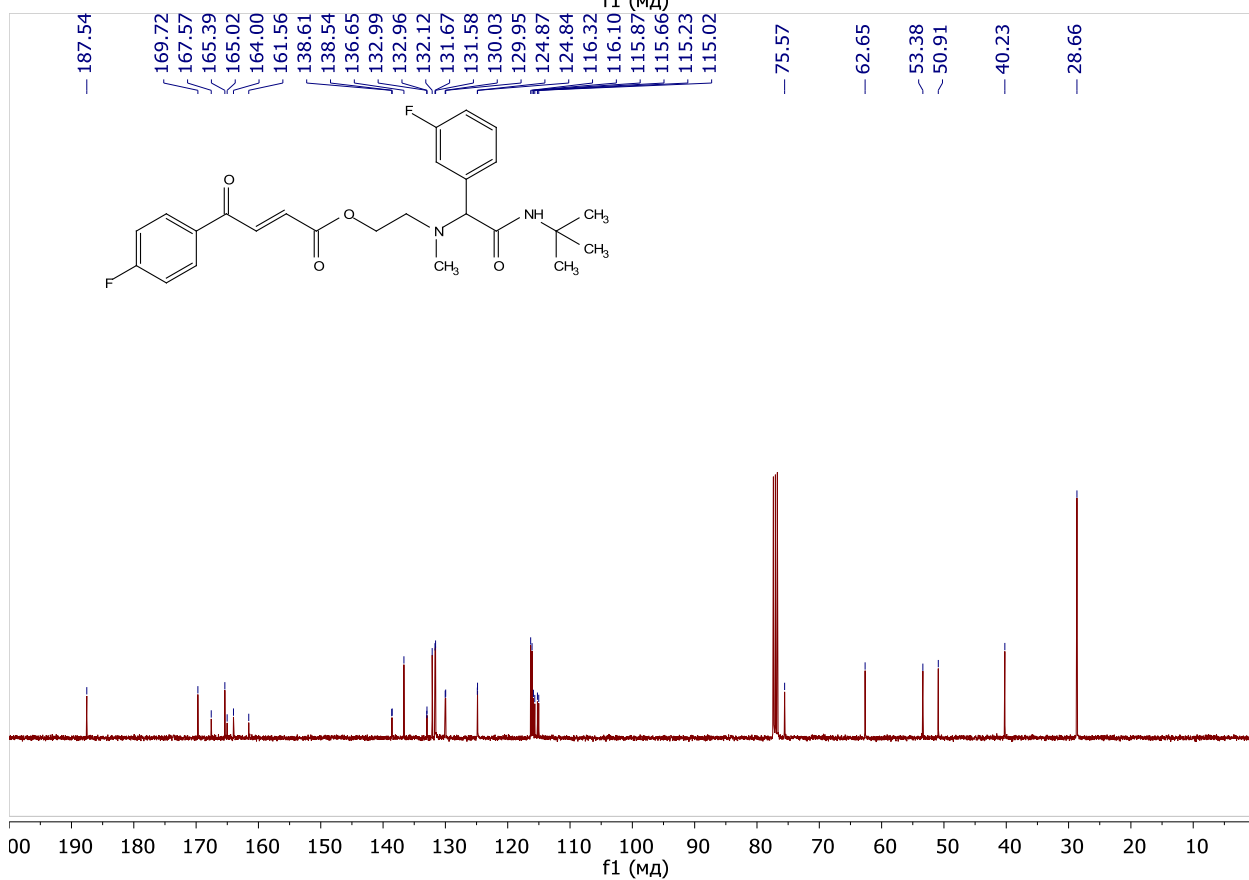
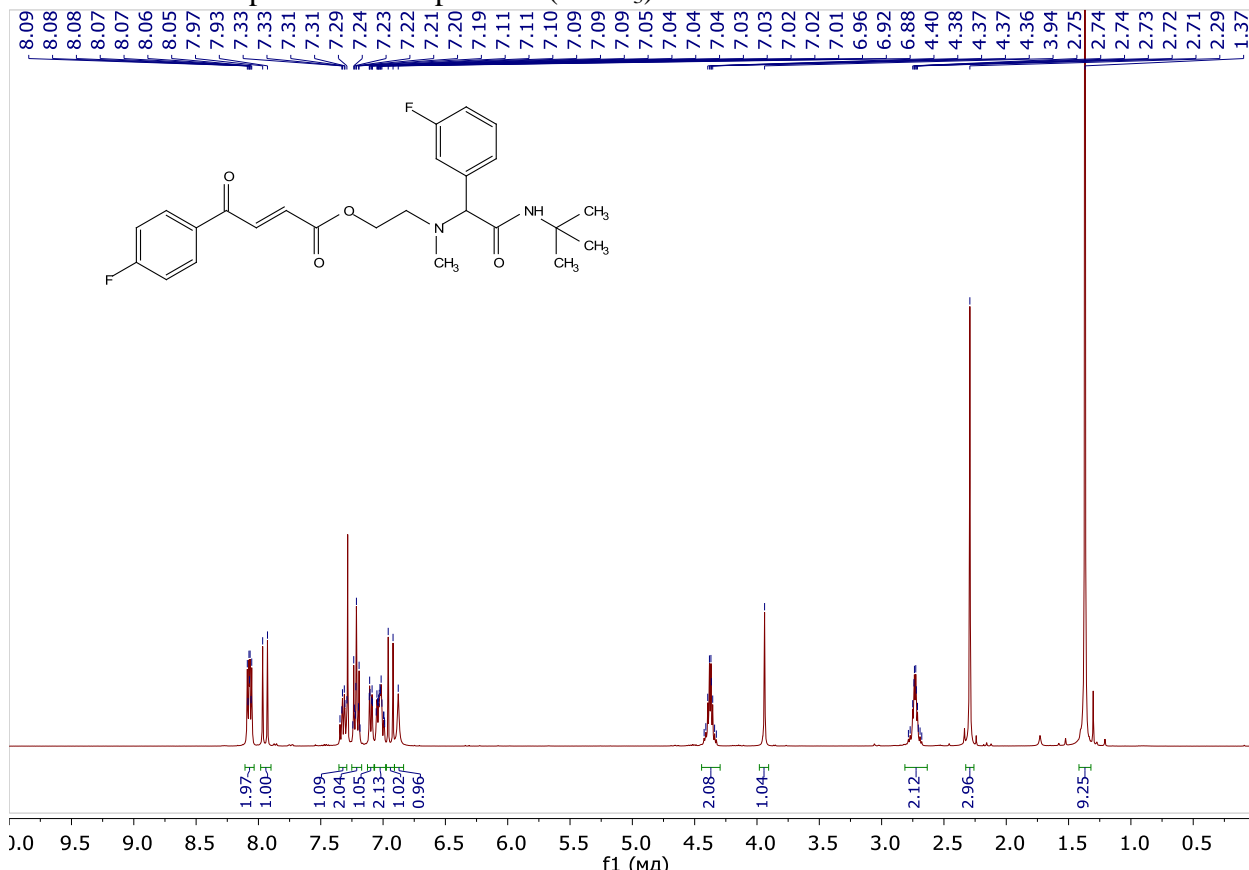
¹H and ¹³C NMR spectra for compound 4 (CDCl₃)



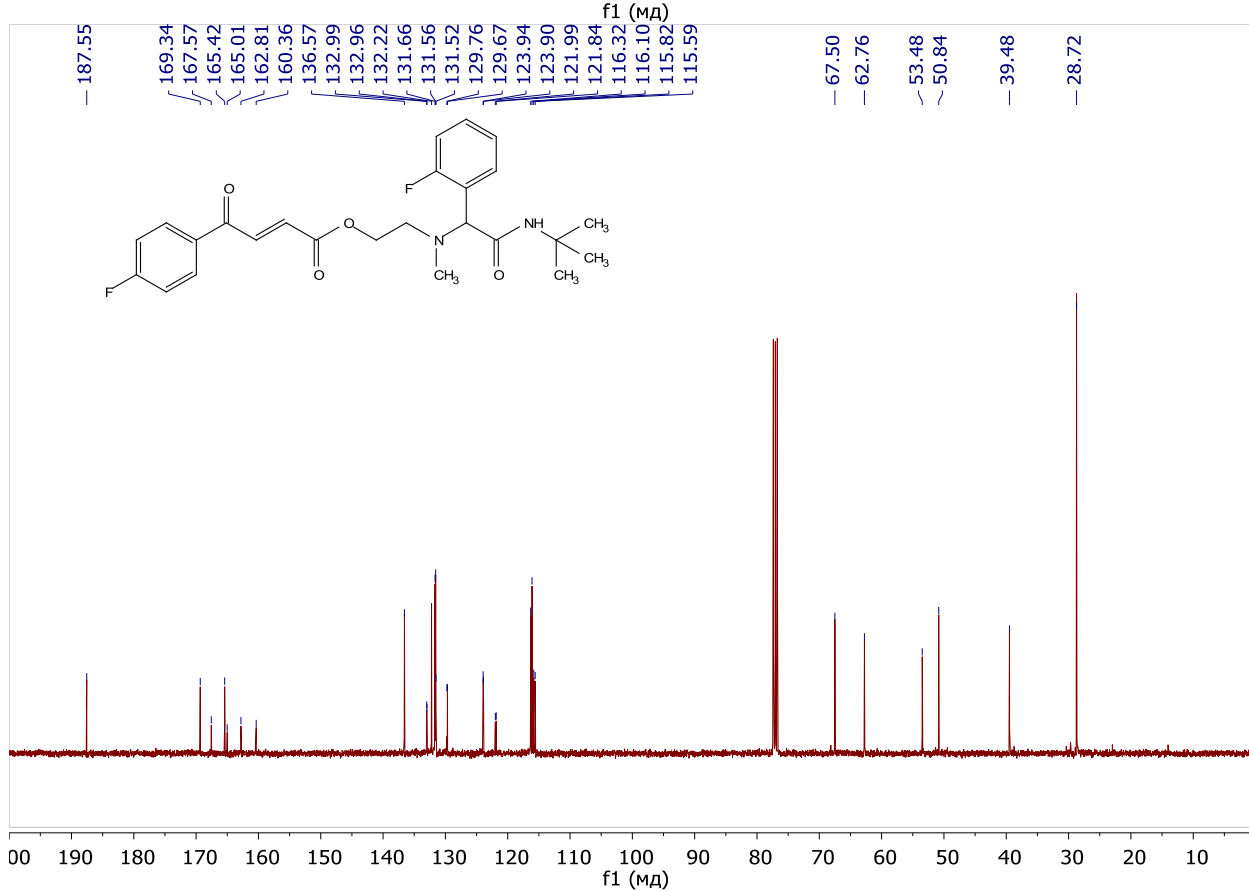
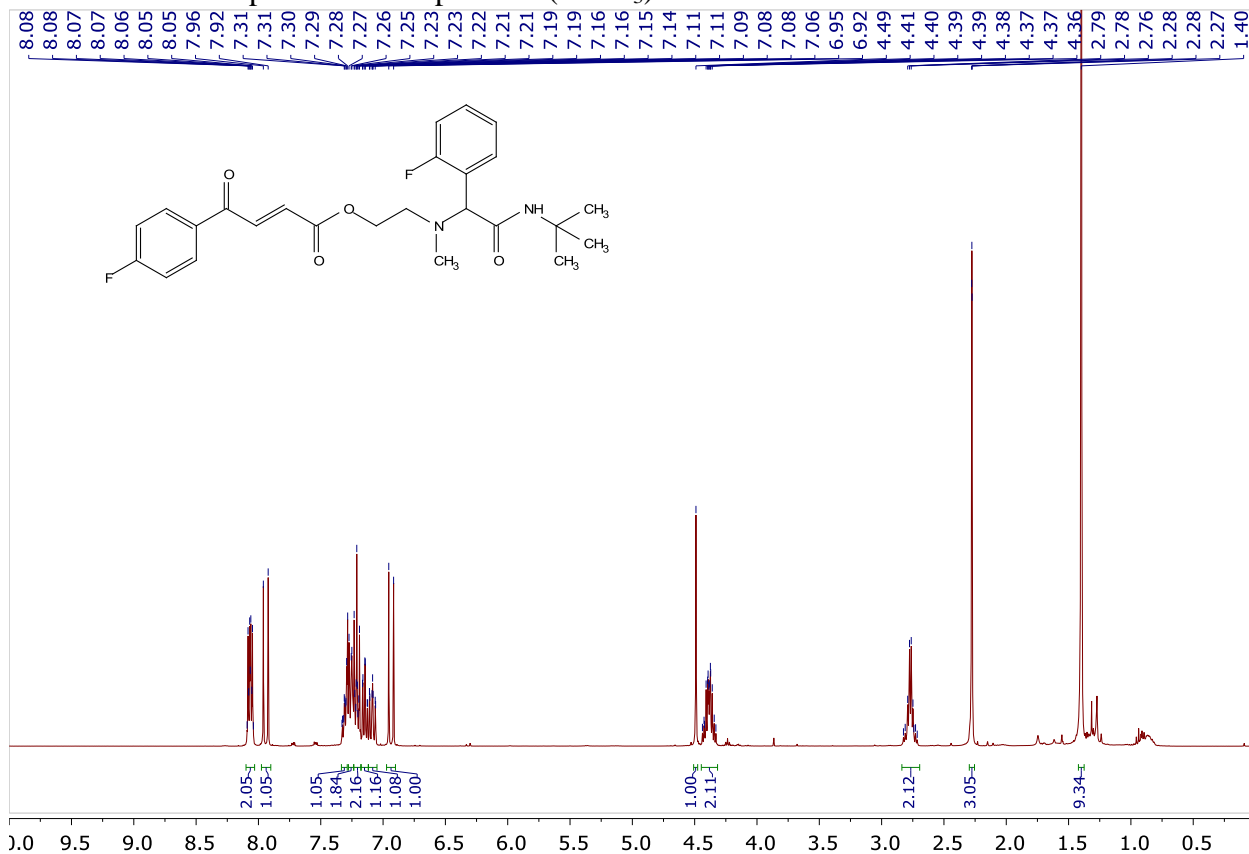
^1H and ^{13}C NMR spectra for compound **5** (CDCl_3)



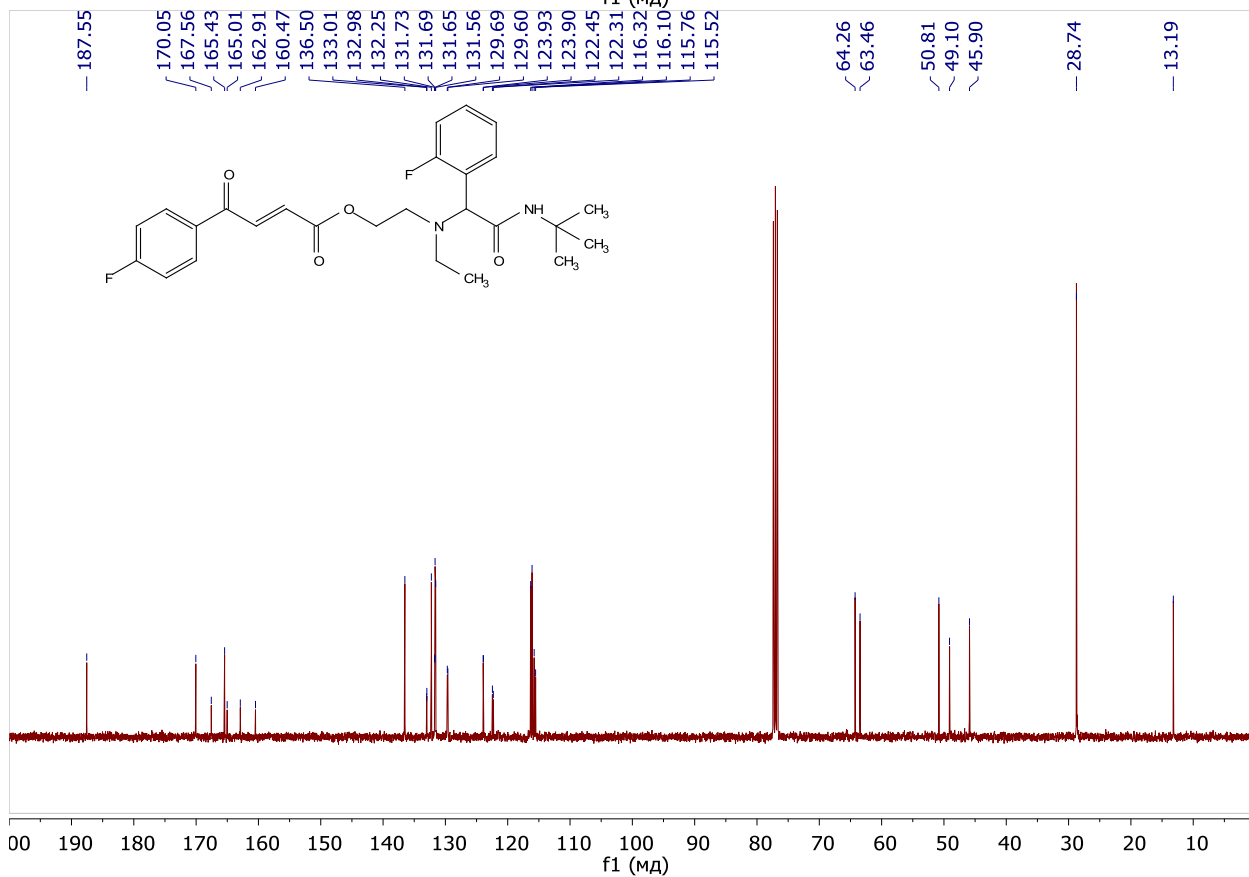
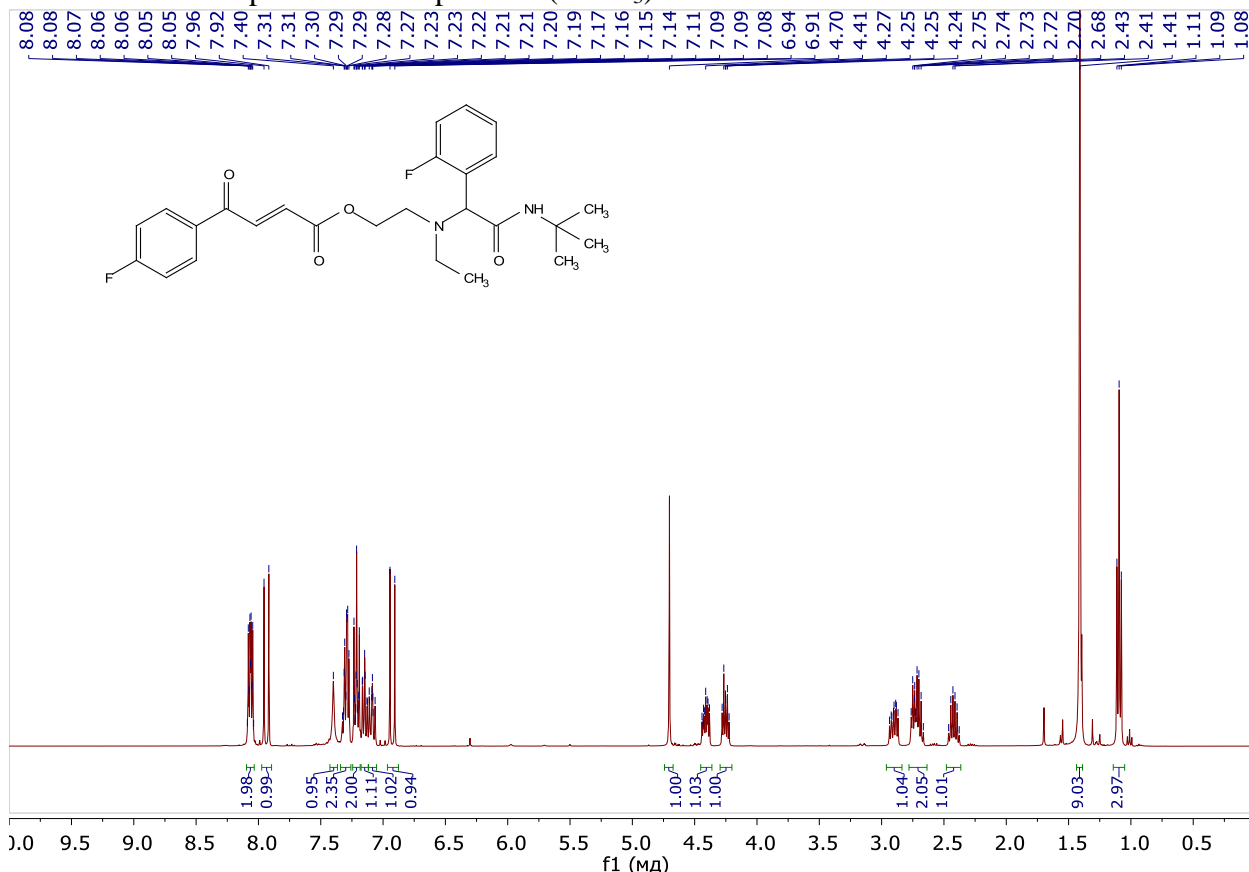
¹H and ¹³C NMR spectra for compound **6** (CDCl₃)



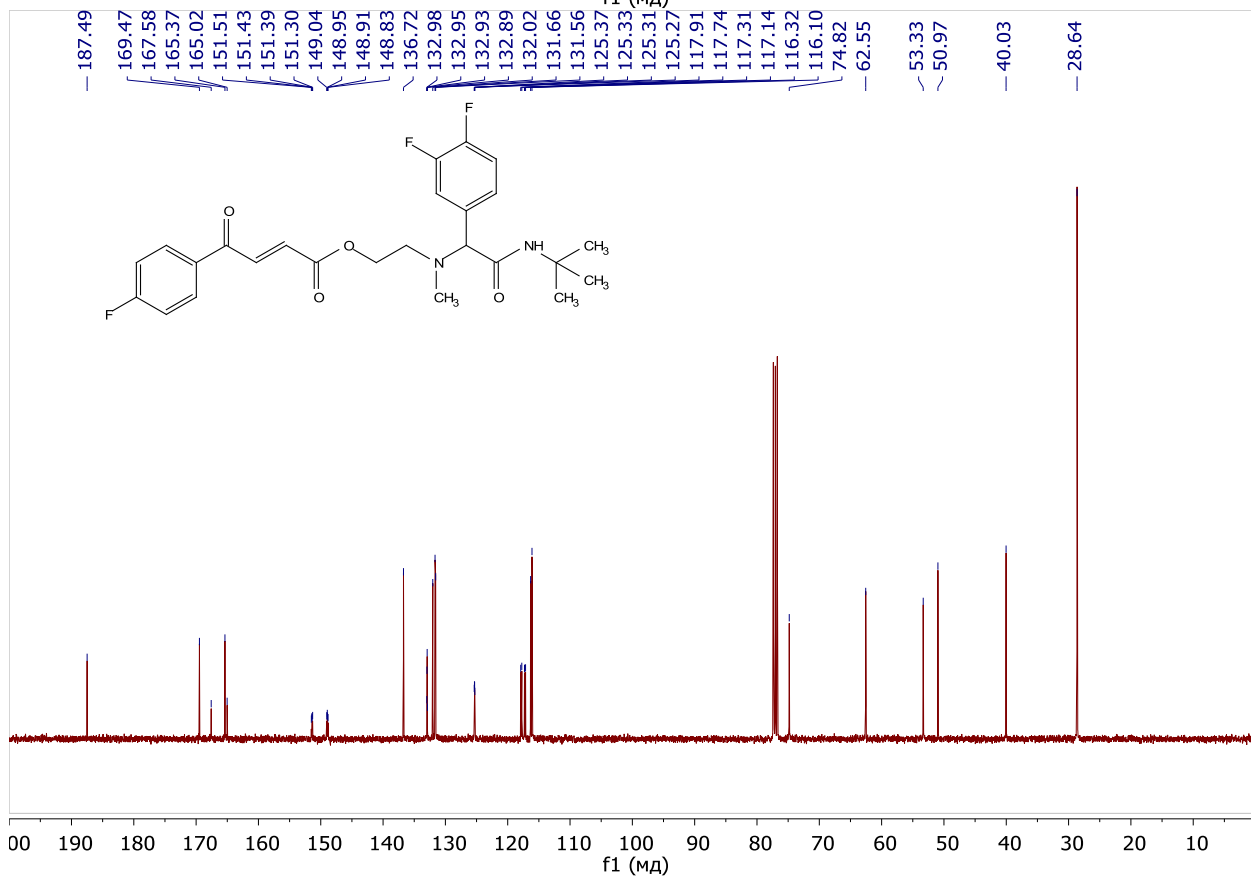
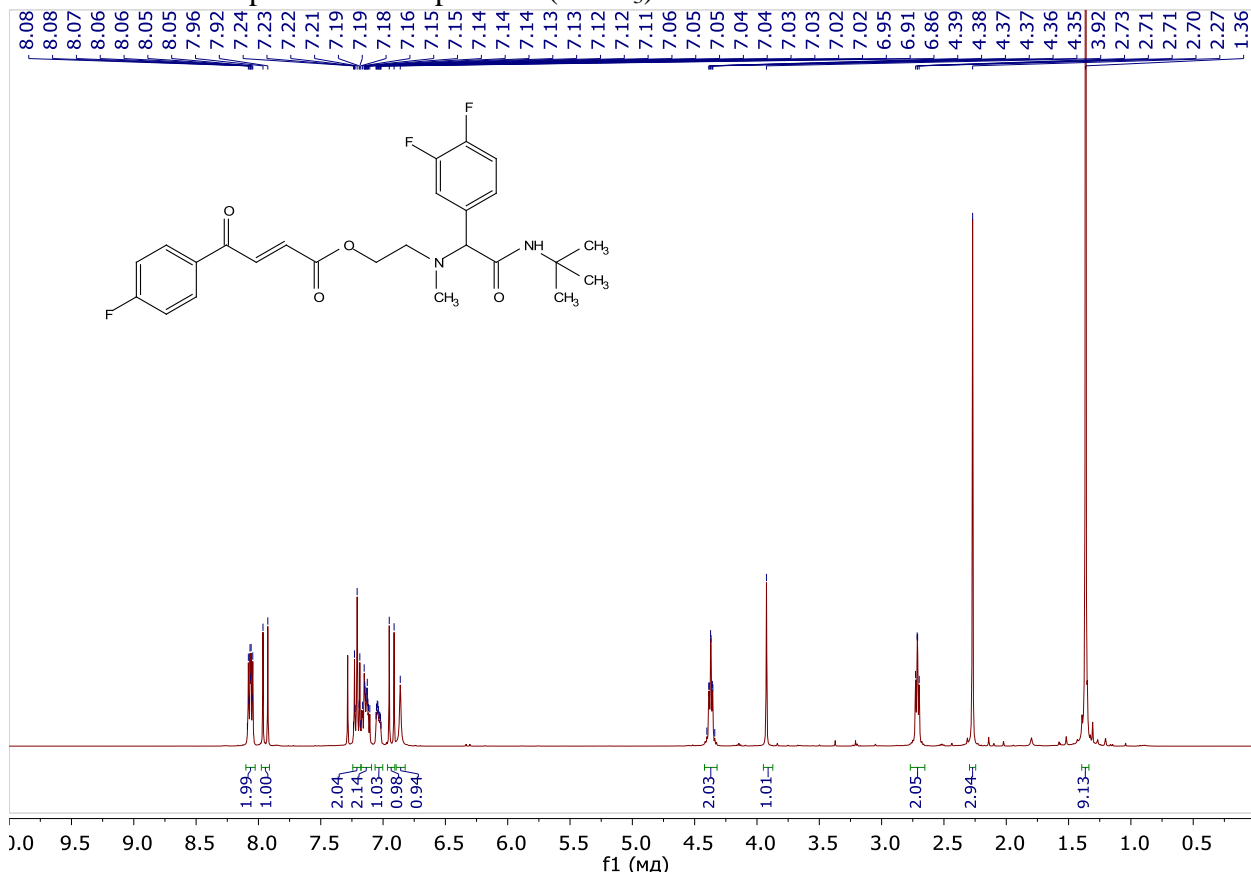
¹H and ¹³C NMR spectra for compound 7 (CDCl₃)



