

Supporting information

Synthesis and biological evaluation of dehydroabietic acid-pyrimidine hybrids as antitumor agents

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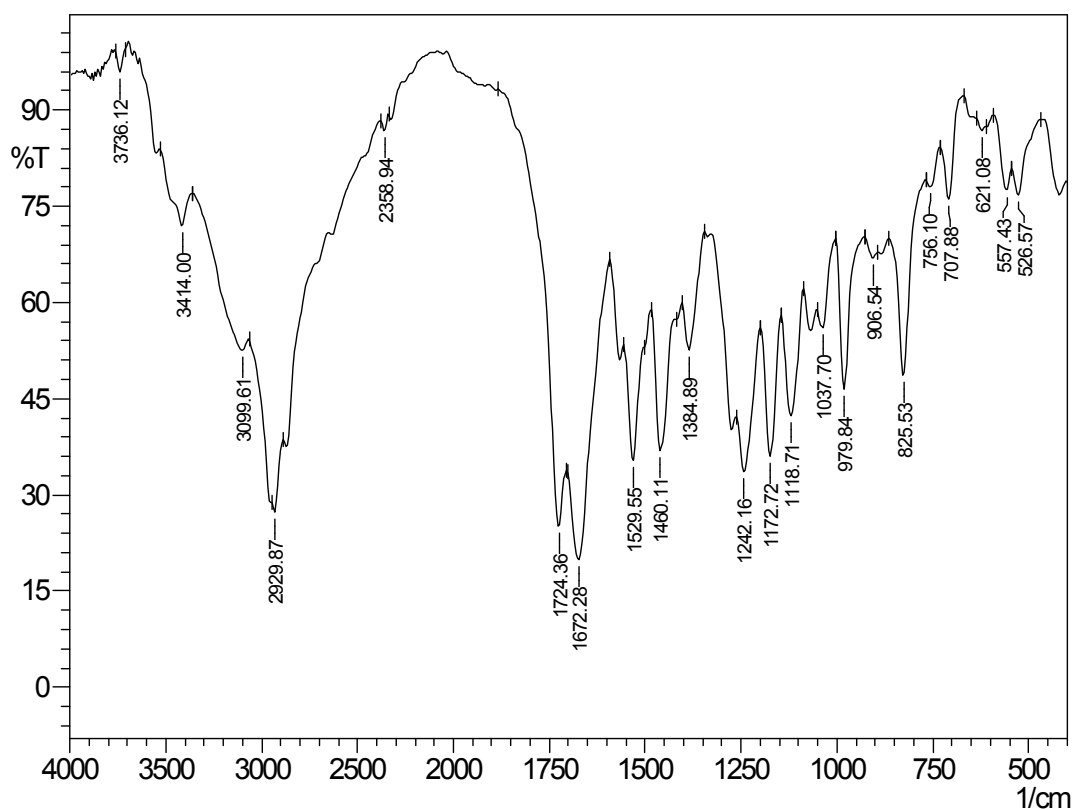


Figure S1. FTIR spectrum of the target compound (3a)