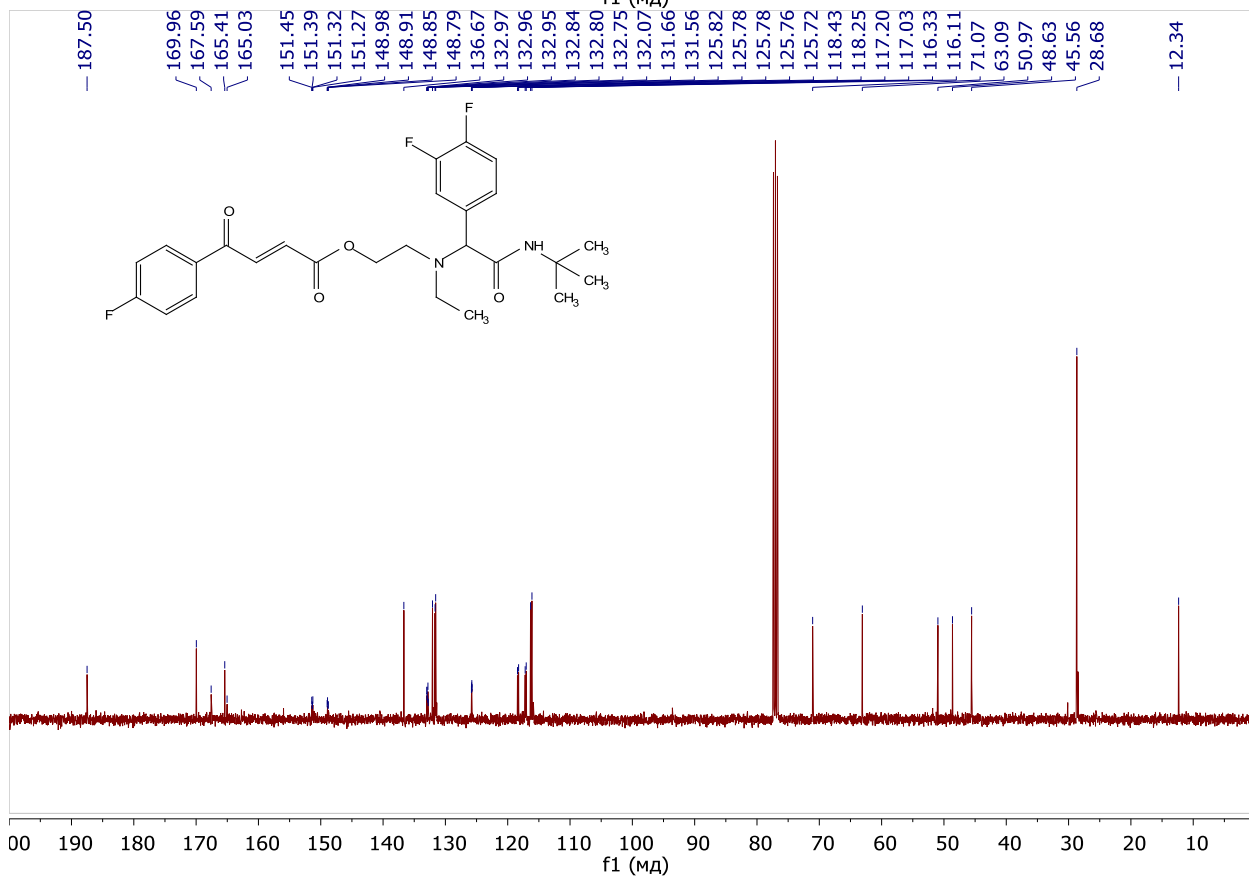
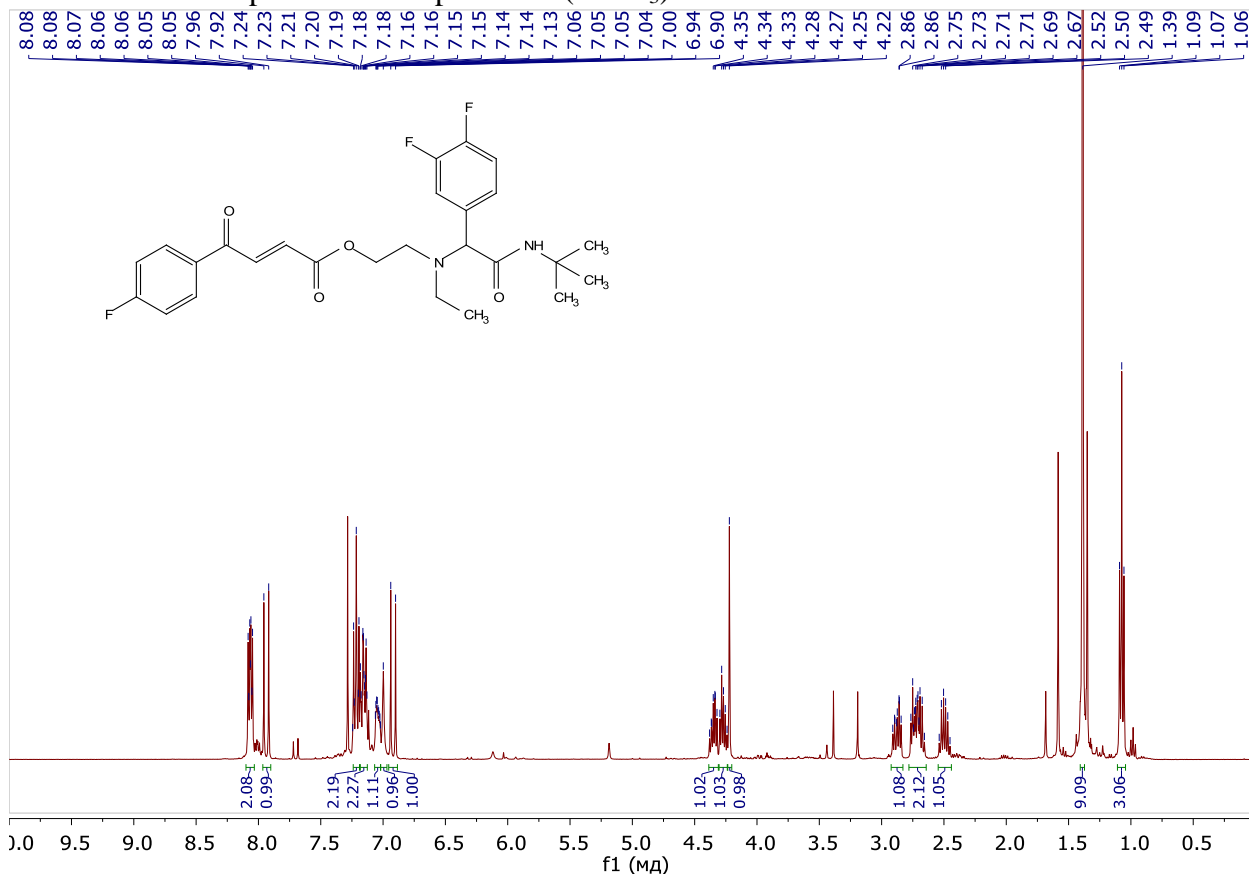
^1H and ^{13}C NMR spectra for compound **8** (CDCl_3)



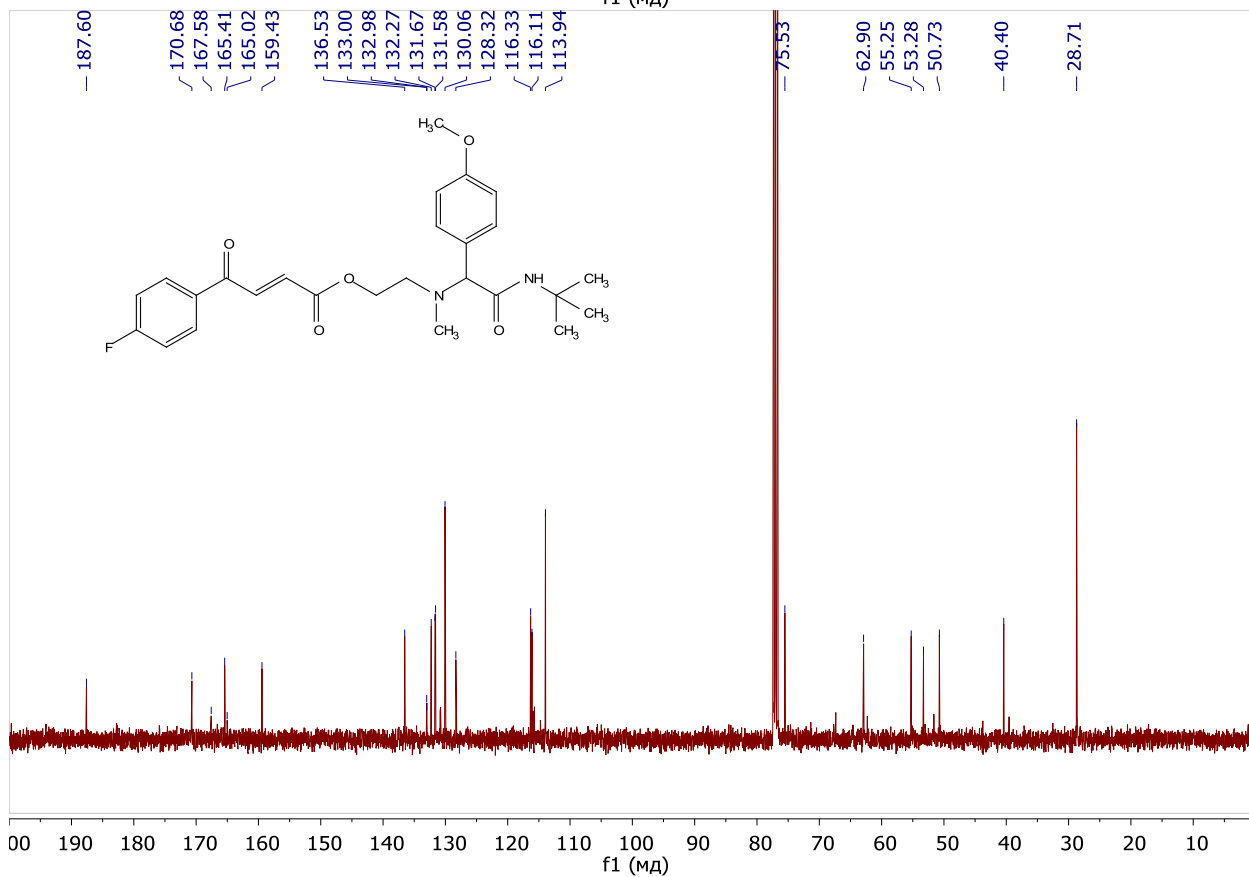
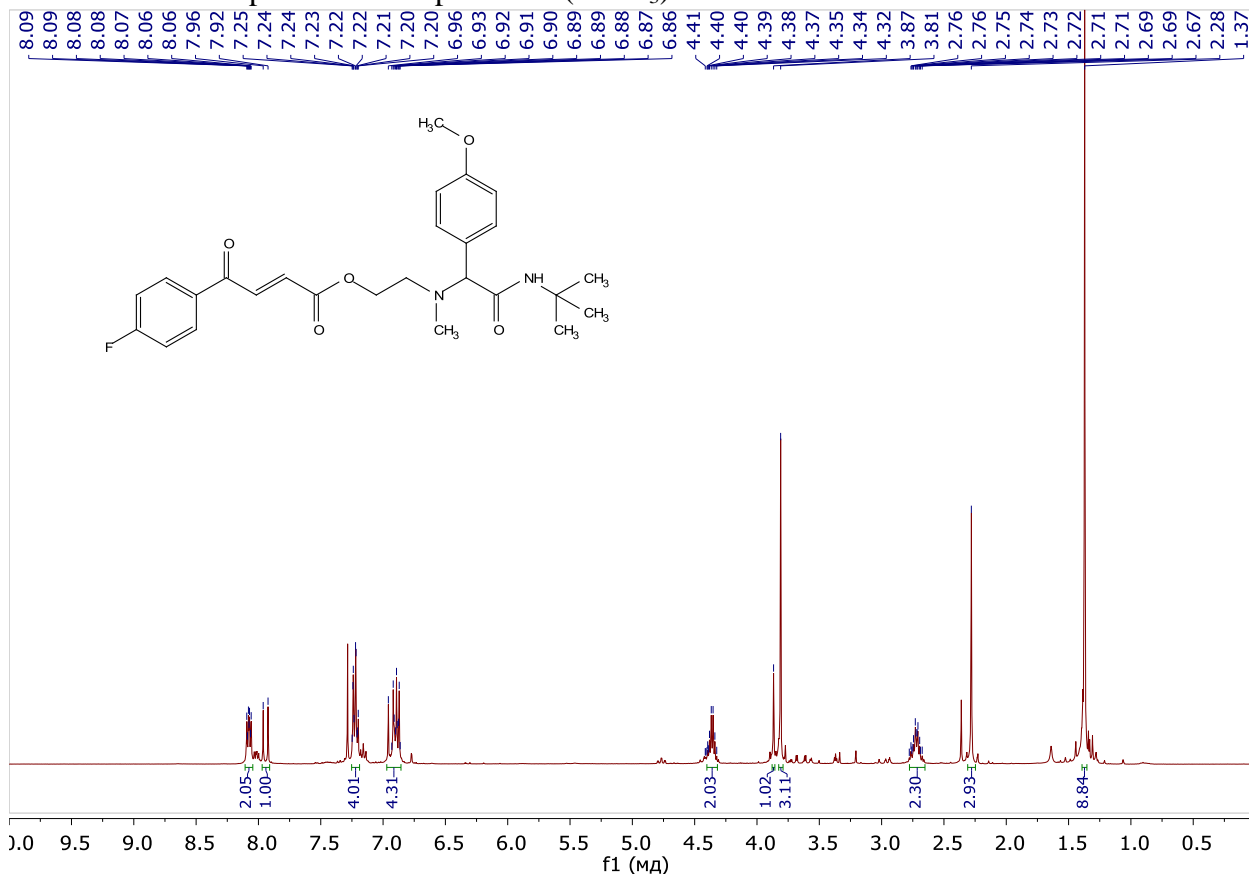
¹H and ¹³C NMR spectra for compound **9** (CDCl₃)



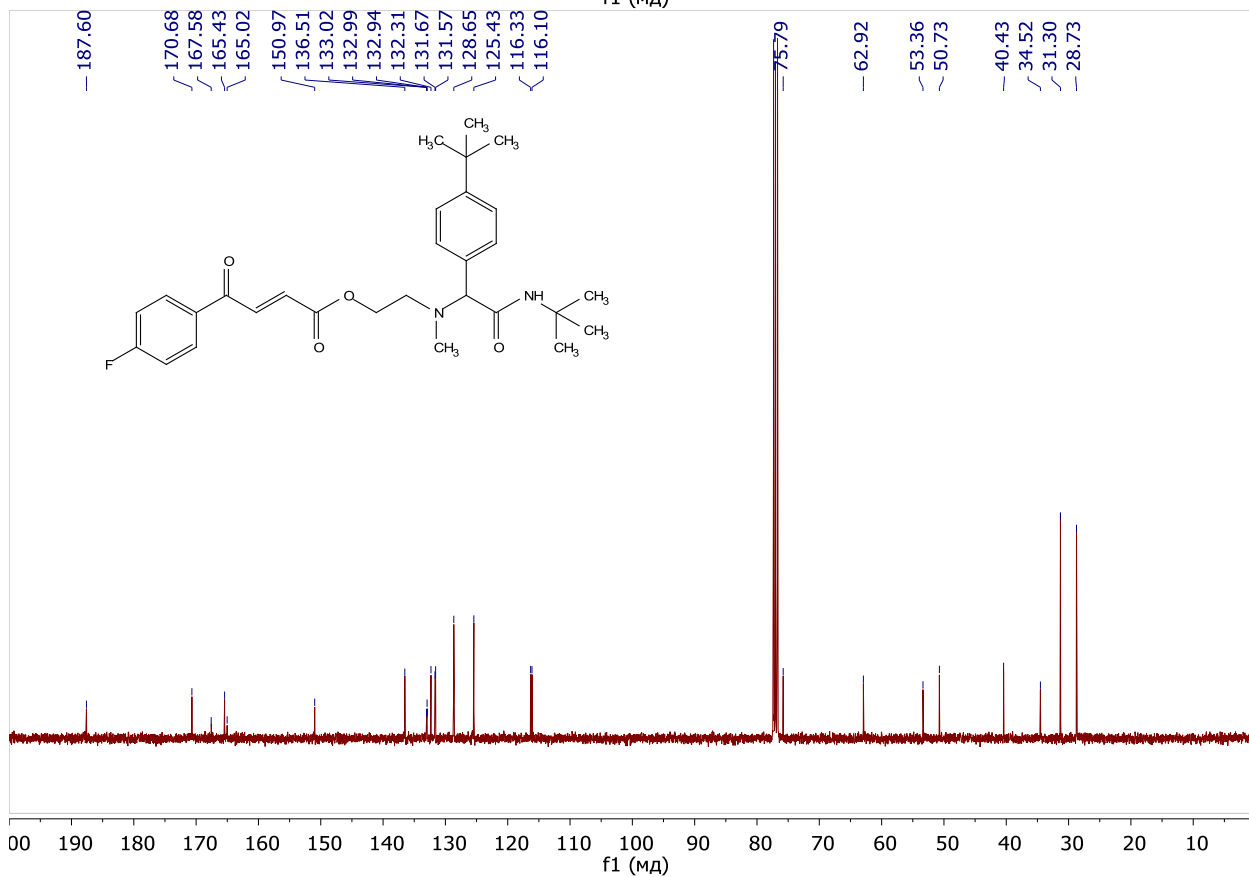
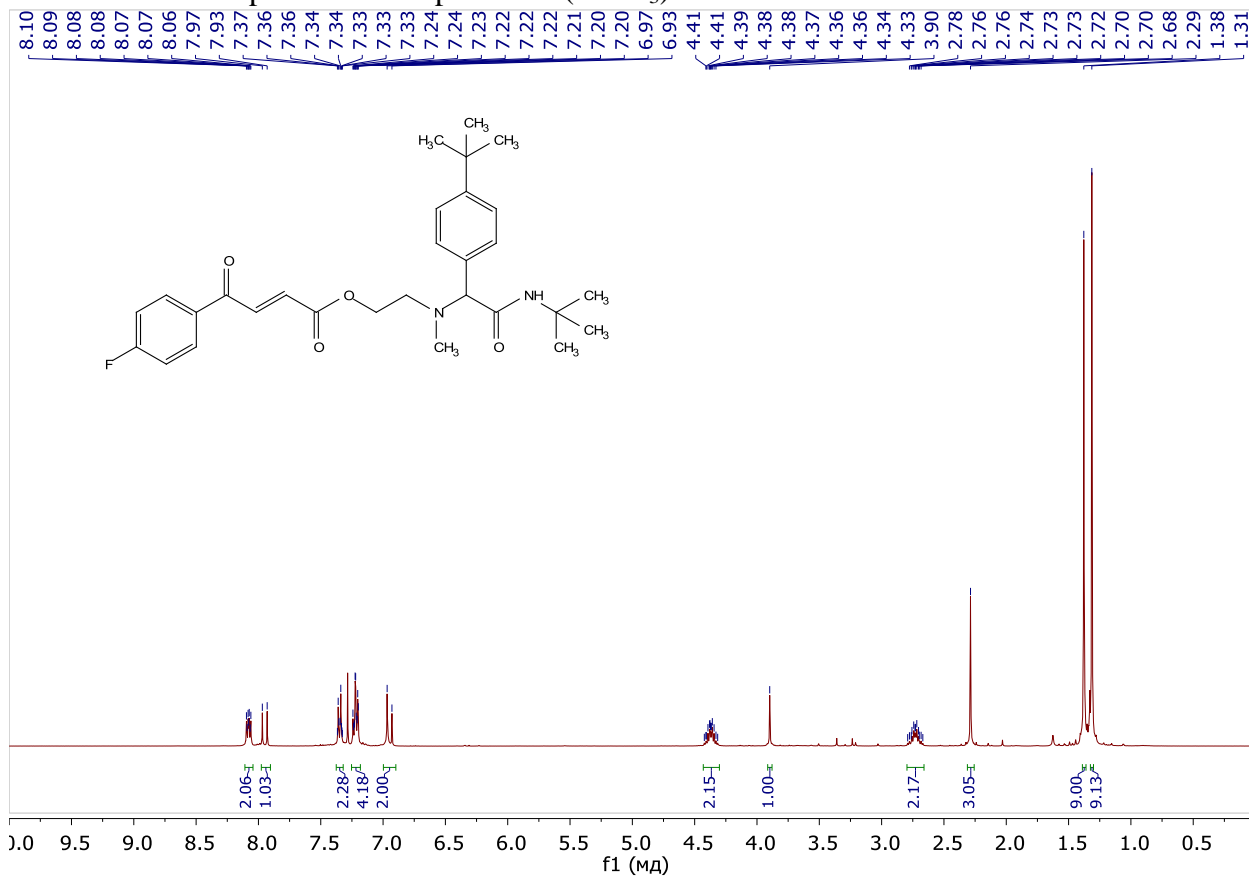
¹H and ¹³C NMR spectra for compound **10** (CDCl₃)



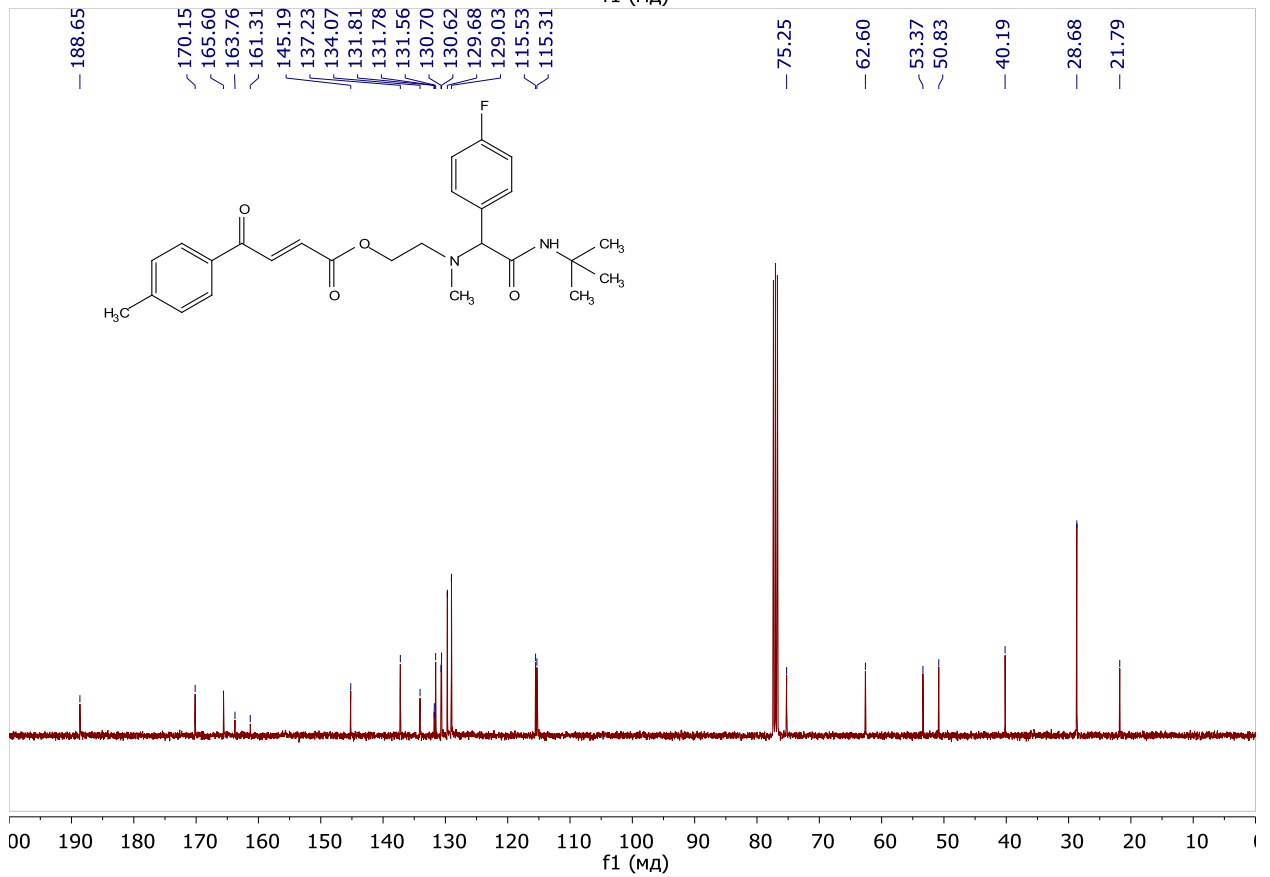
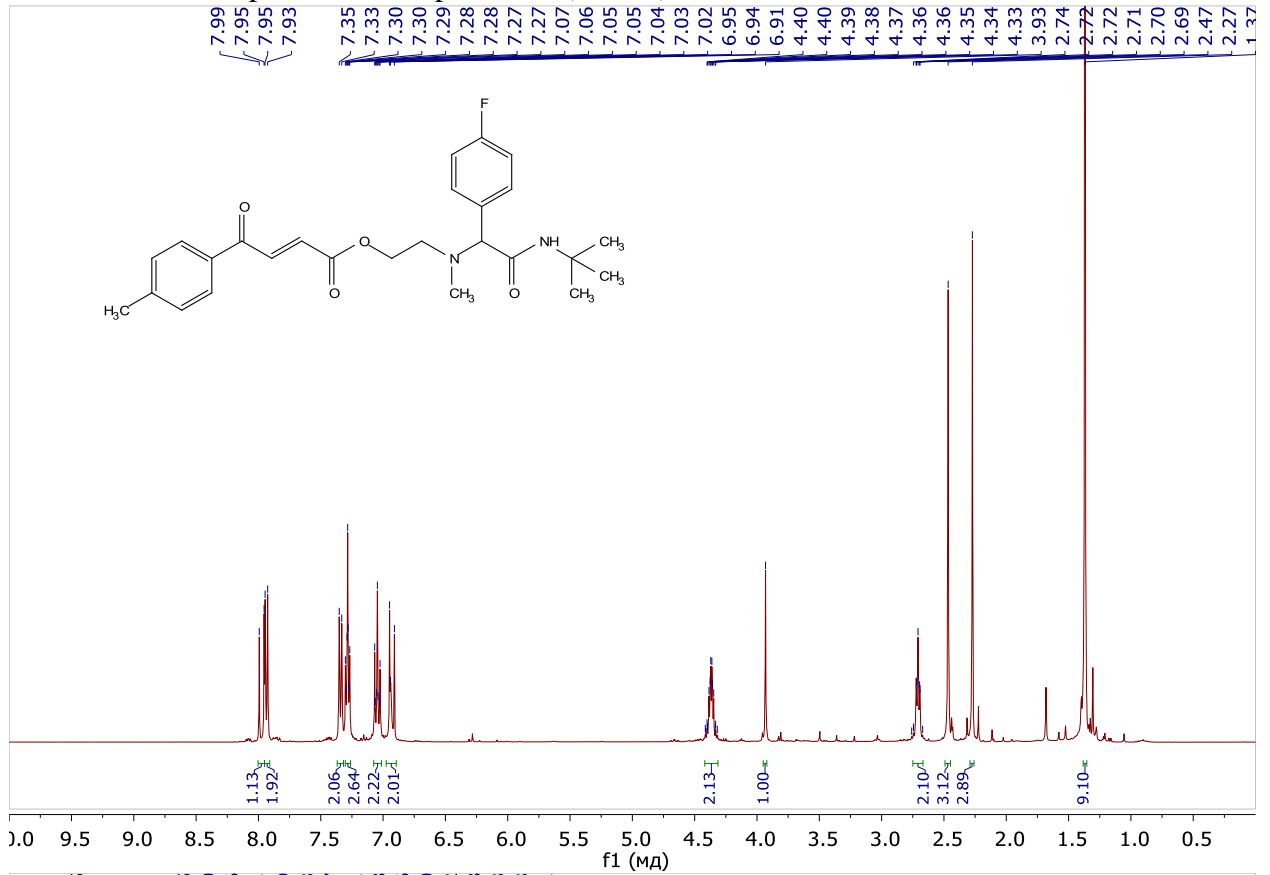
¹H and ¹³C NMR spectra for compound 11 (CDCl₃)



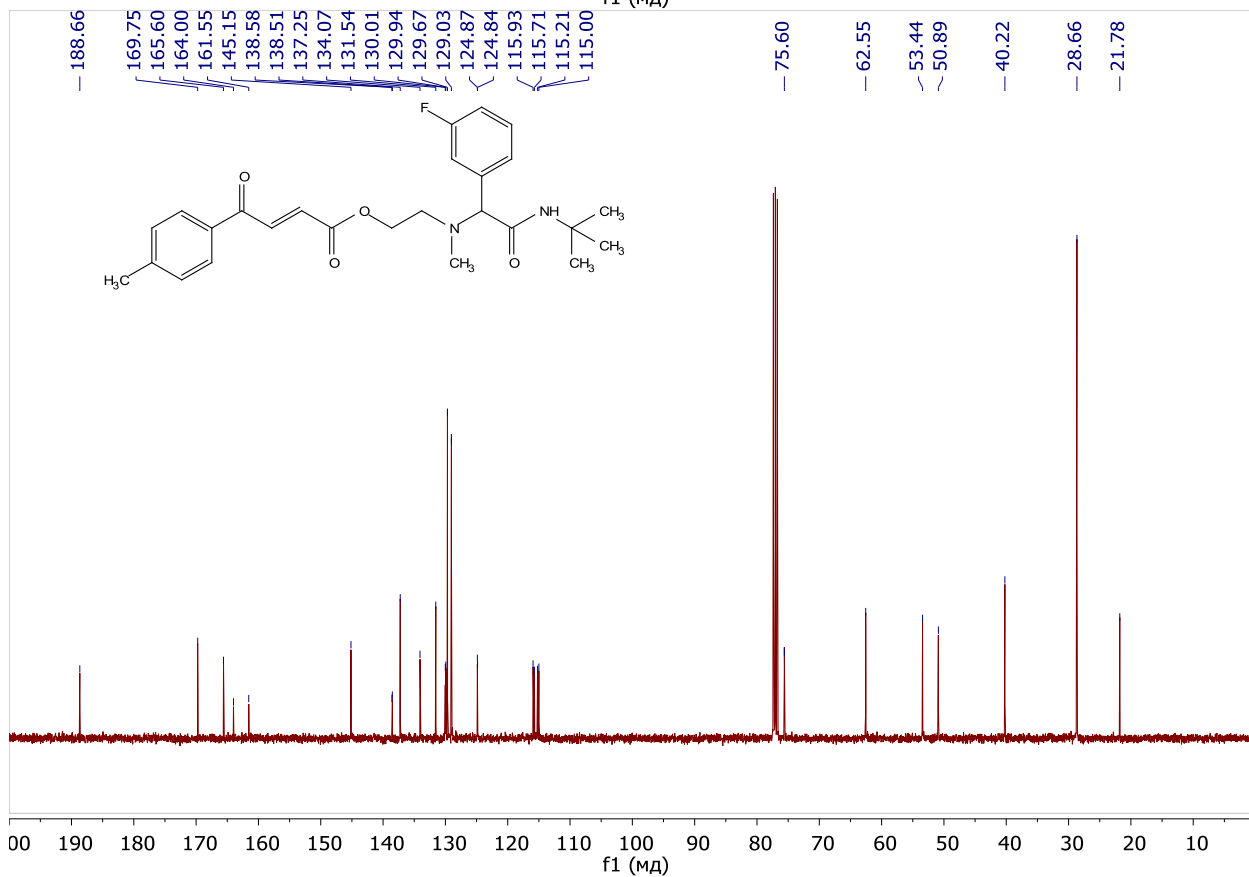
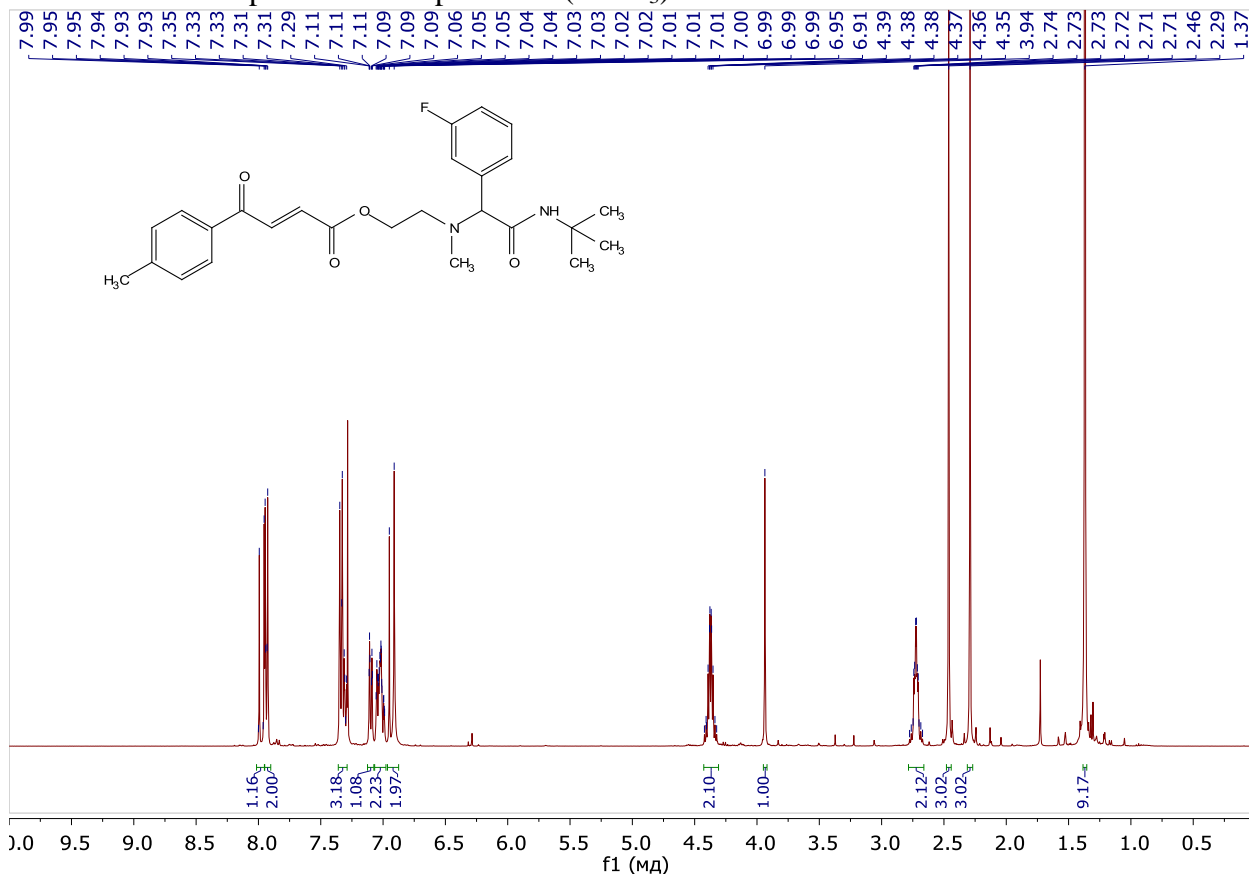
^1H and ^{13}C NMR spectra for compound **12** (CDCl_3)



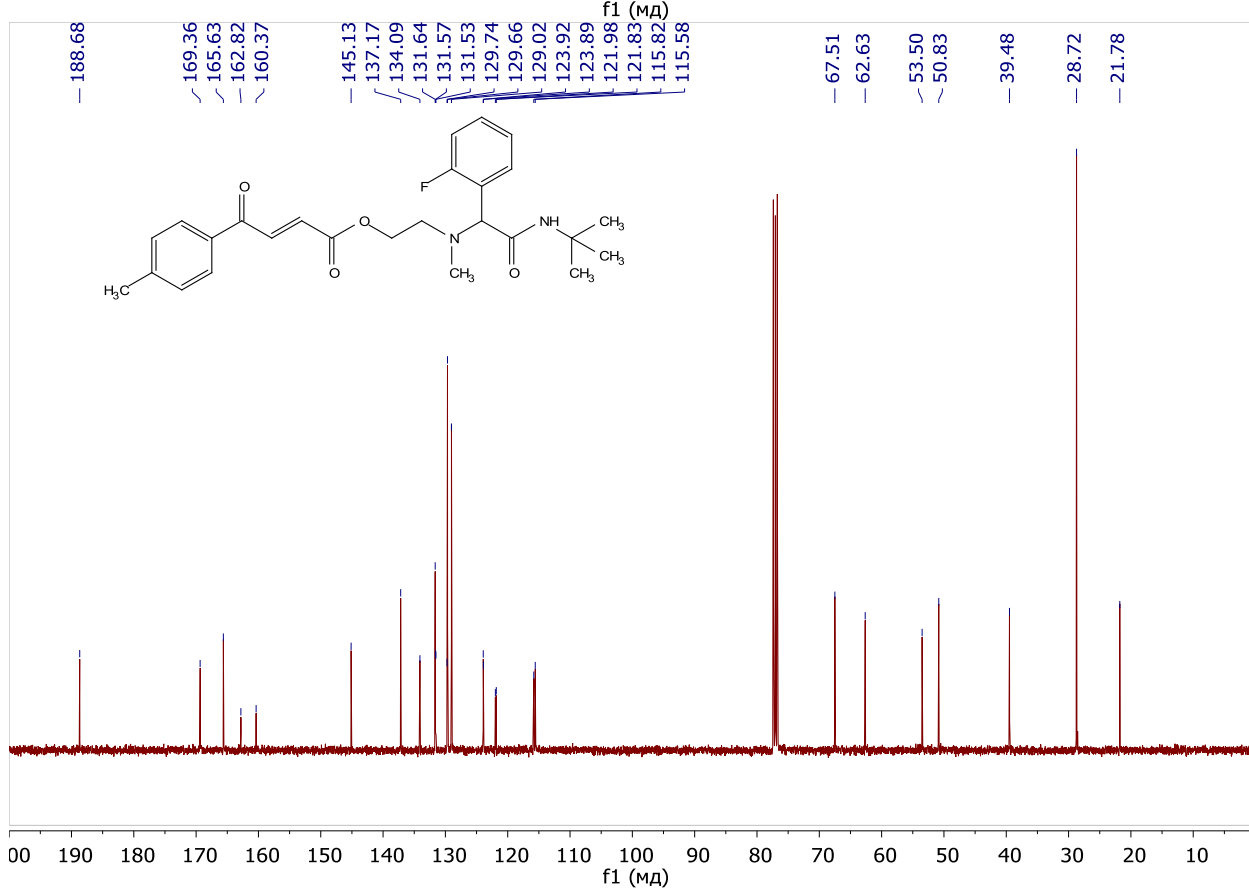
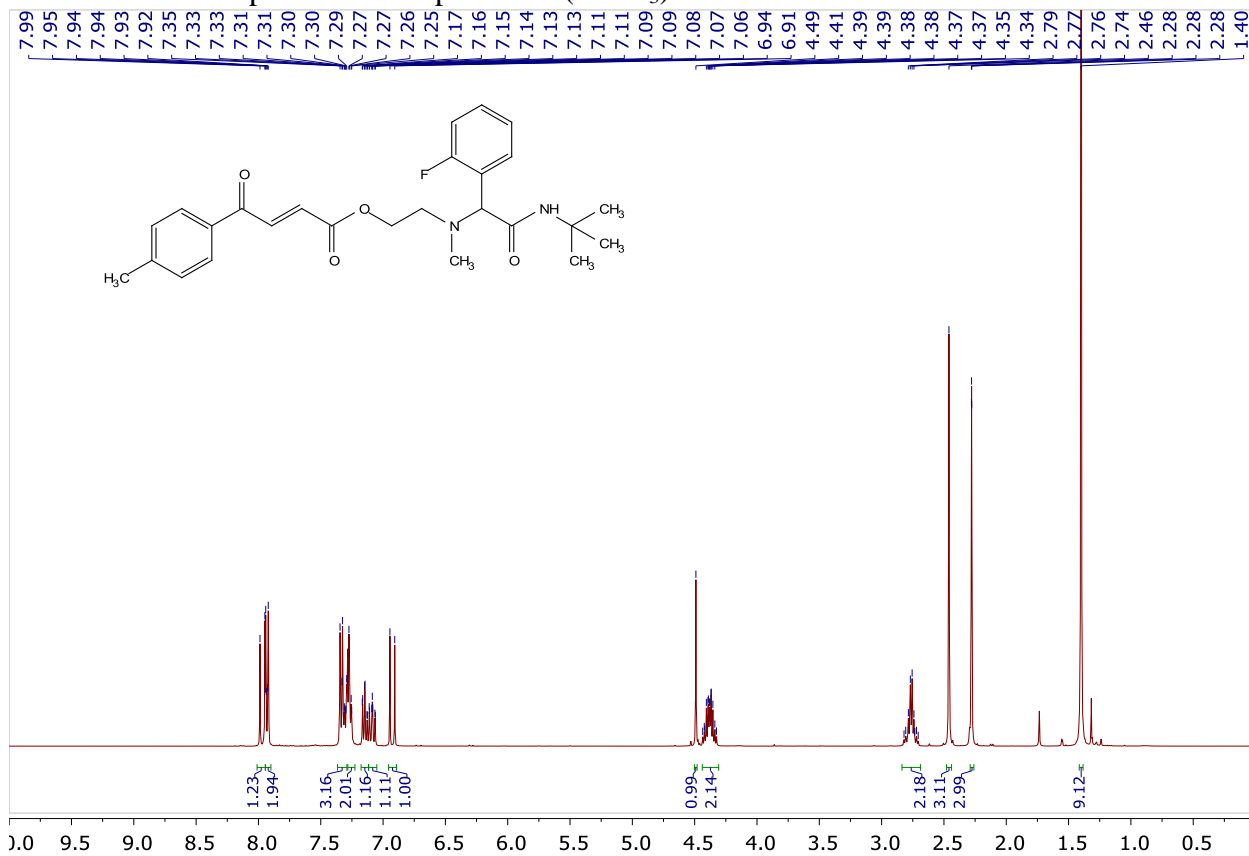
¹H and ¹³C NMR spectra for compound **13** (CDCl₃)



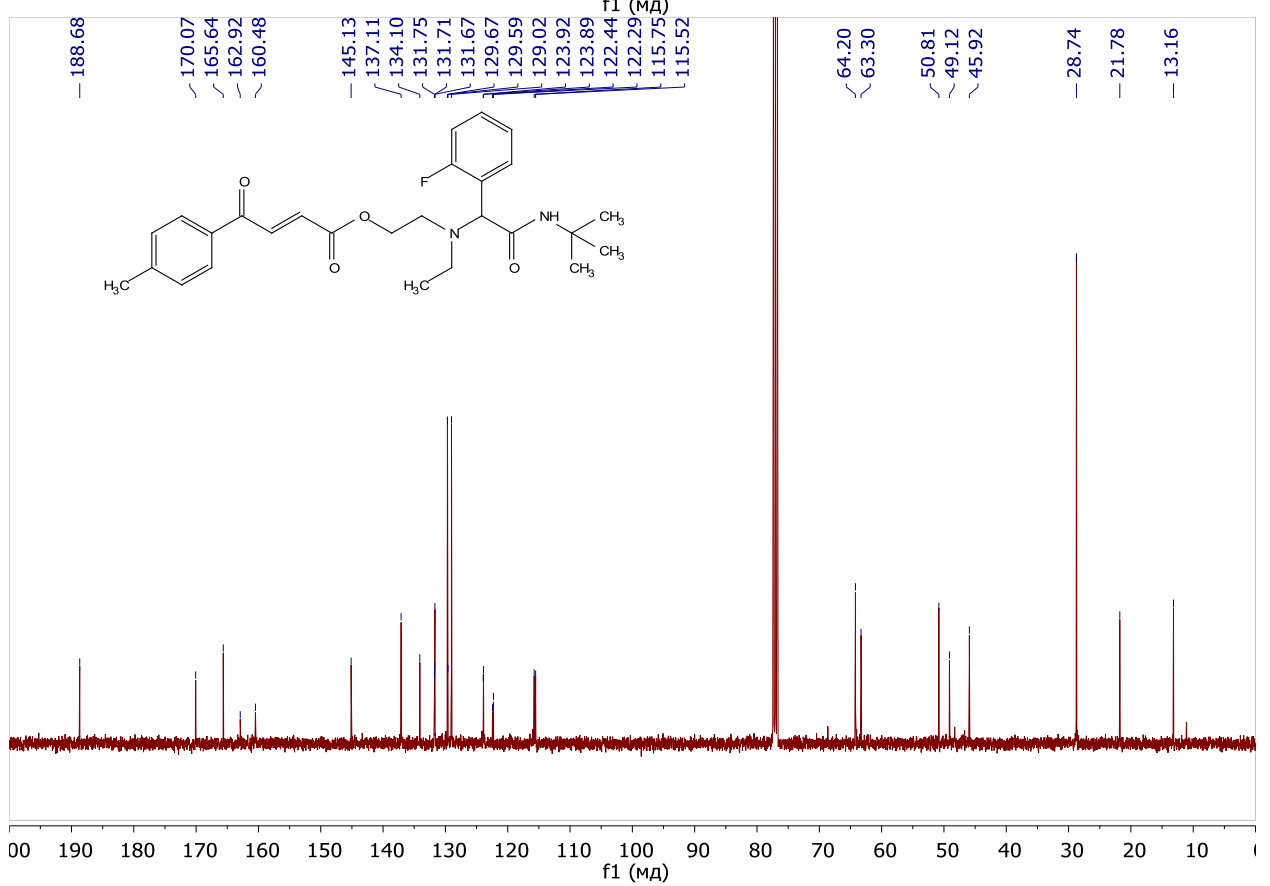
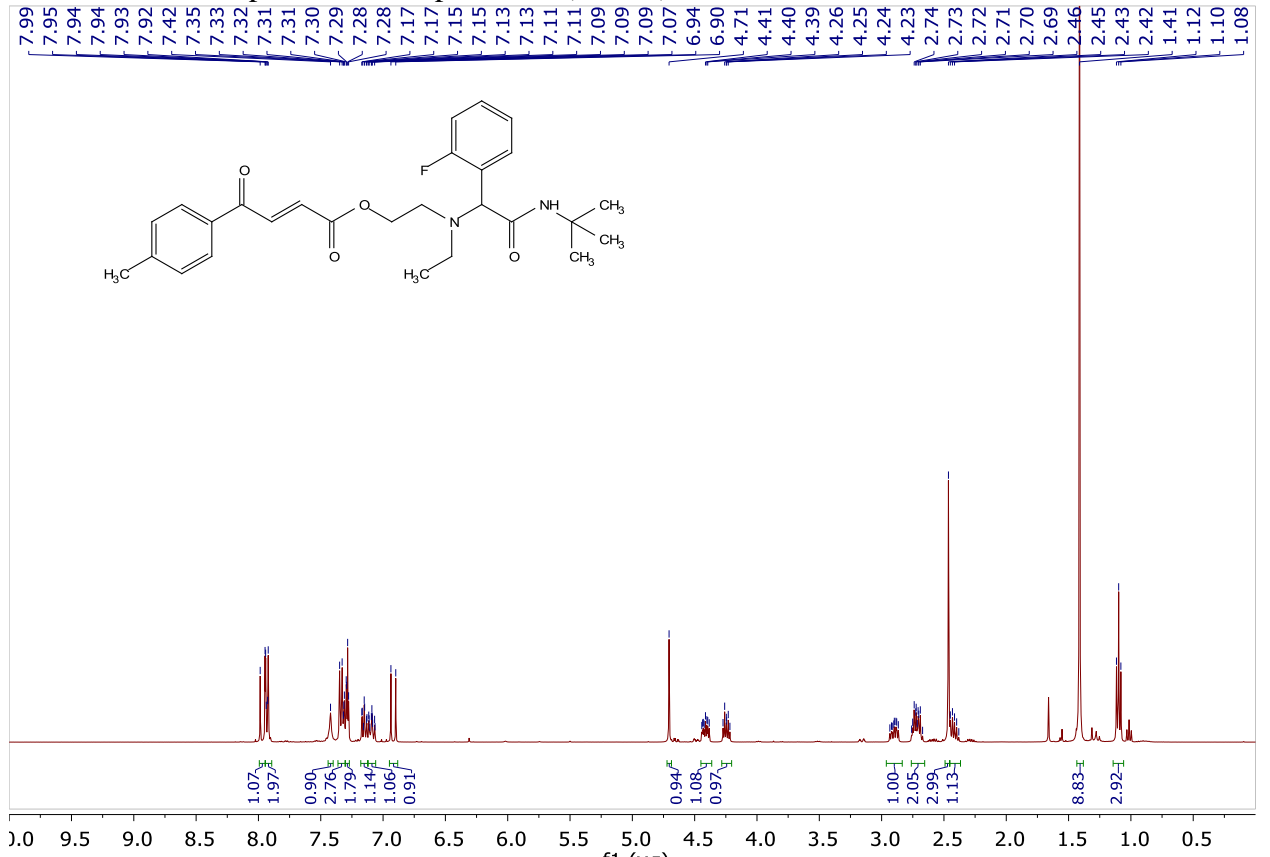
¹H and ¹³C NMR spectra for compound **14** (CDCl₃)



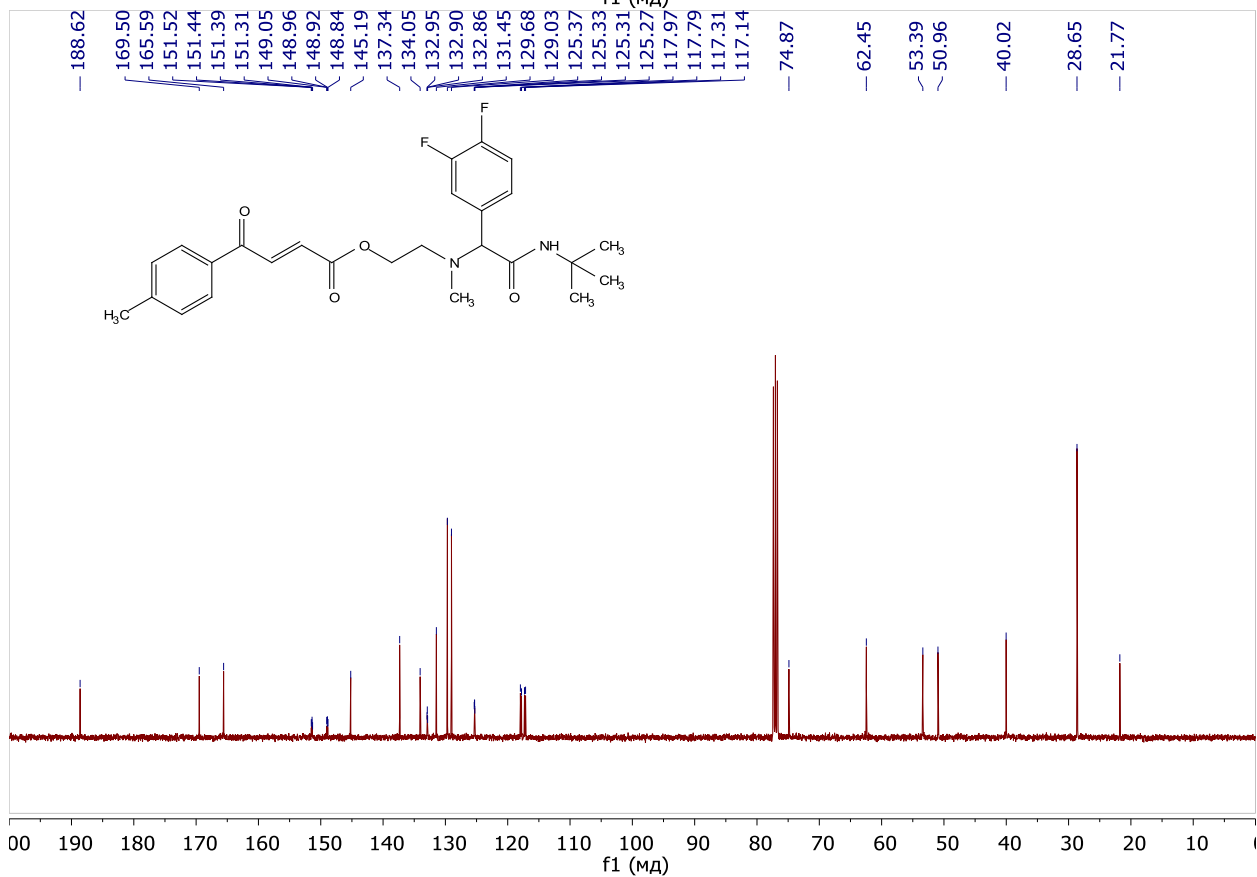
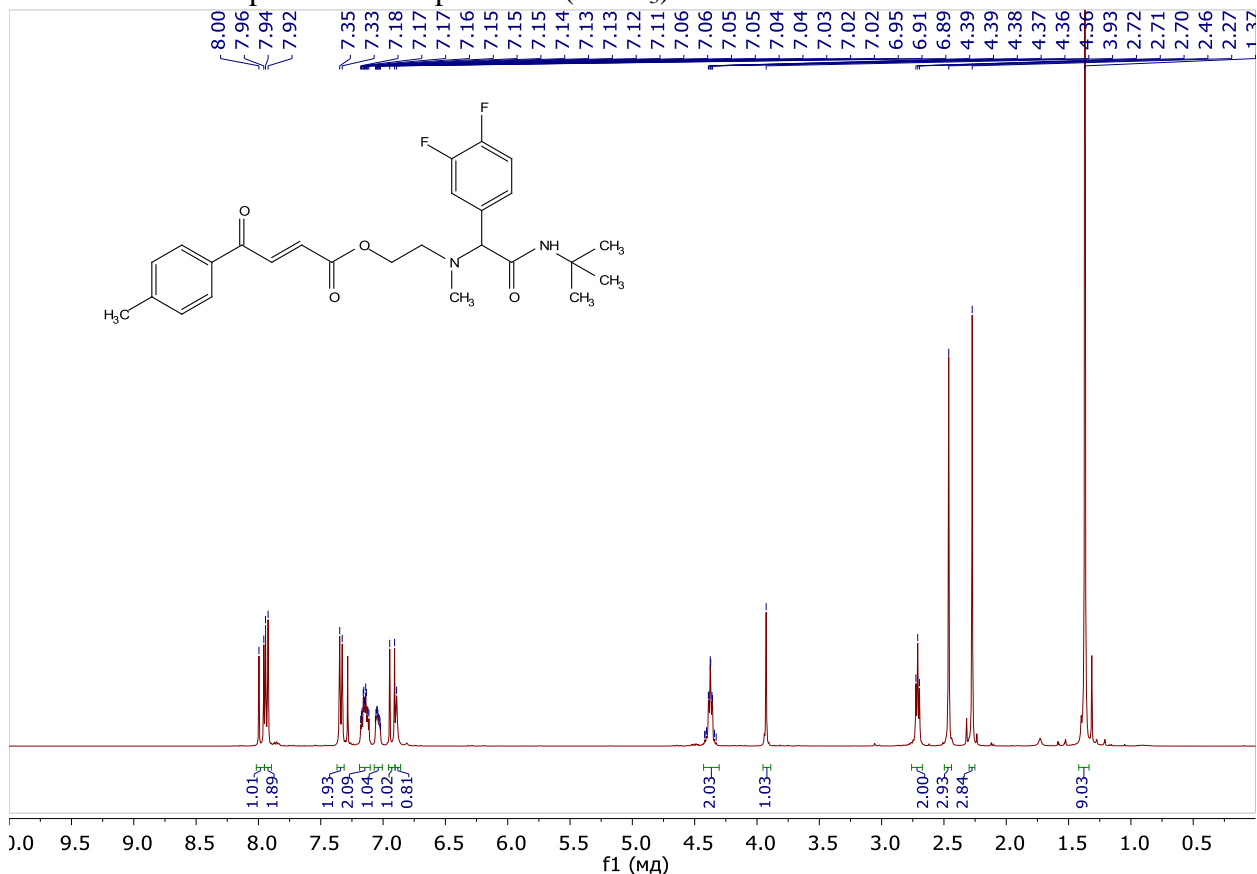
¹H and ¹³C NMR spectra for compound **15** (CDCl₃)



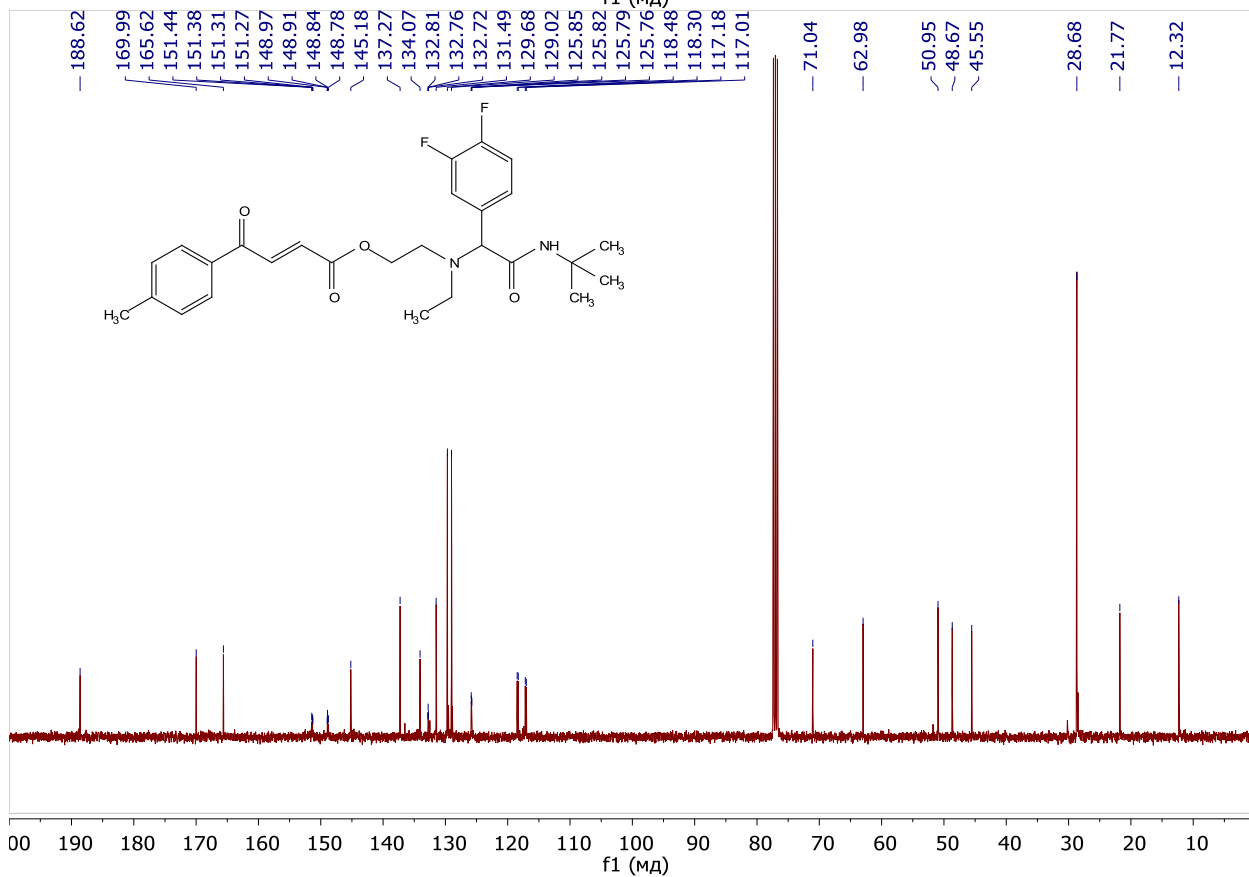
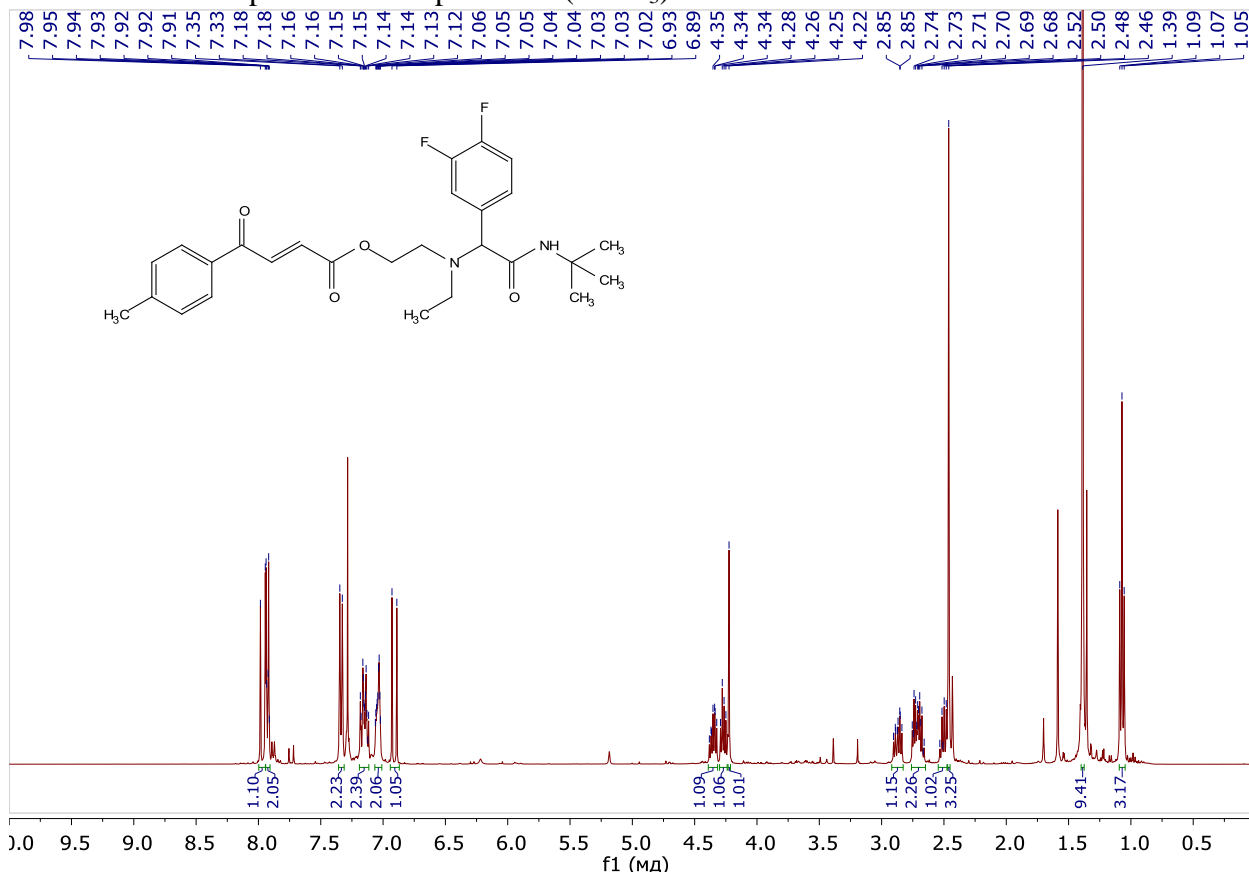
¹H and ¹³C NMR spectra for compound **16** (CDCl₃)



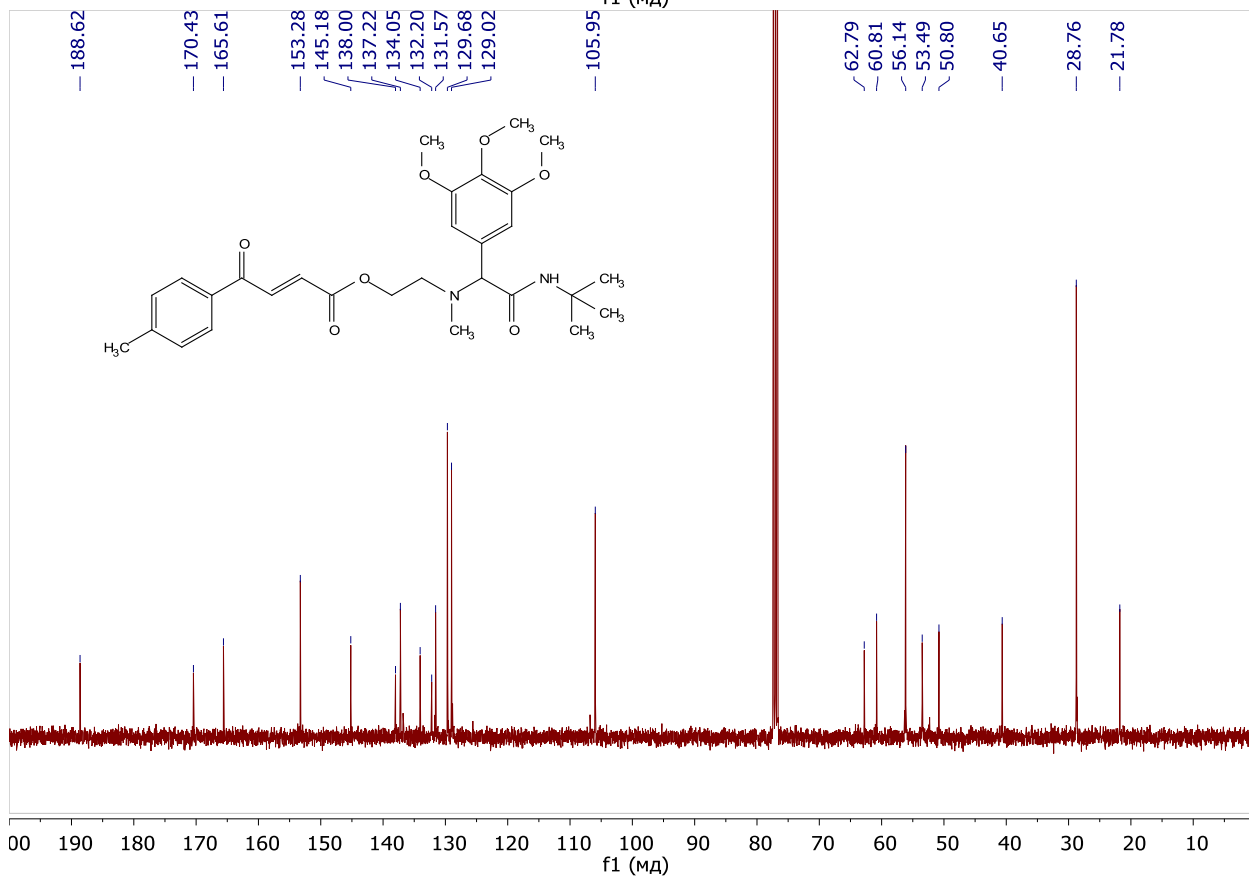
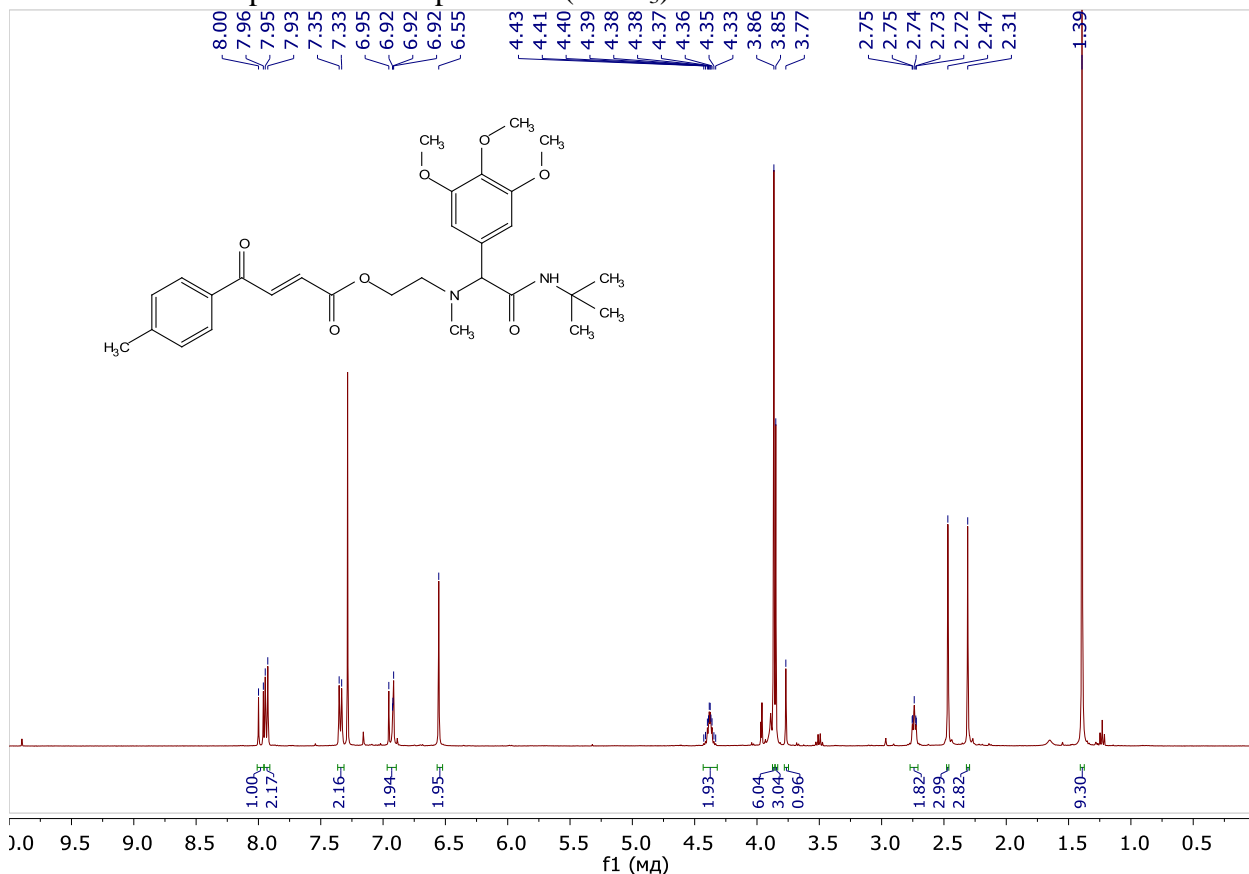
¹H and ¹³C NMR spectra for compound **17** (CDCl₃)



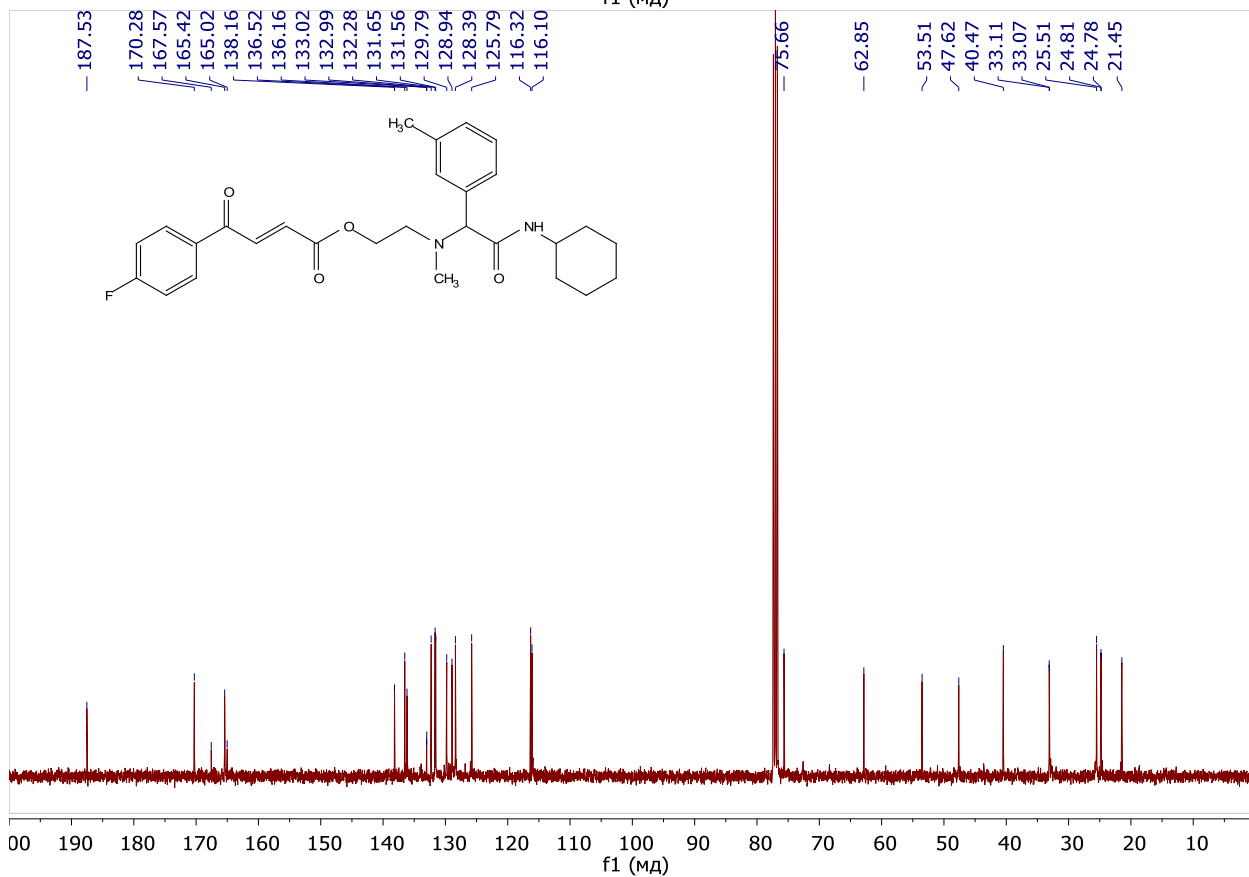
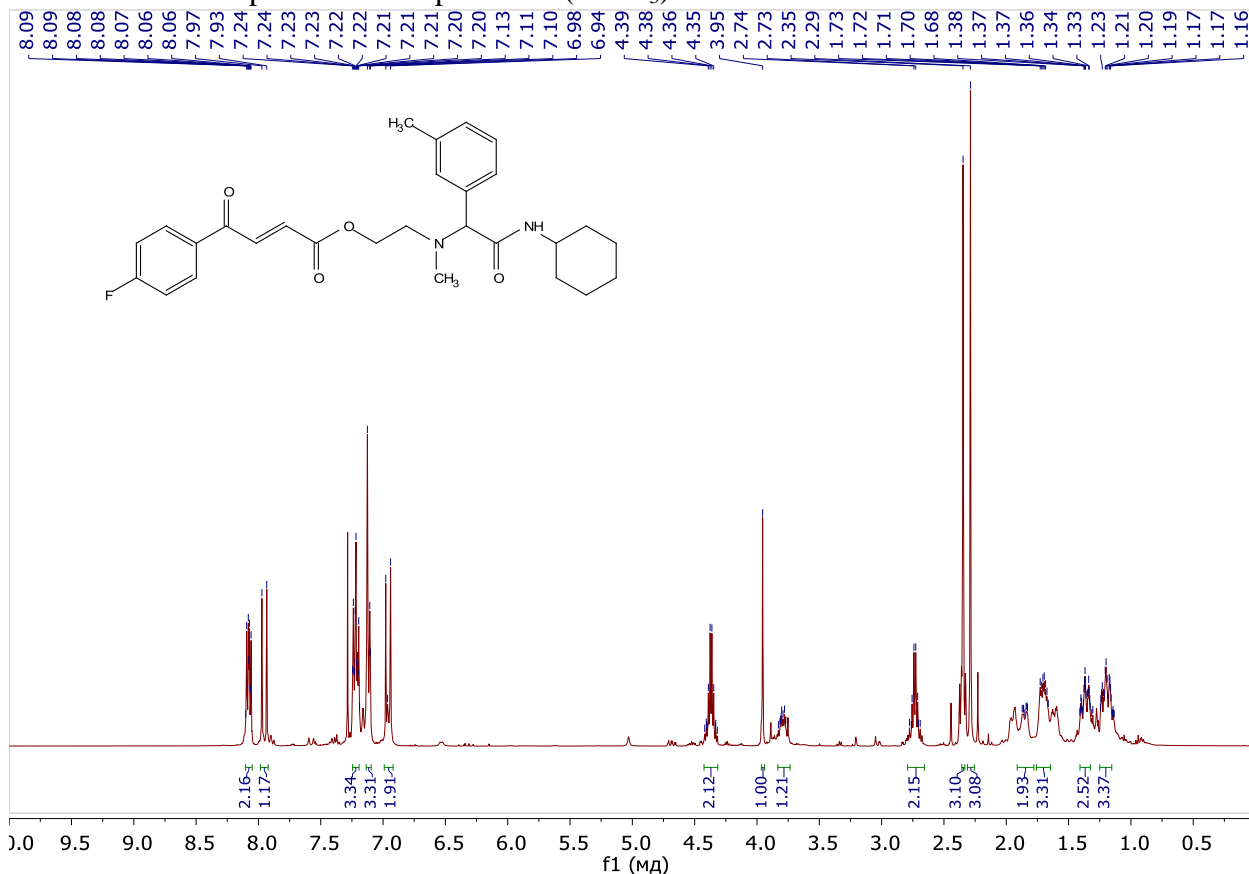
¹H and ¹³C NMR spectra for compound **18** (CDCl₃)



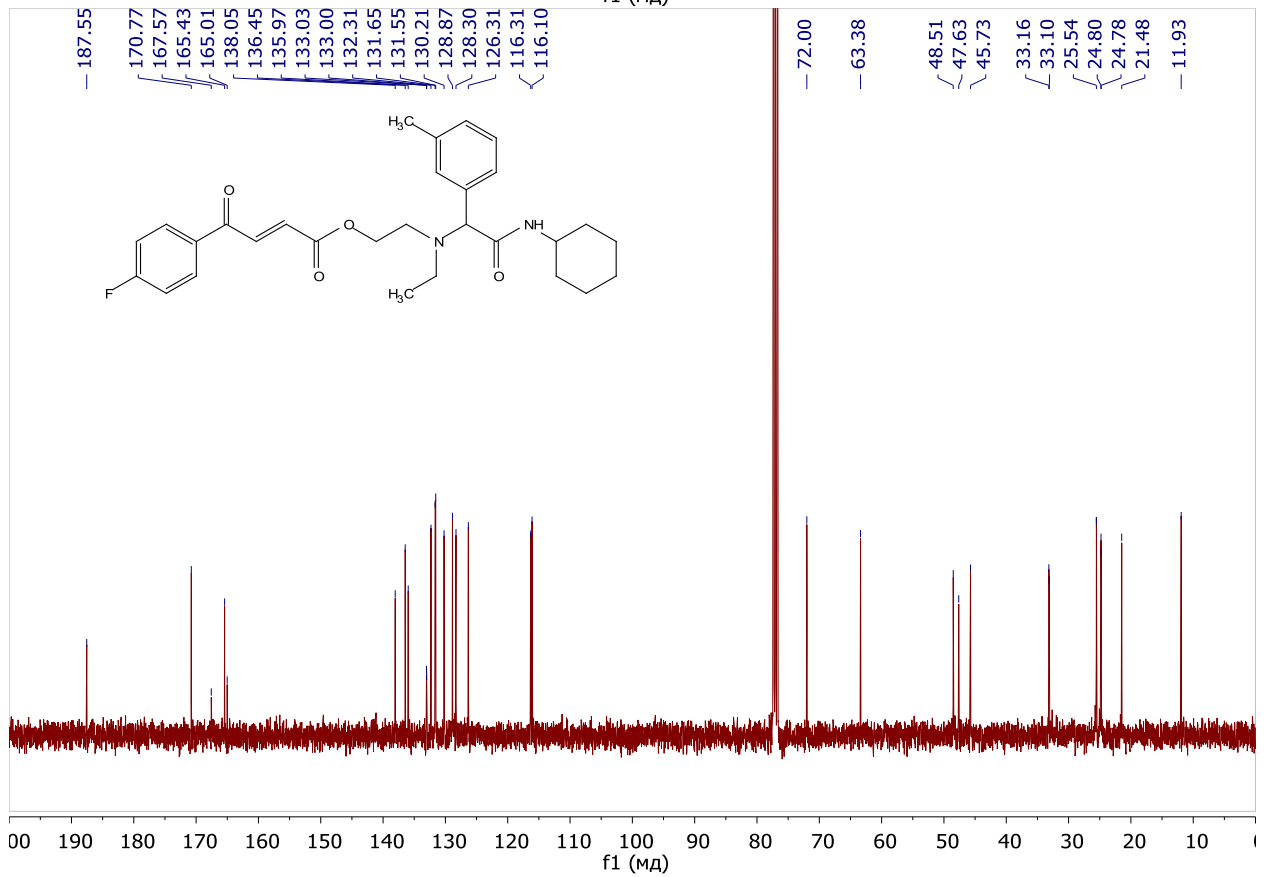
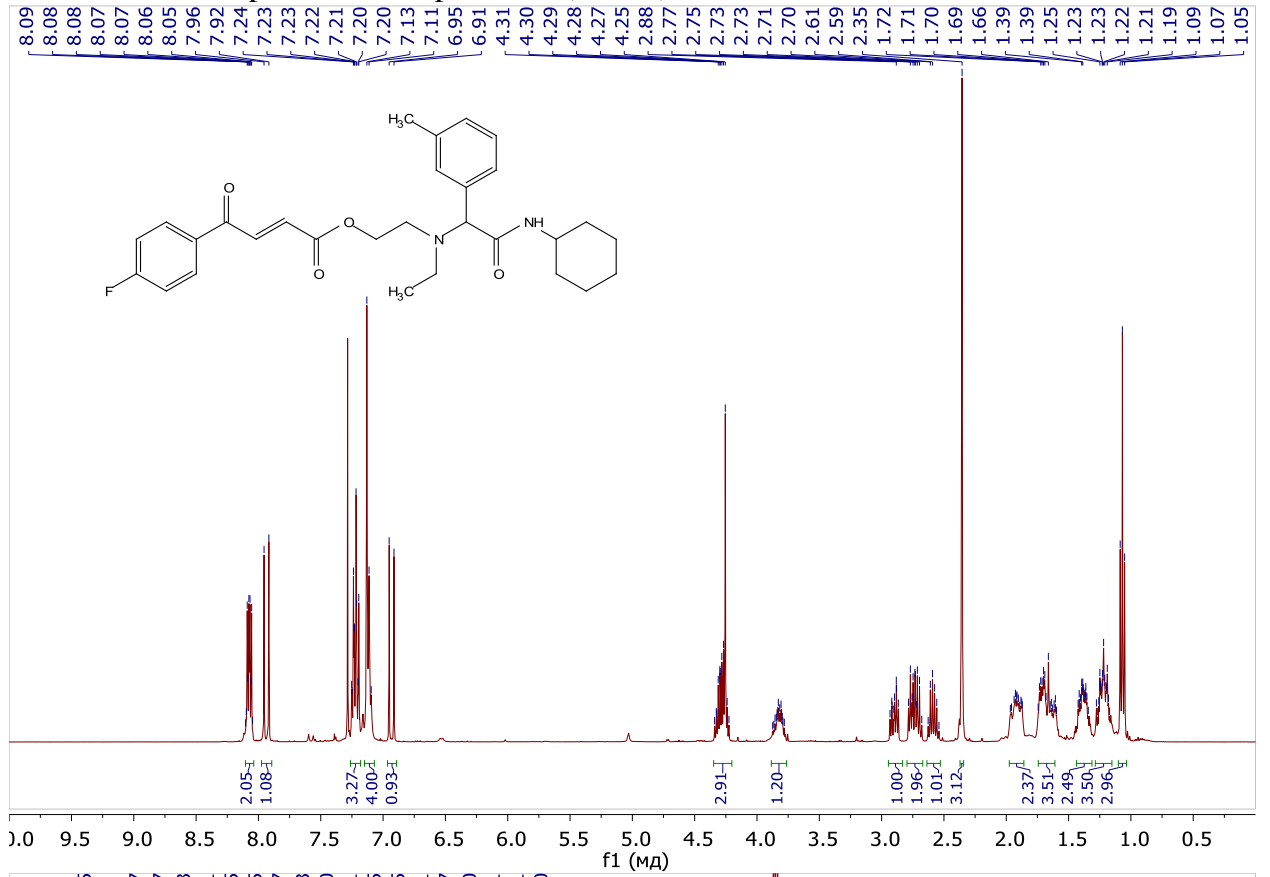
¹H and ¹³C NMR spectra for compound **19** (CDCl₃)



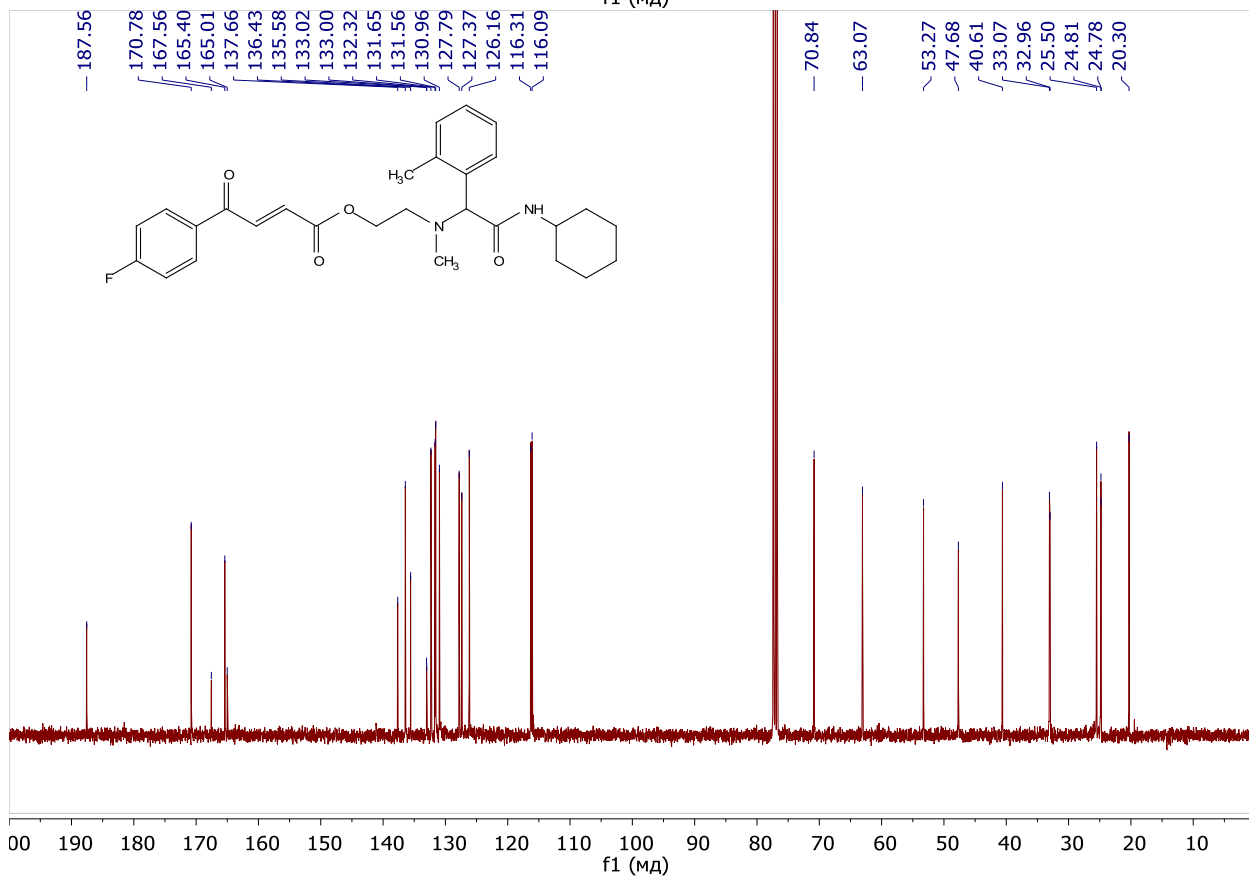
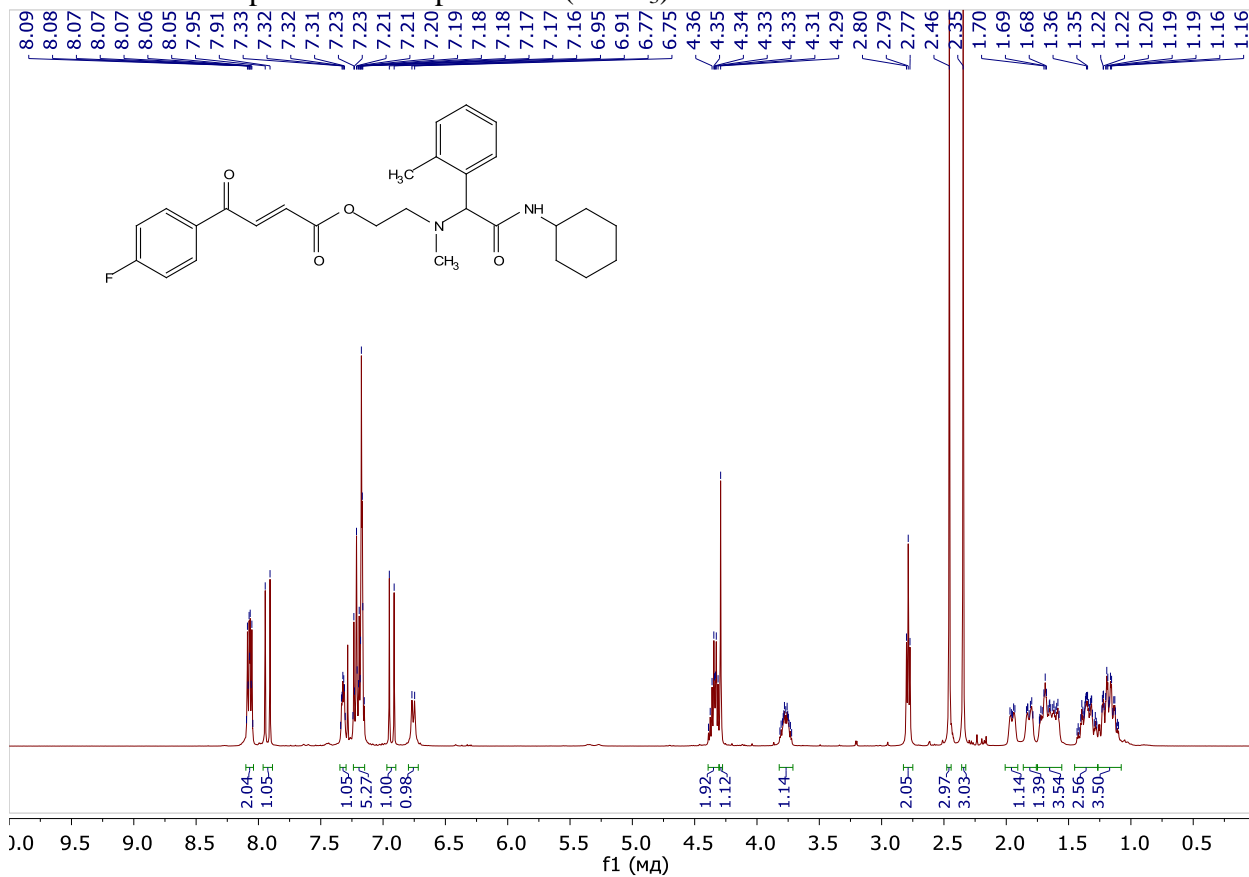
¹H and ¹³C NMR spectra for compound **20** (CDCl₃)



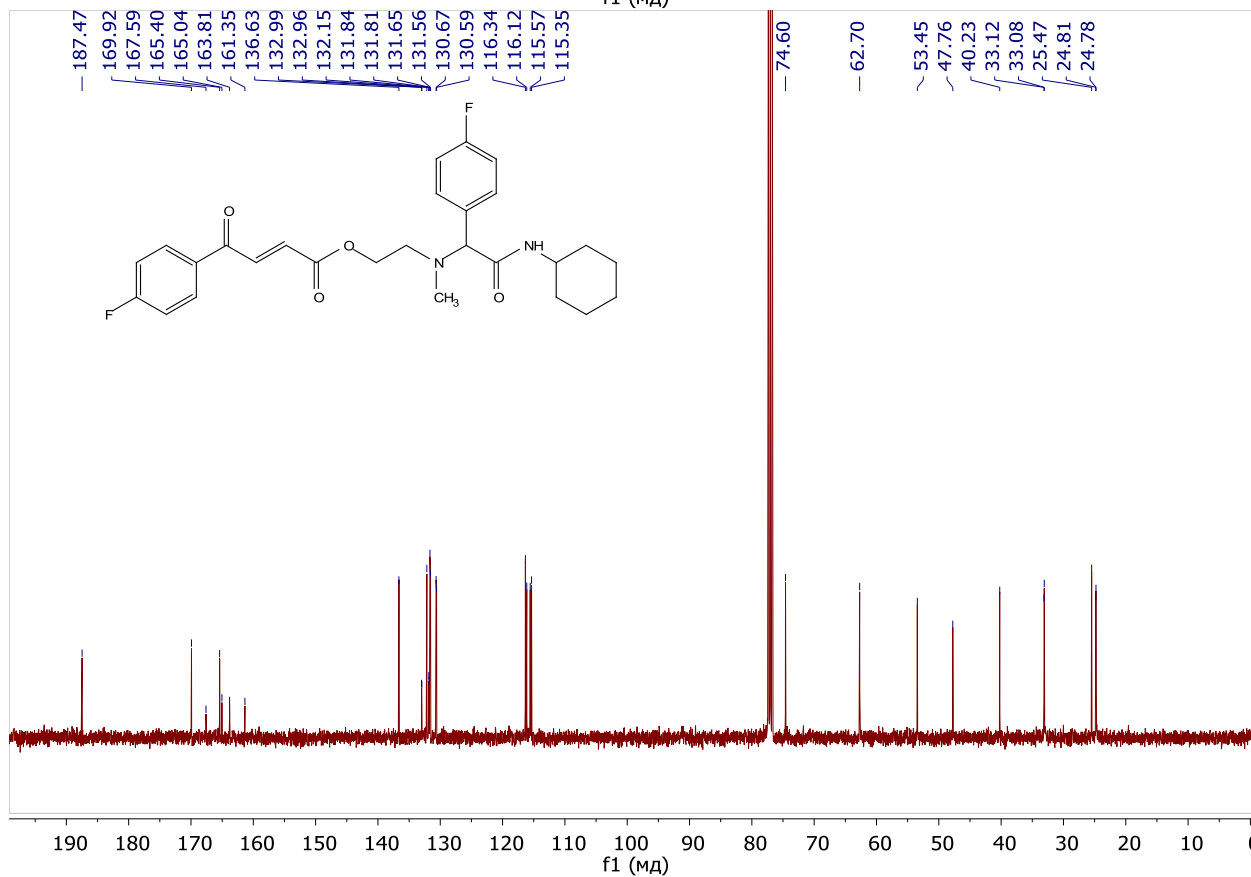
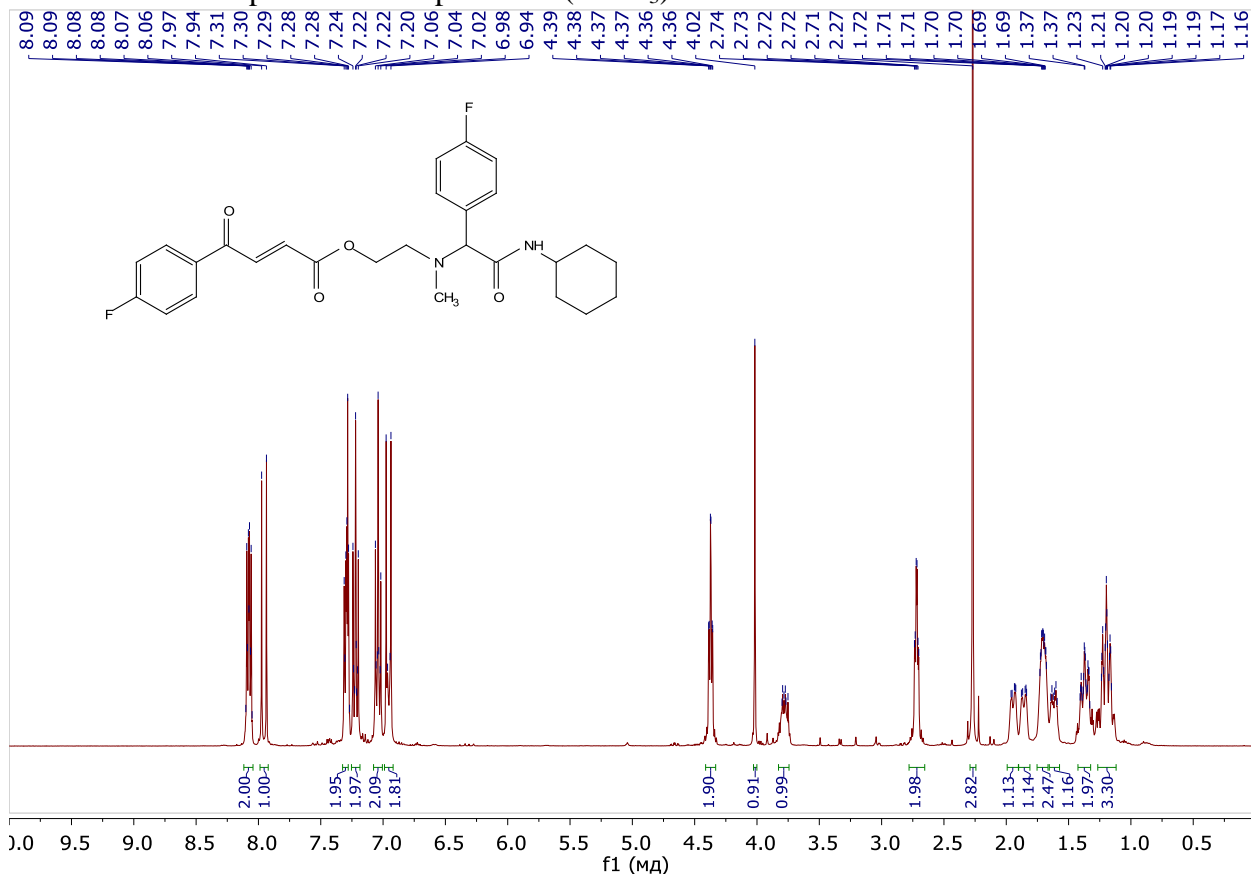
¹H and ¹³C NMR spectra for compound **21** (CDCl₃)



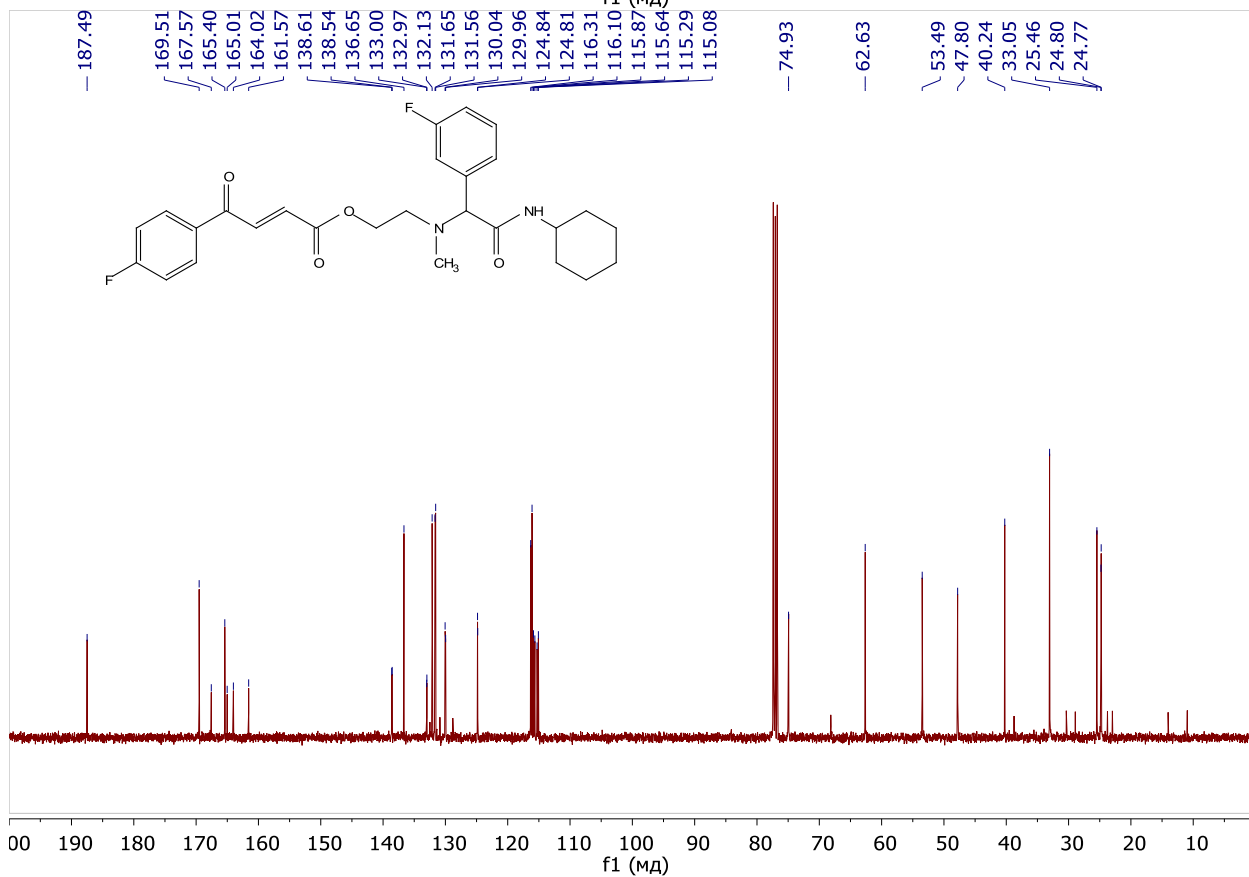
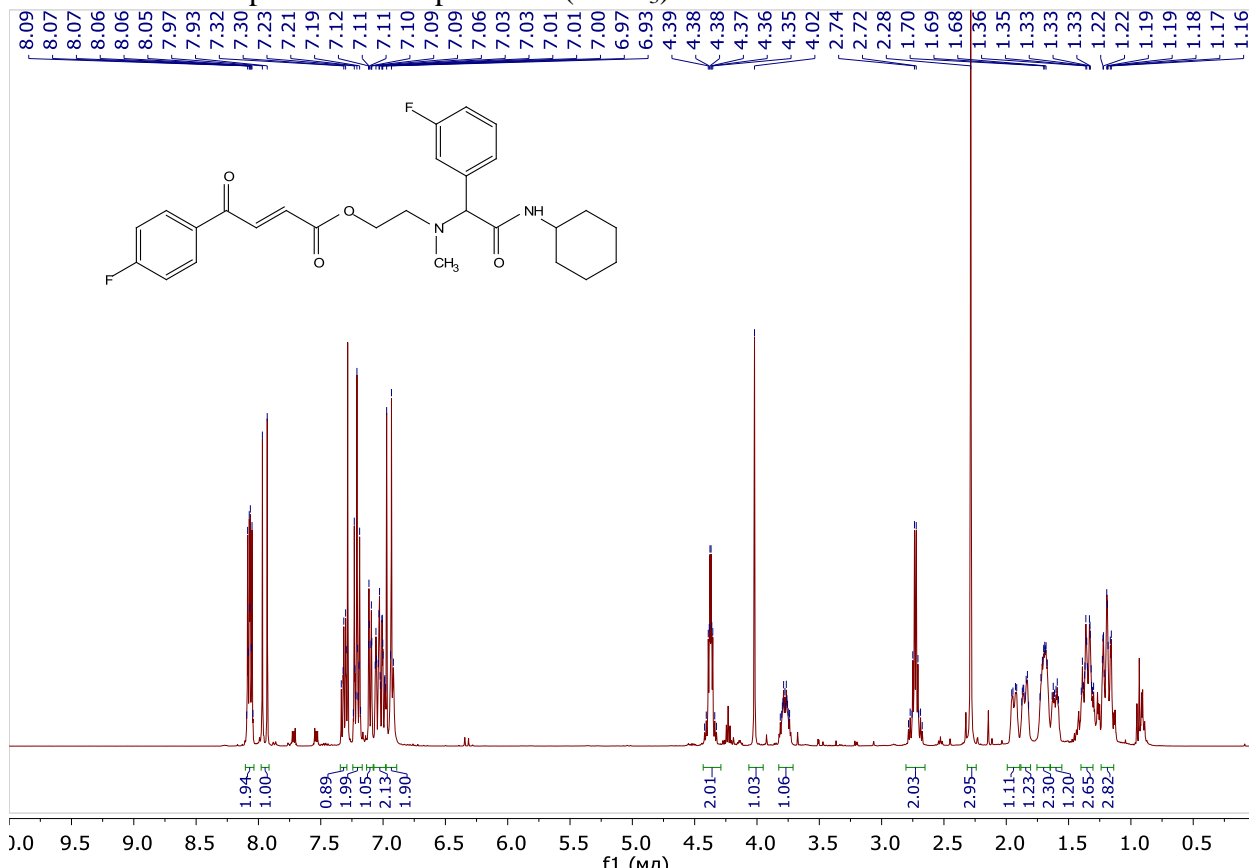
¹H and ¹³C NMR spectra for compound **22** (CDCl₃)



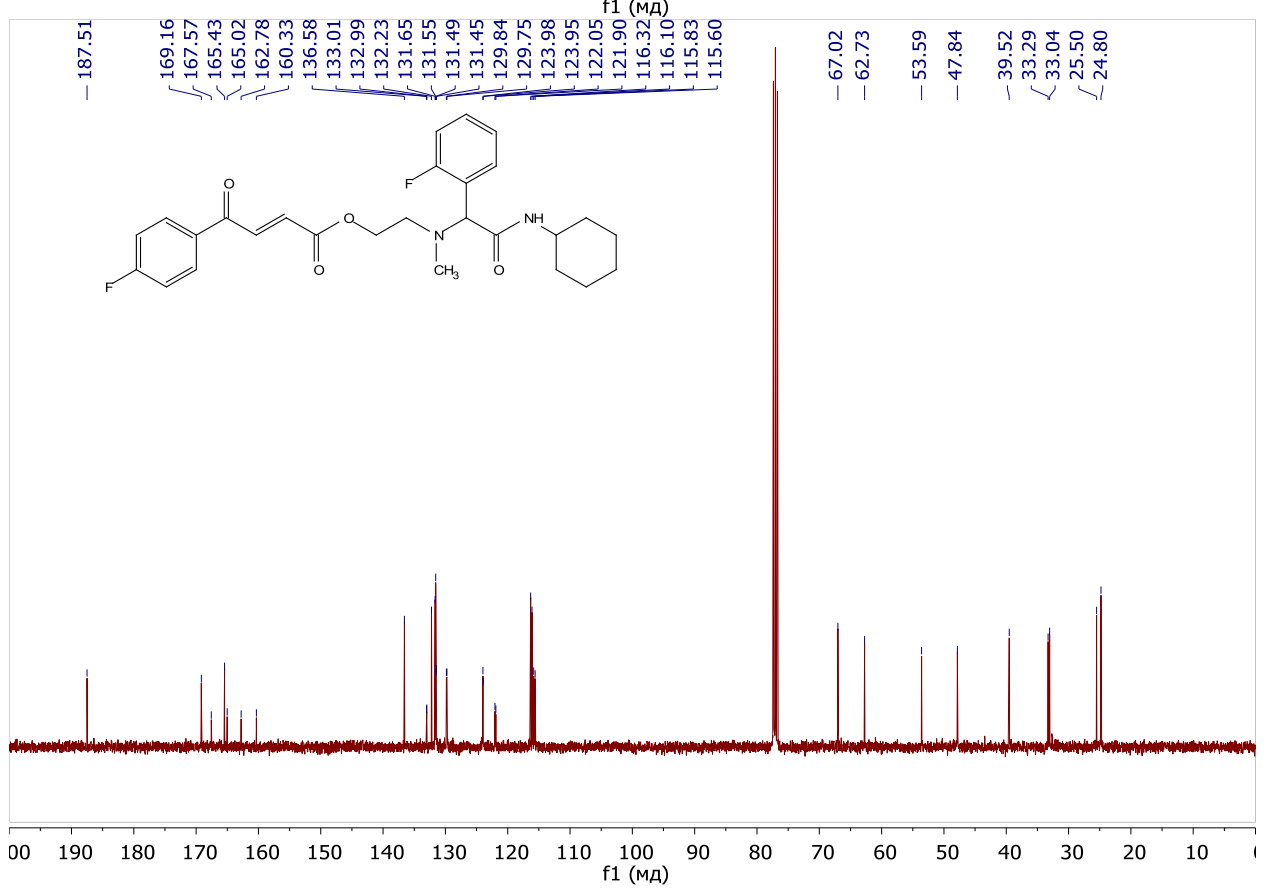
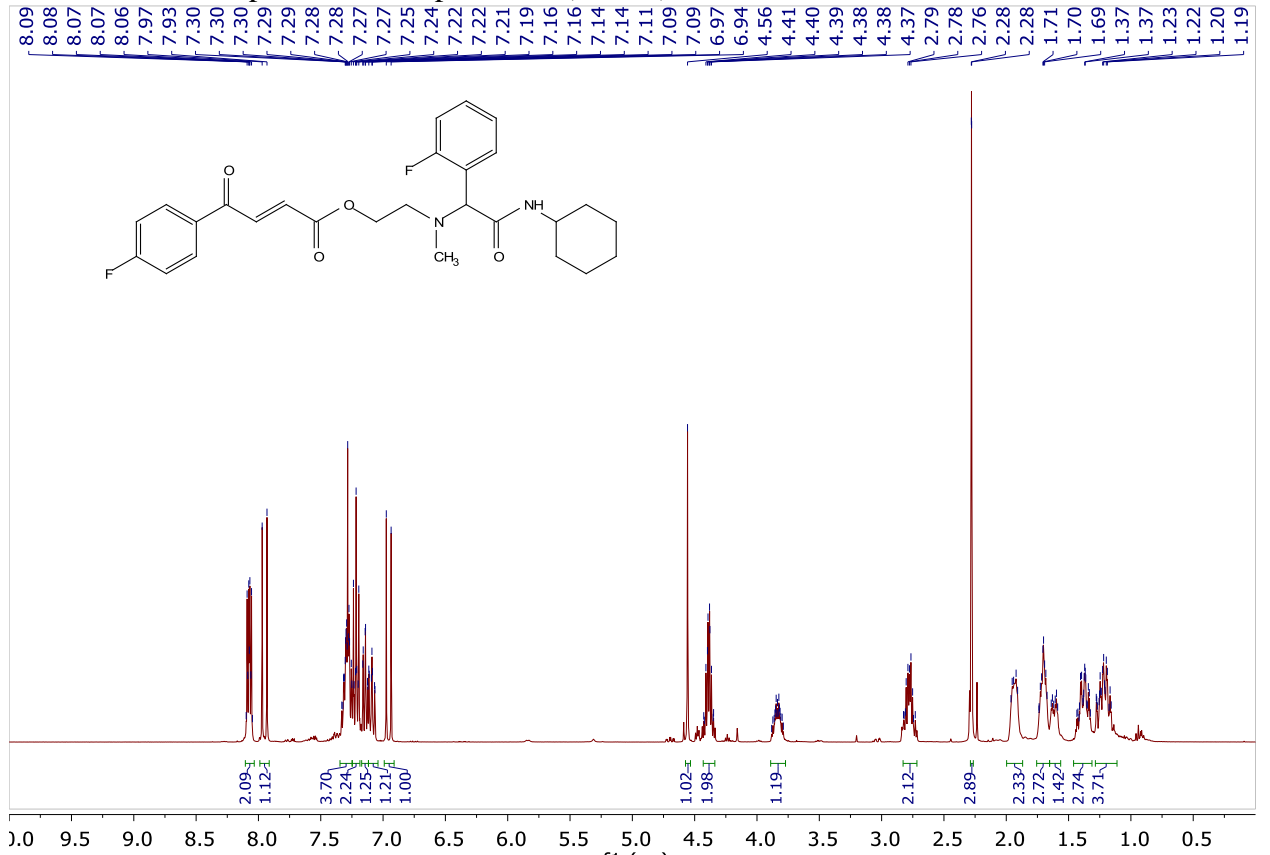
¹H and ¹³C NMR spectra for compound **23** (CDCl₃)



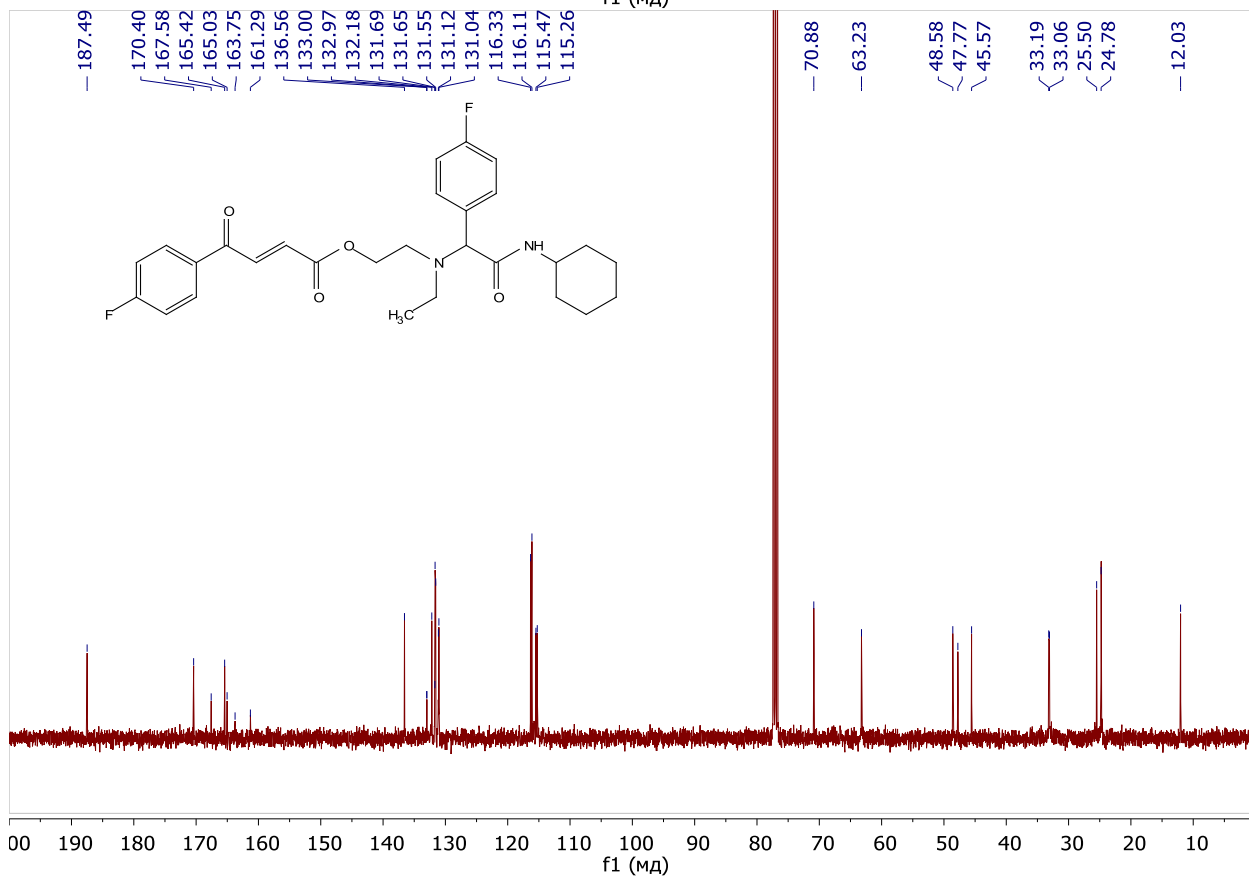
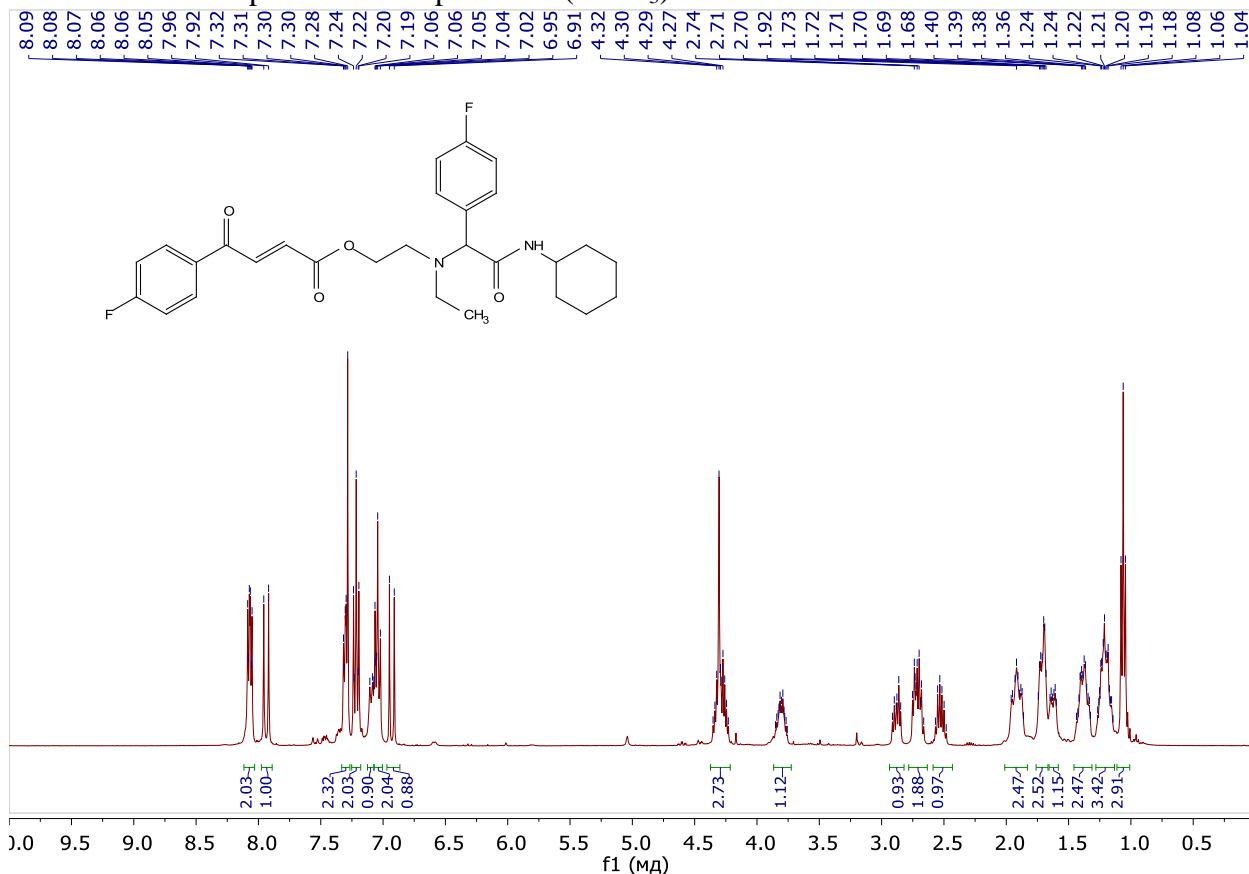
¹H and ¹³C NMR spectra for compound **24** (CDCl₃)



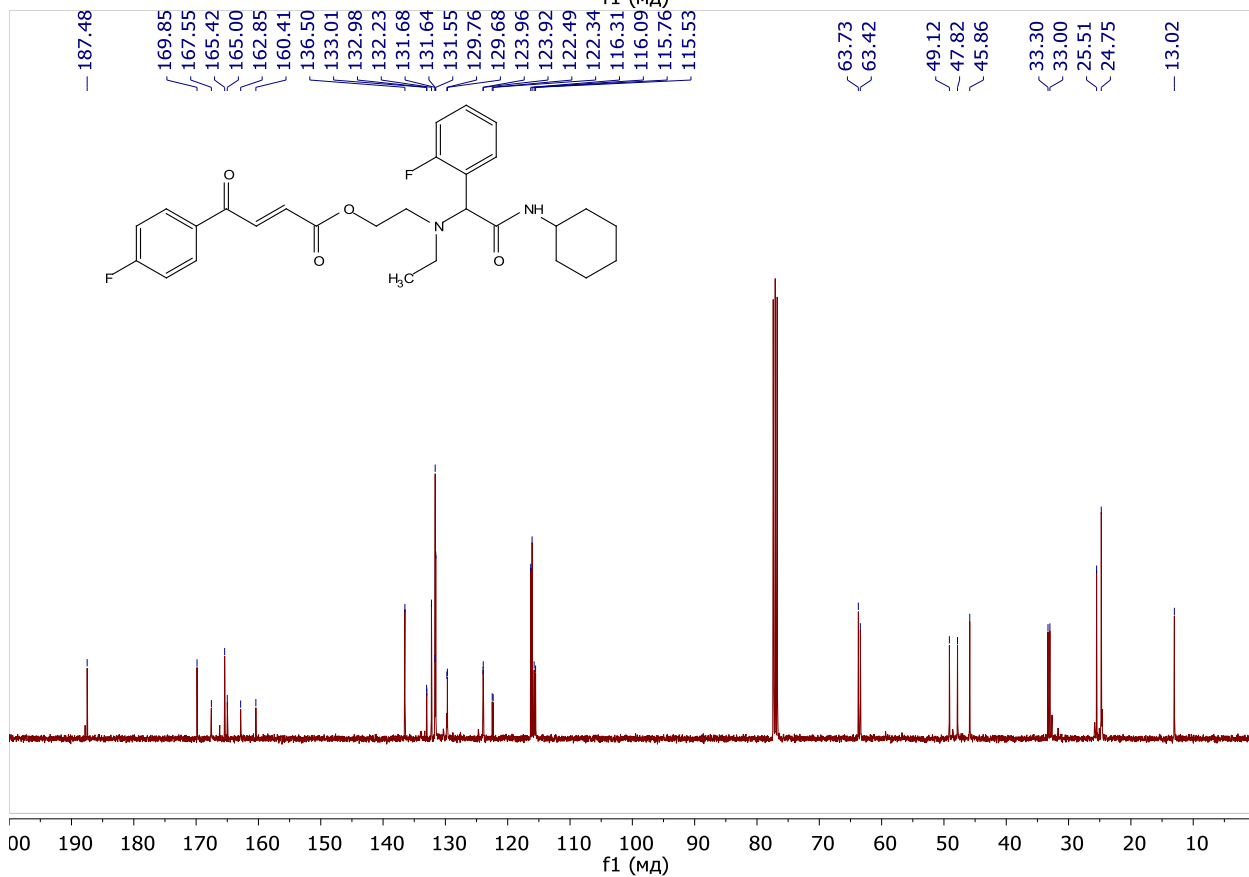
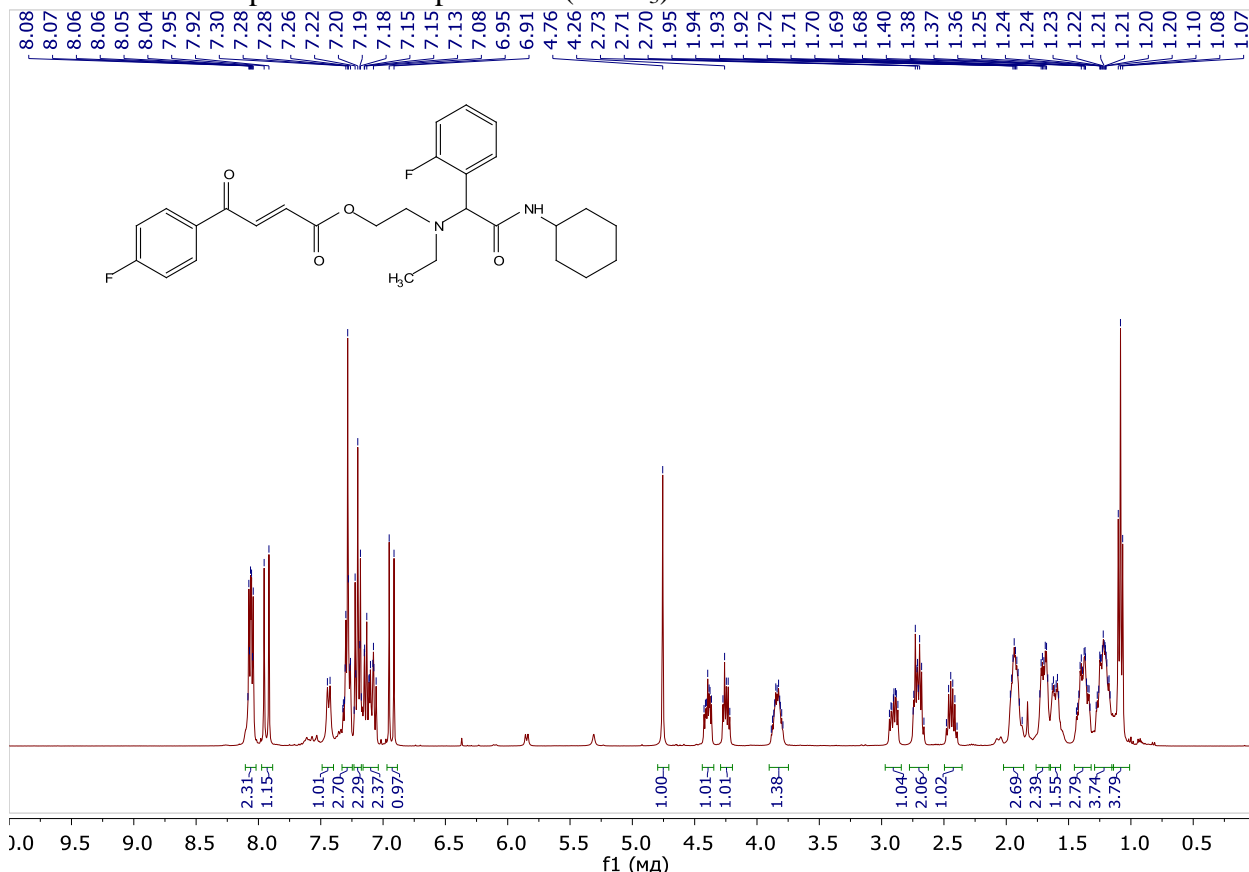
¹H and ¹³C NMR spectra for compound **25** (CDCl₃)



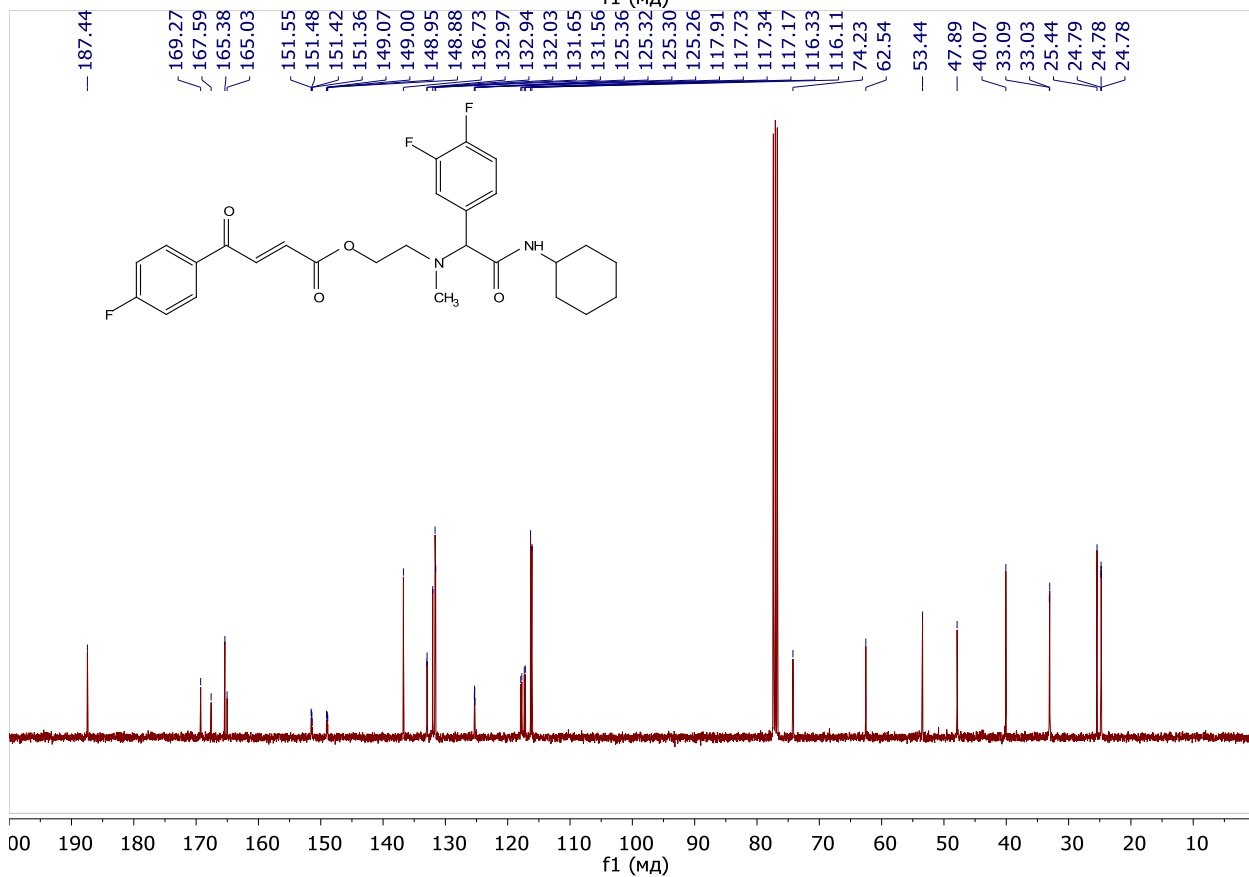
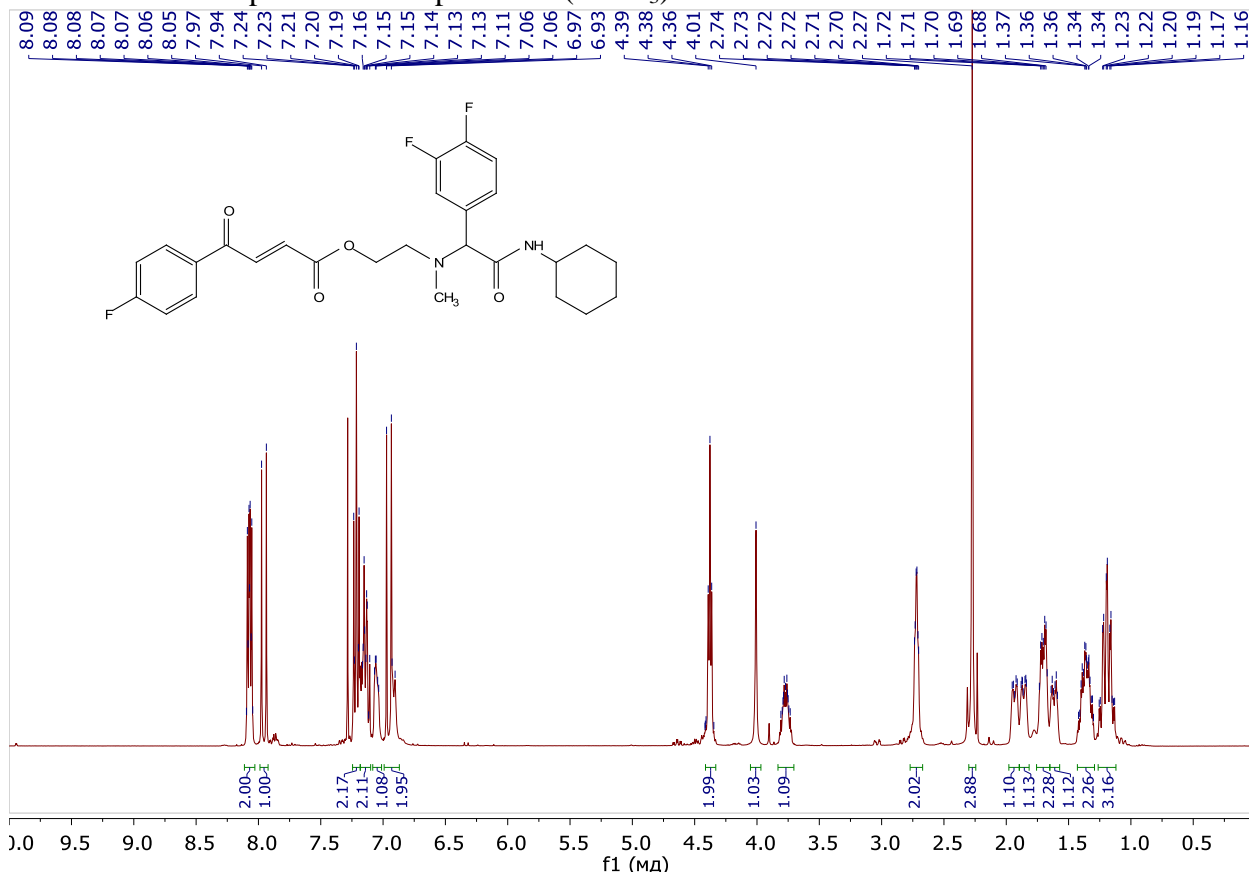
¹H and ¹³C NMR spectra for compound **26** (CDCl₃)



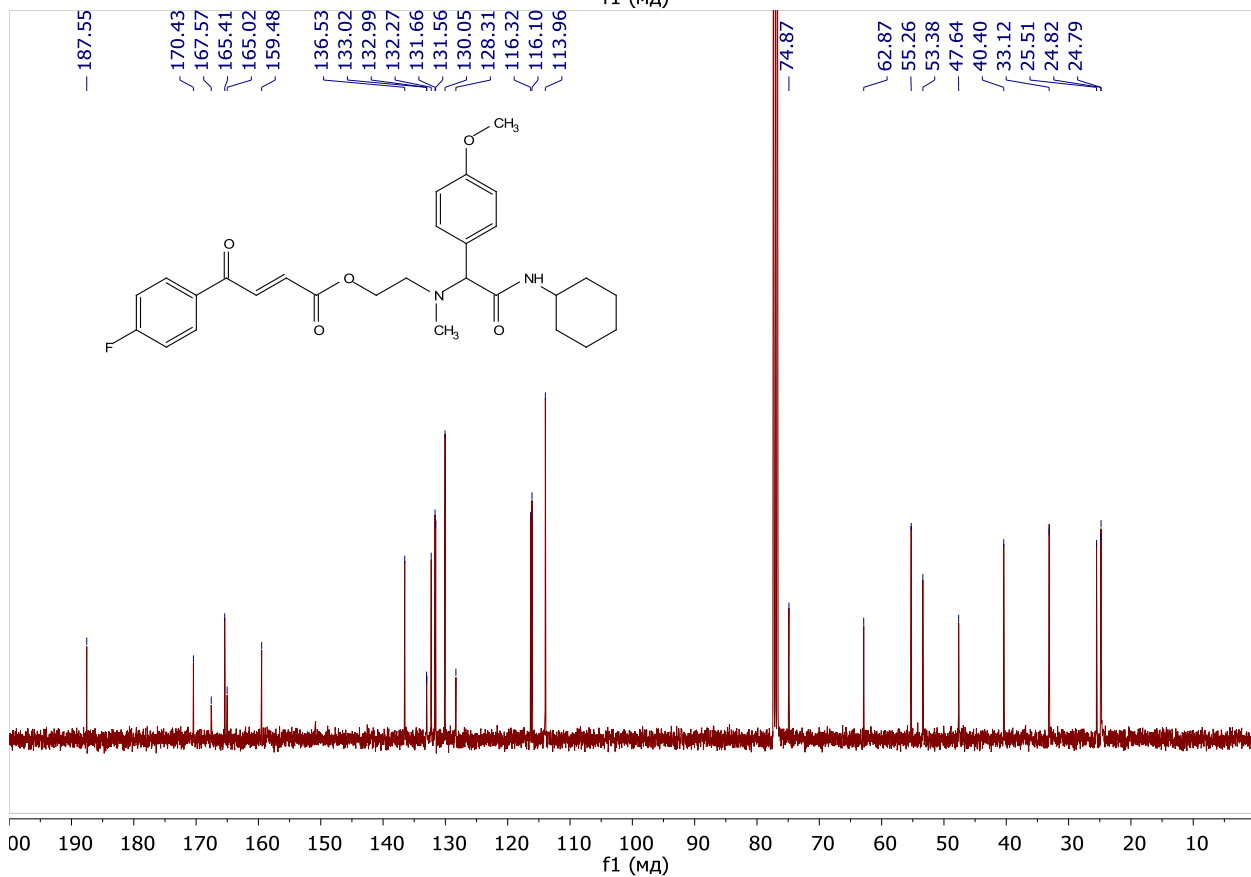
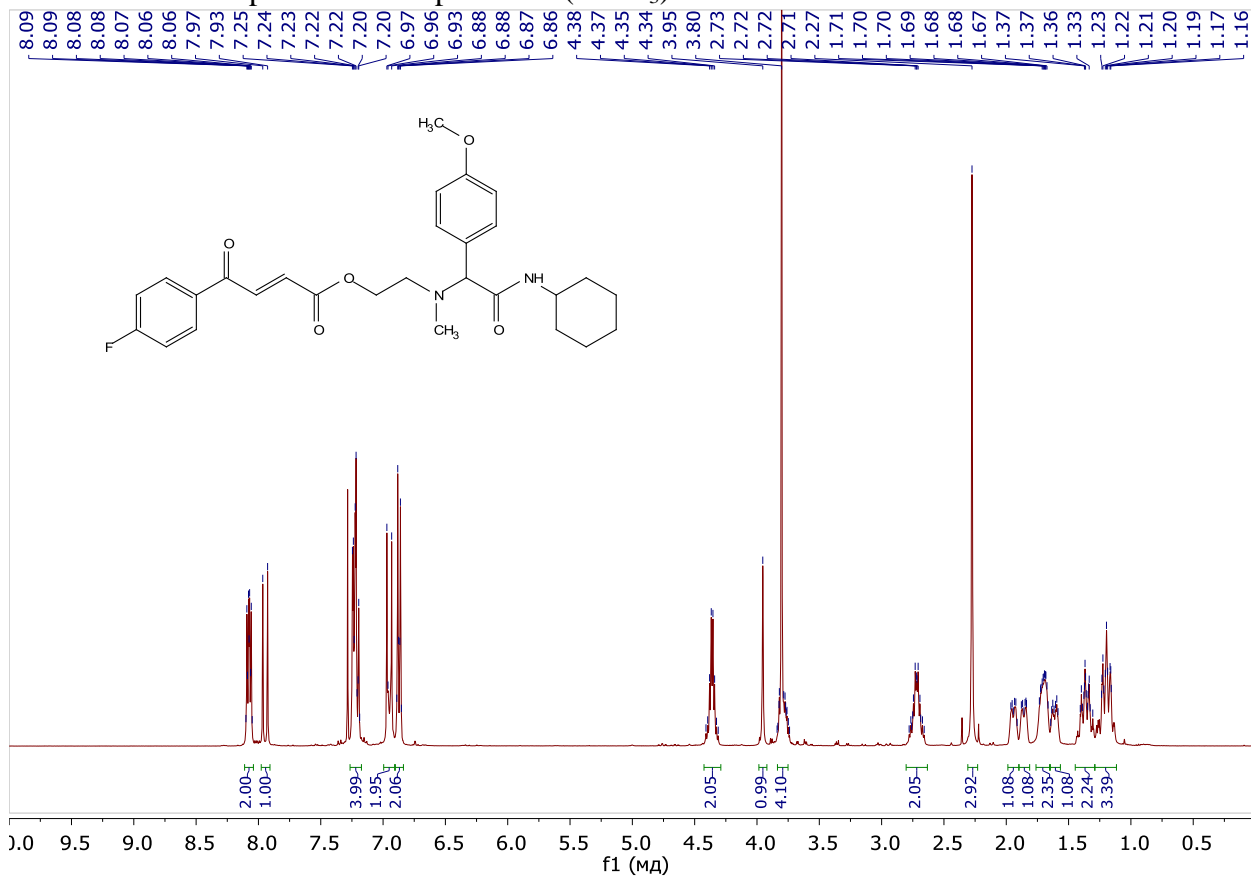
¹H and ¹³C NMR spectra for compound **27** (CDCl₃)



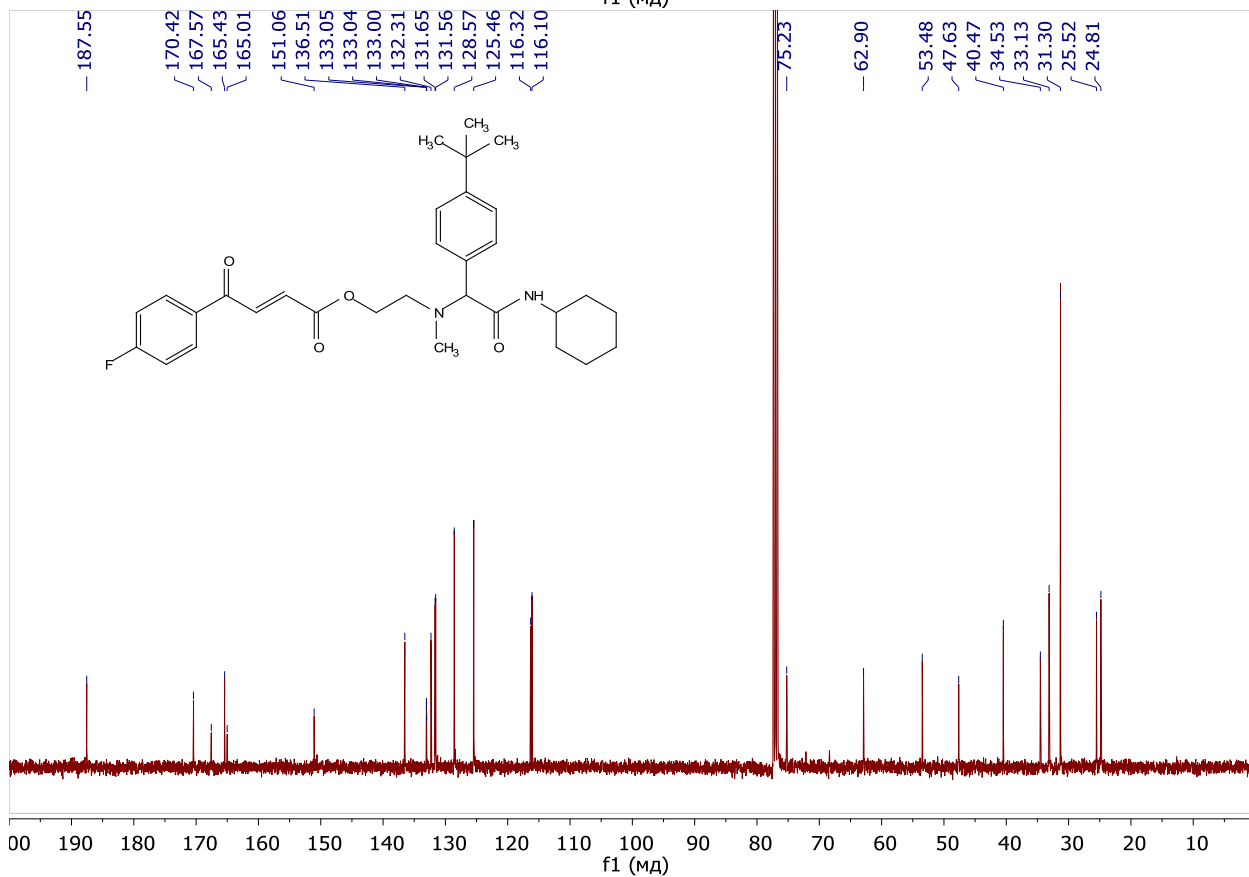
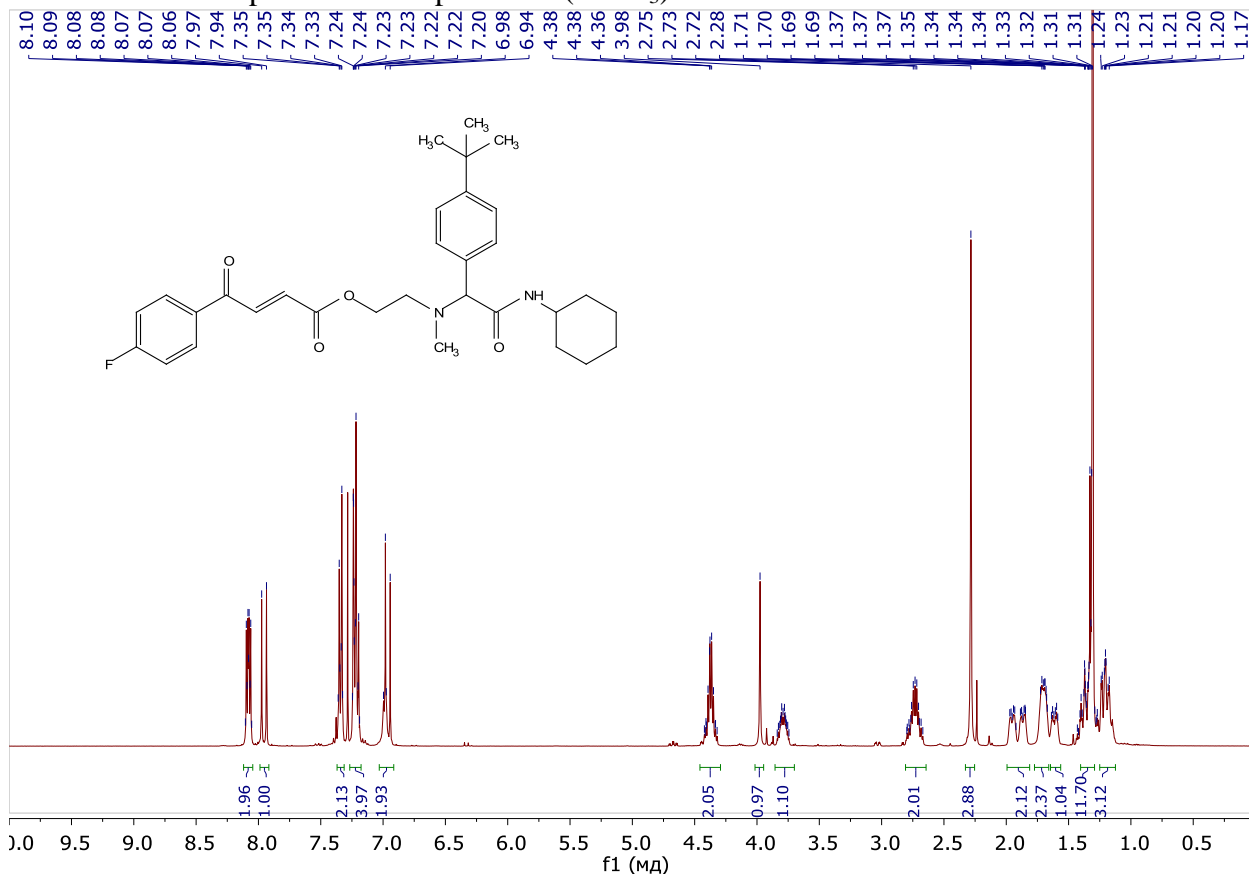
¹H and ¹³C NMR spectra for compound **28** (CDCl₃)



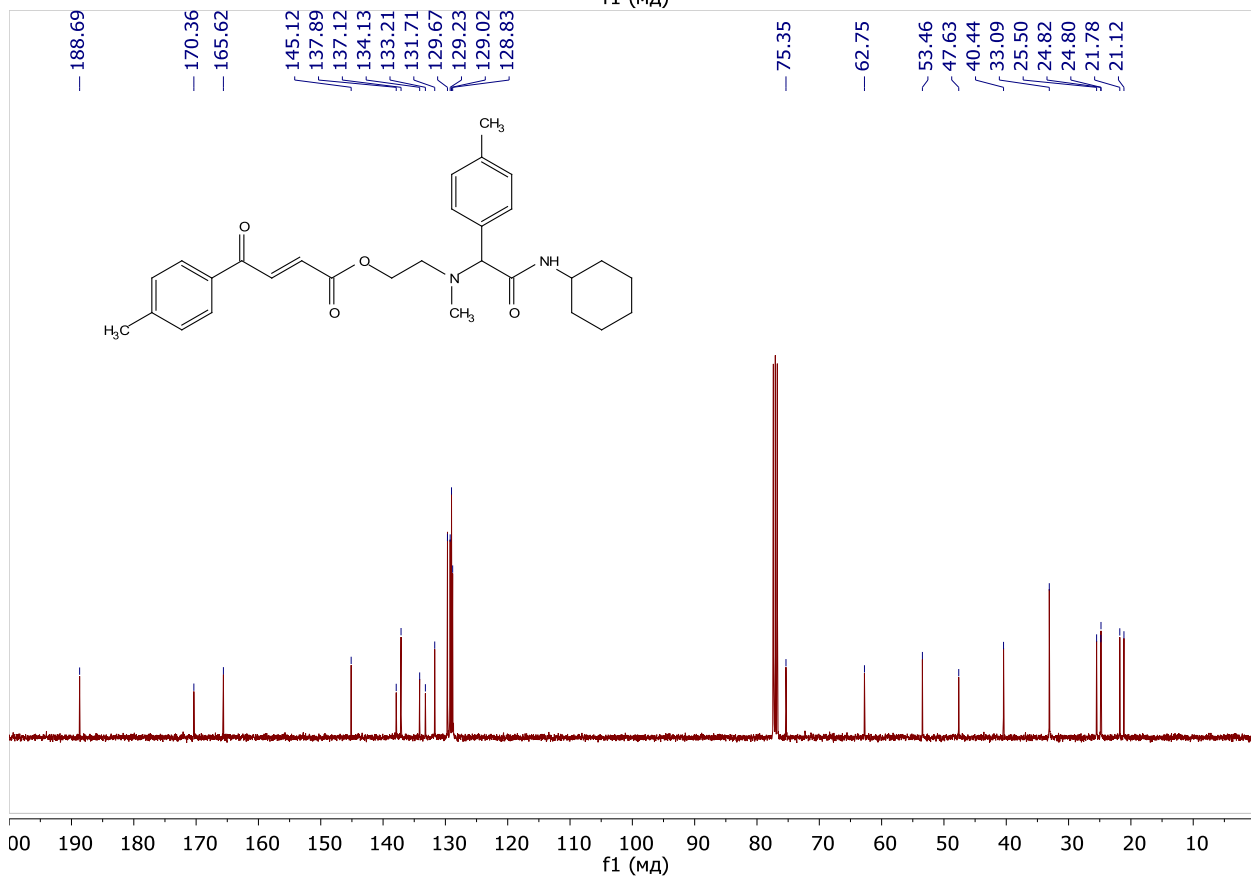
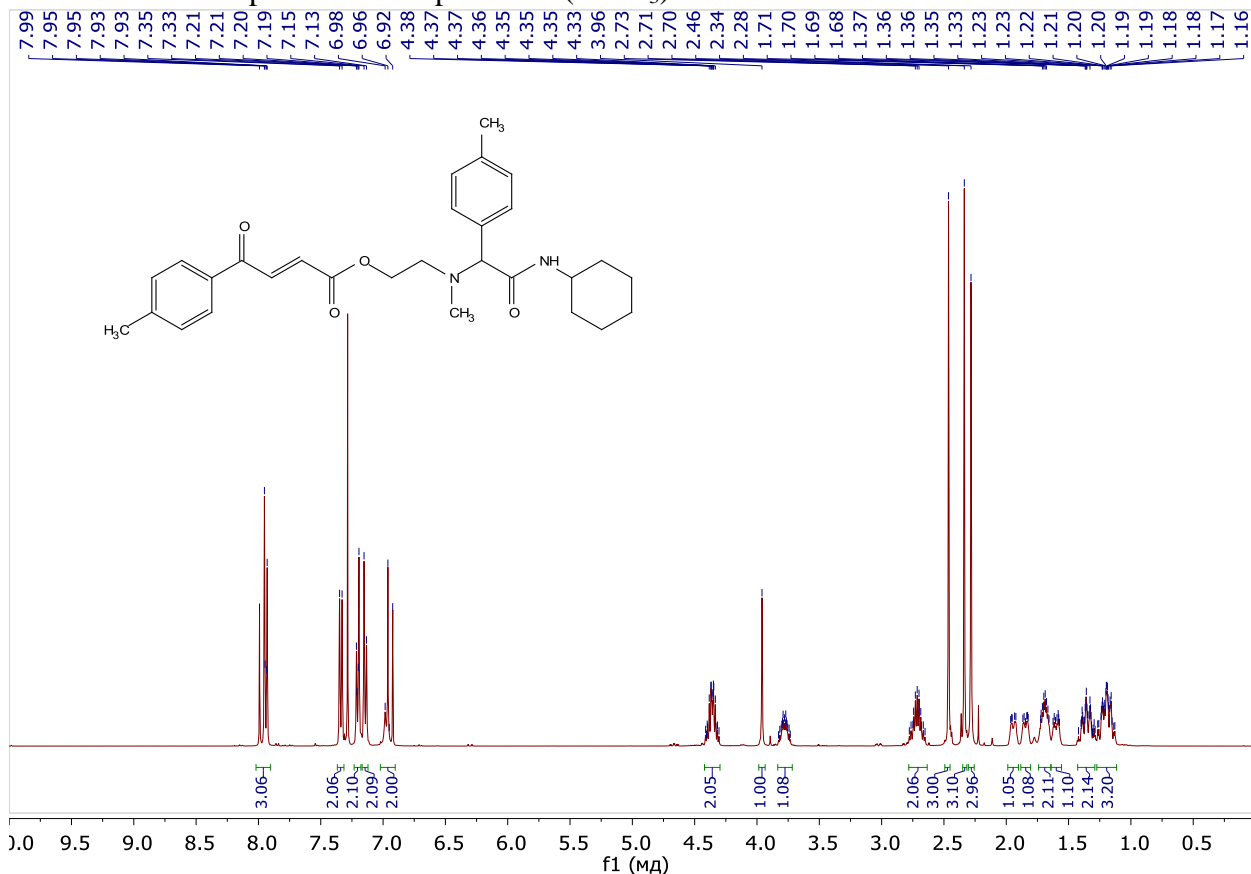
^1H and ^{13}C NMR spectra for compound **29** (CDCl_3)



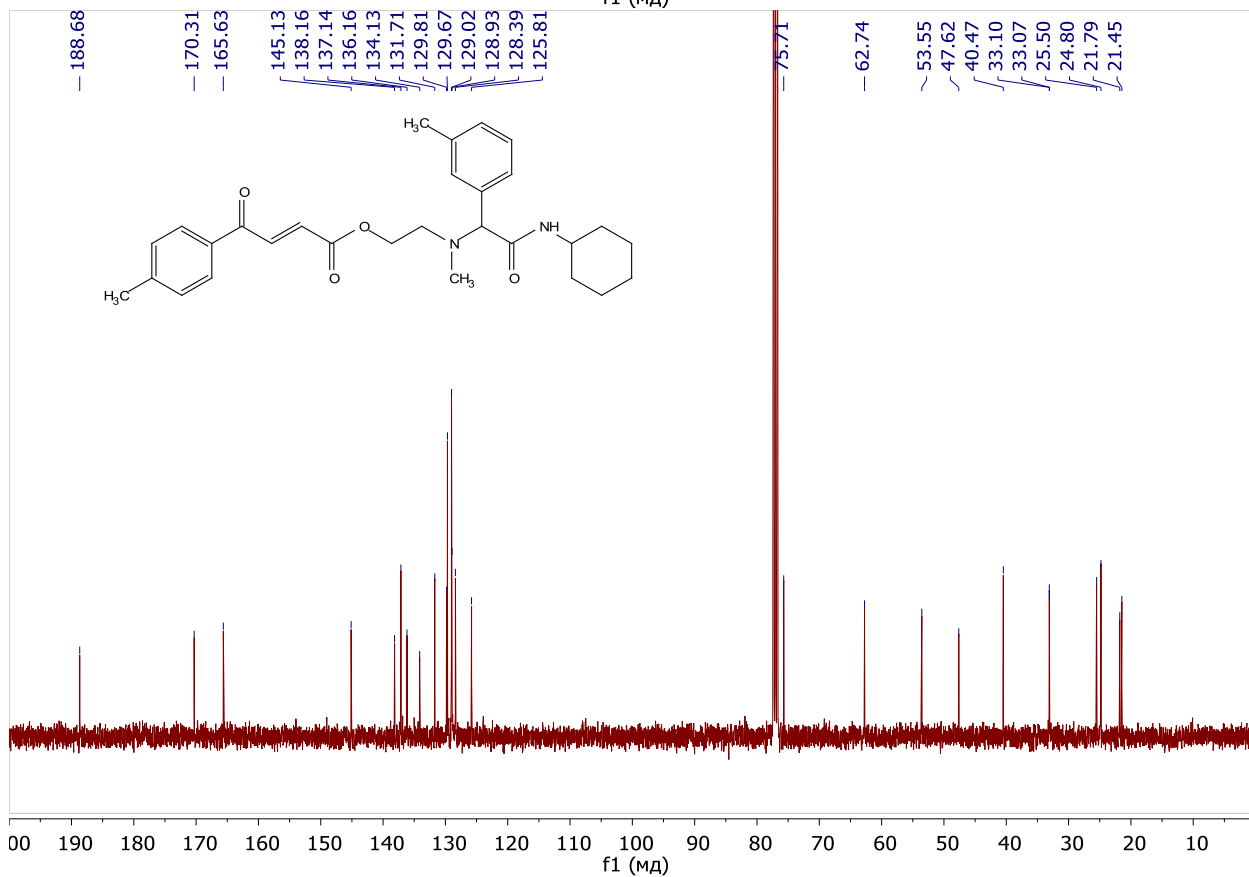
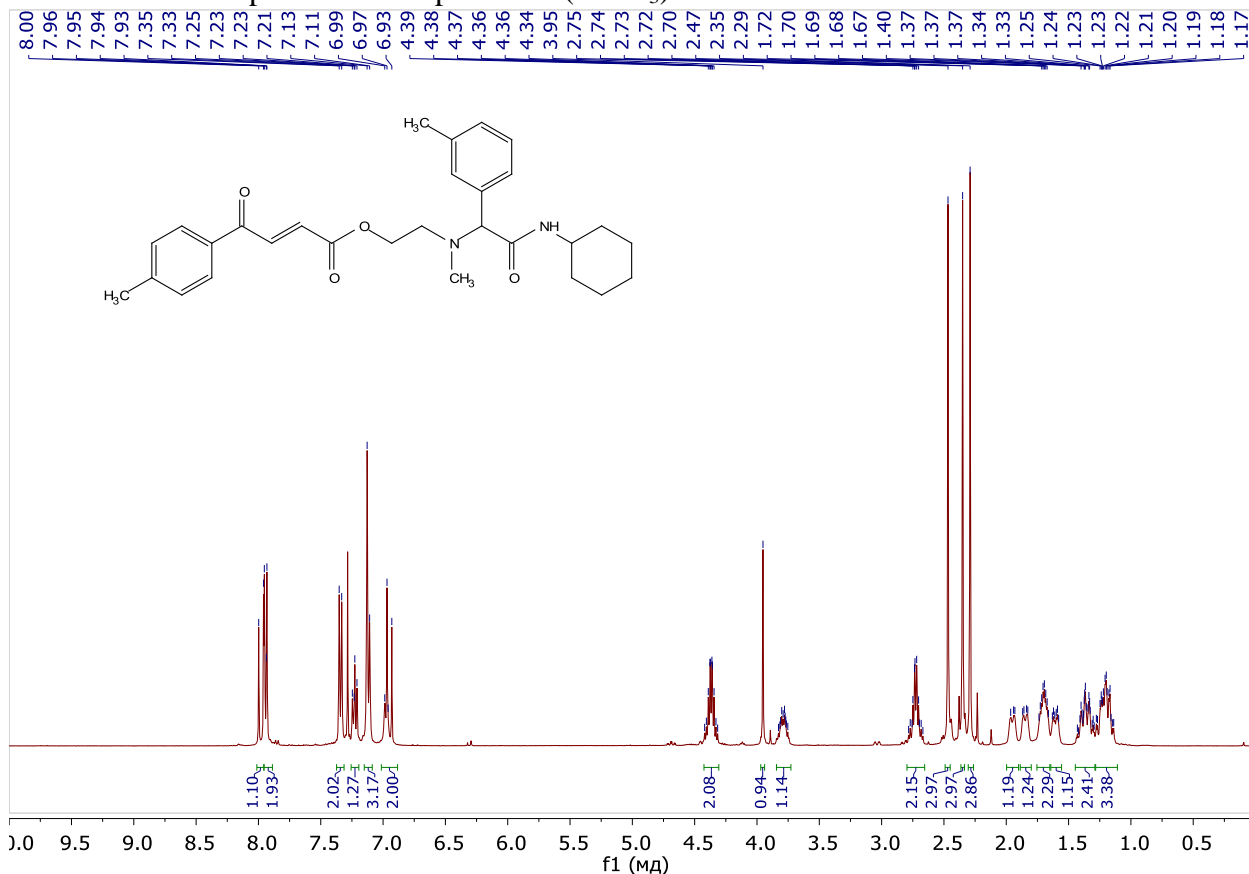
¹H and ¹³C NMR spectra for compound **30** (CDCl₃)



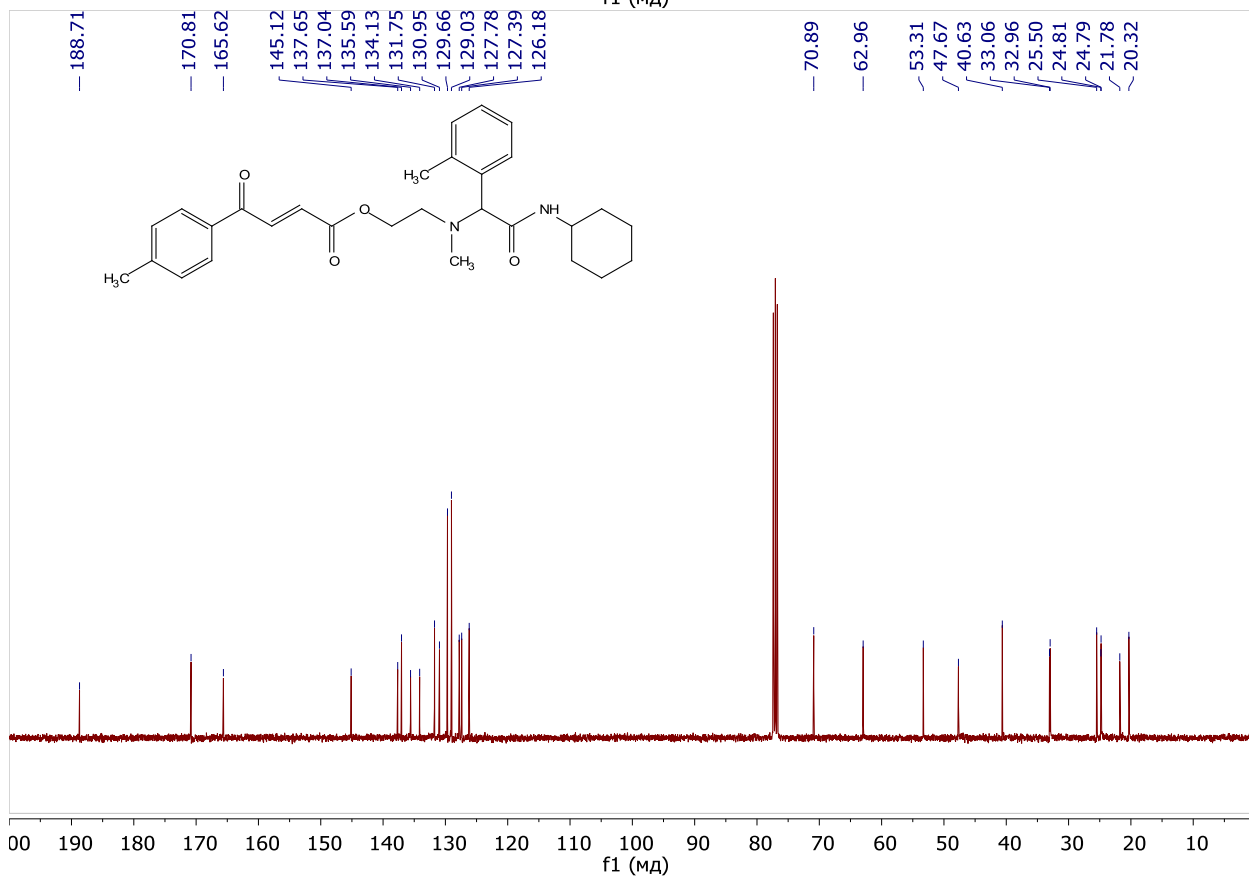
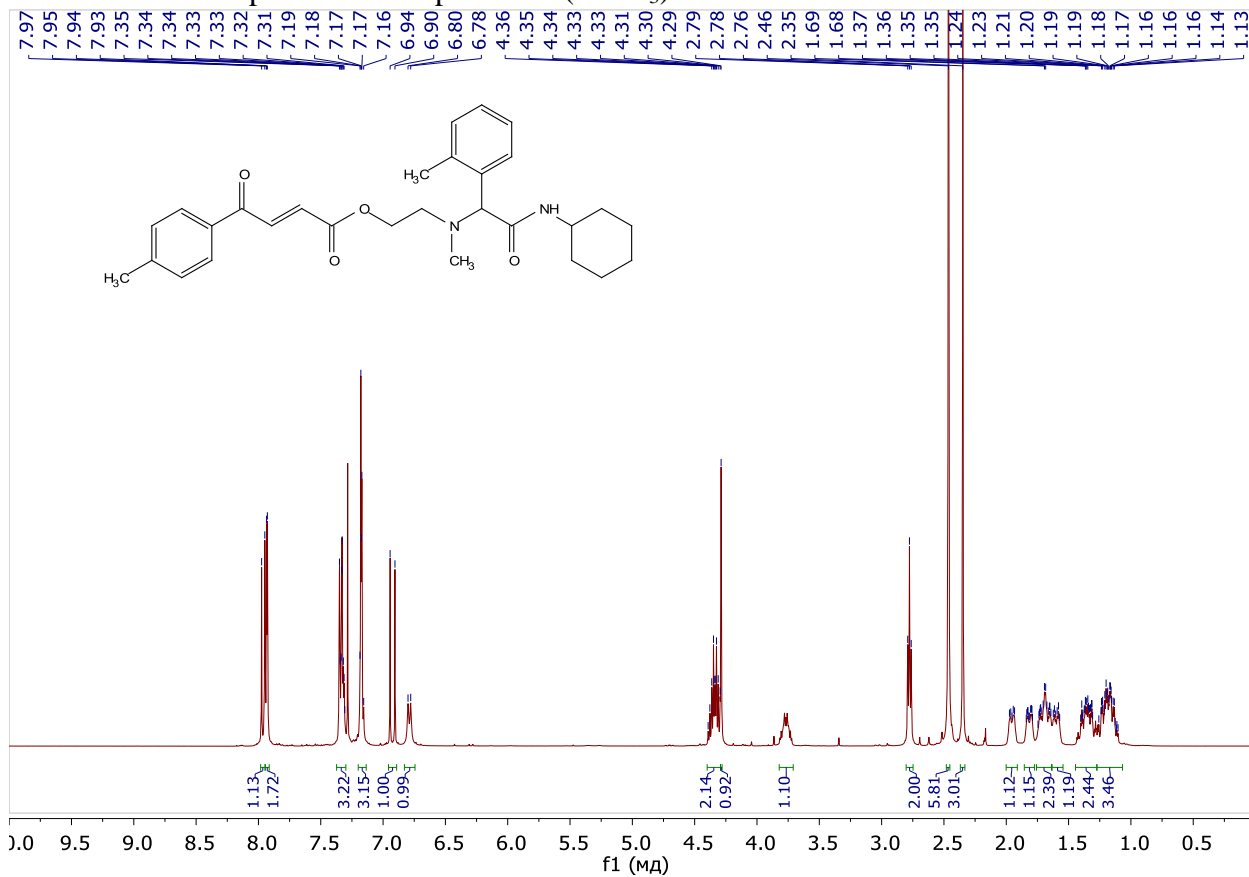
¹H and ¹³C NMR spectra for compound **31** (CDCl₃)



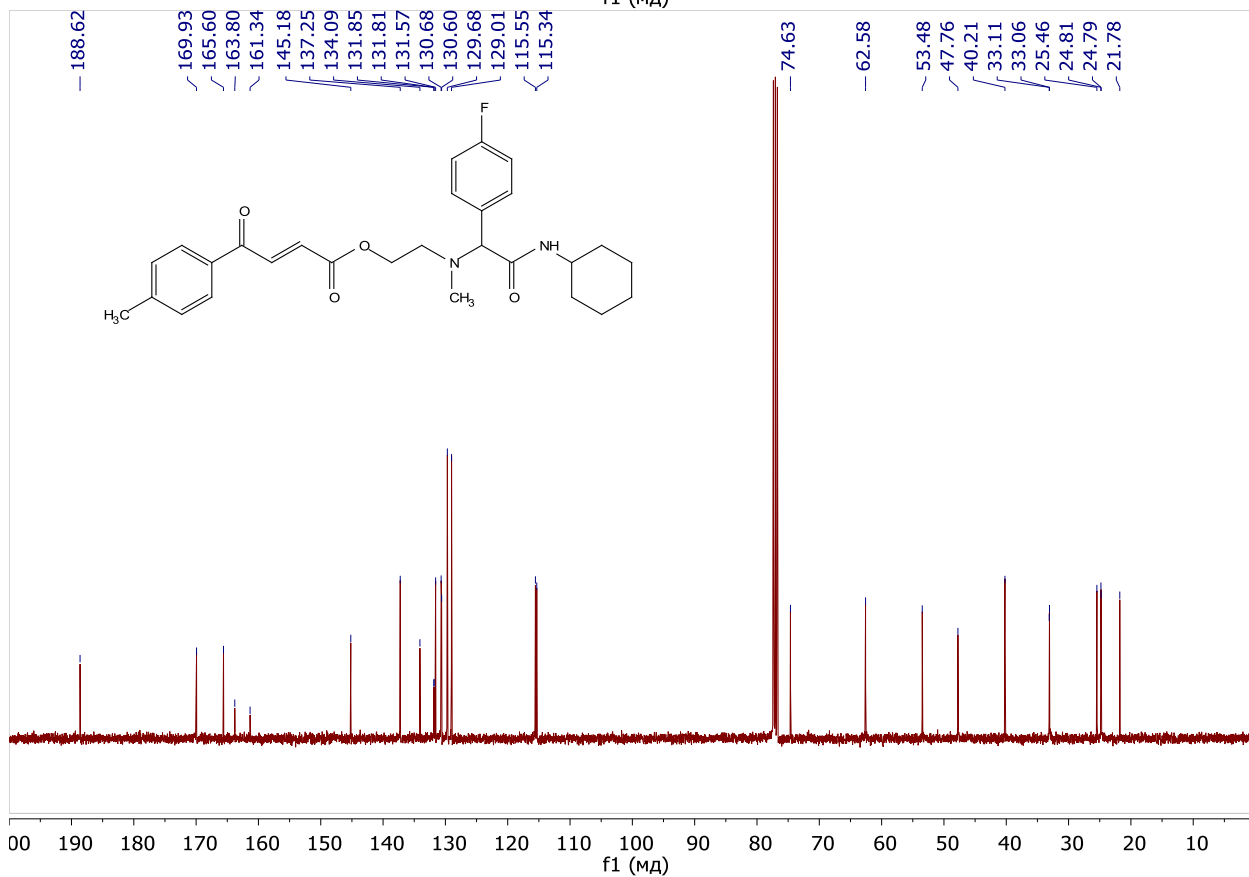
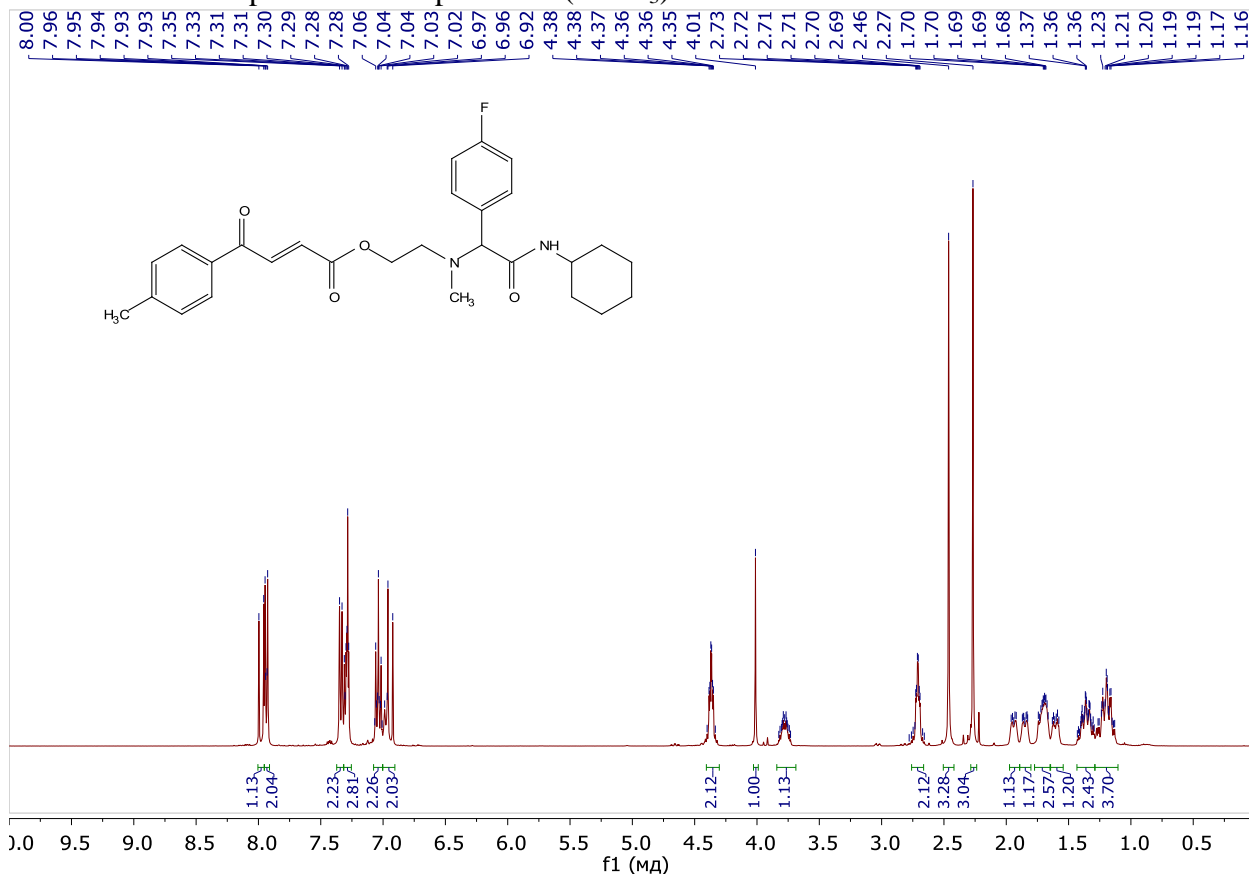
¹H and ¹³C NMR spectra for compound **32** (CDCl₃)



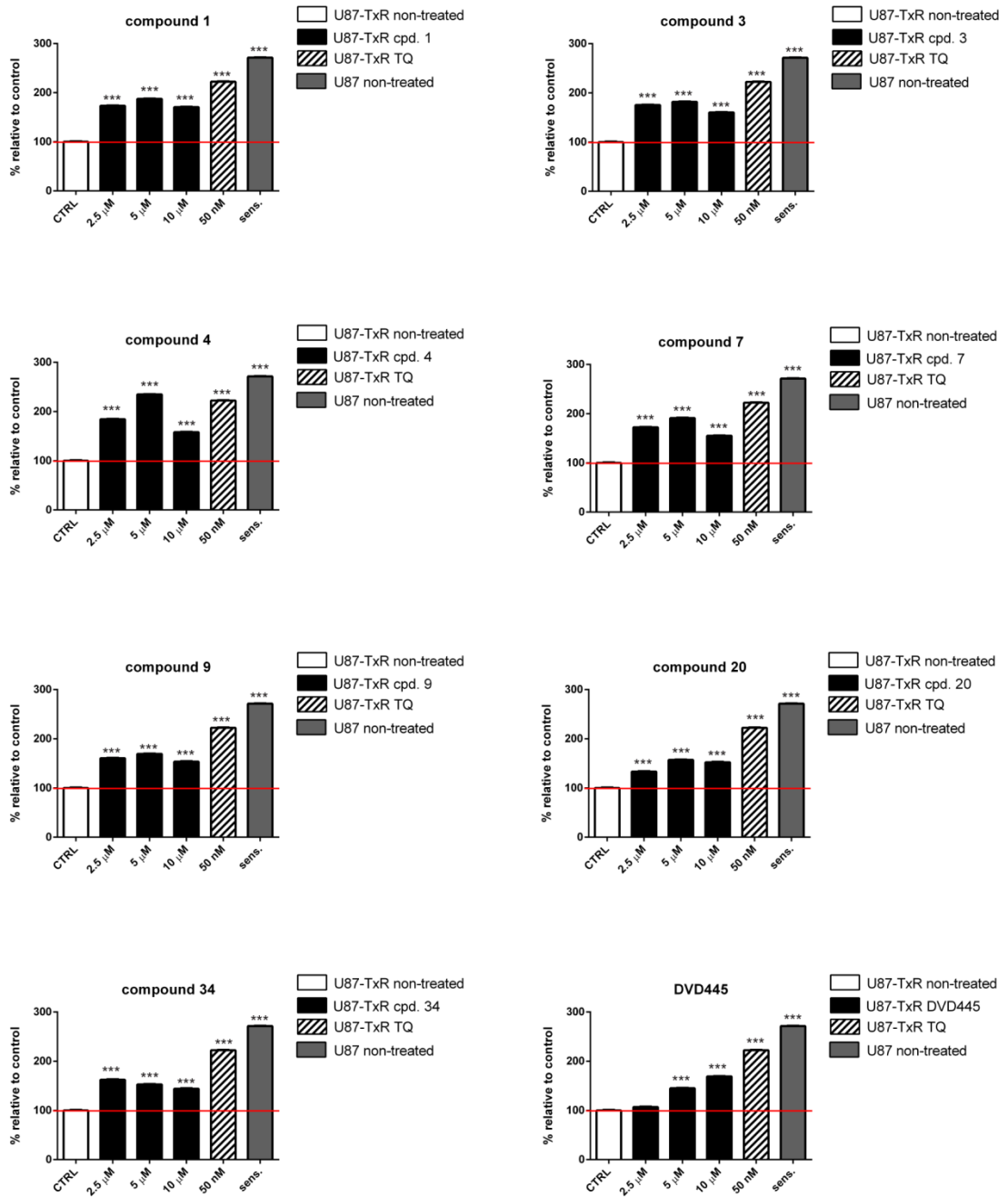
¹H and ¹³C NMR spectra for compound **33** (CDCl₃)



¹H and ¹³C NMR spectra for compound **34** (CDCl₃)



Effect of variable concentrations of UMAs on Rho123 uptake after 30 min treatment



Rho123 accumulation after treatment with DVD-445 and its seven UMA derivatives. U87-TxR cells were exposed to compounds **1, 3, 4, 7, 9, 20, 34** and DVD-445 (2.5, 5 and 10 μM) or TQ (50 nM) and incubated with Rho123 for 30 min. Sensitive U87 cell were used as a positive control for the Rho123 accumulation. Statistical significance was determined by Two-way ANOVA using Dunnett's multiple comparisons test. Significant difference compared to control (untreated U87-TxR cells) is expressed as *** (p<0.001).