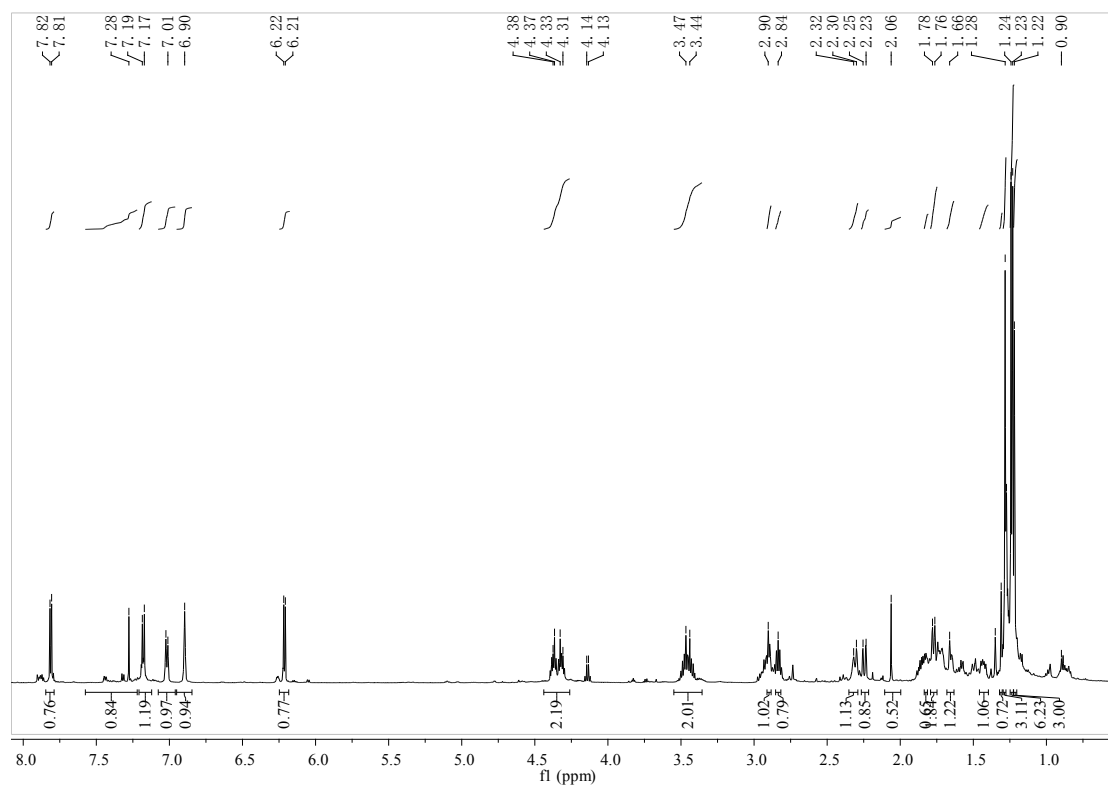


Figure S2. ^1H -NMR spectrum of the target compound (**3a**) in CDCl_3

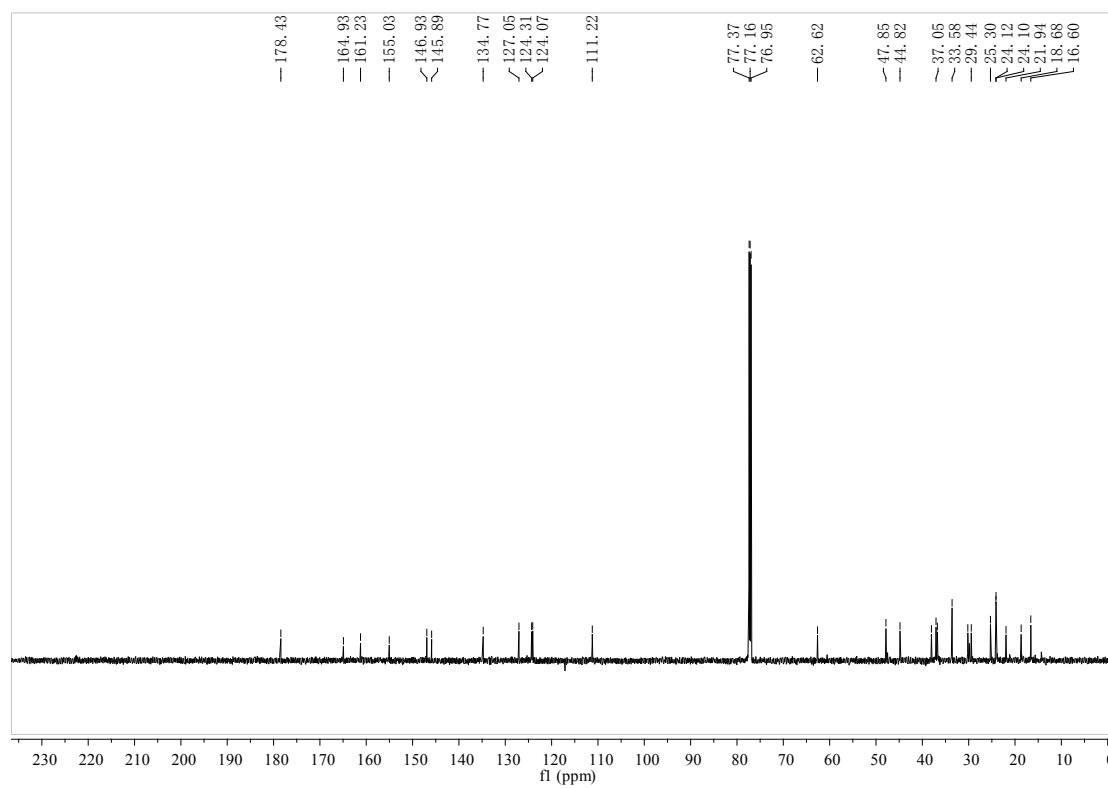


Figure S3. ^{13}C -NMR spectrum of the target compound (**3a**) in CDCl_3

Sample Name	LFY01	Position	P1-A1	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY01.d
ACQ Method	yljing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 3:06:01 PM

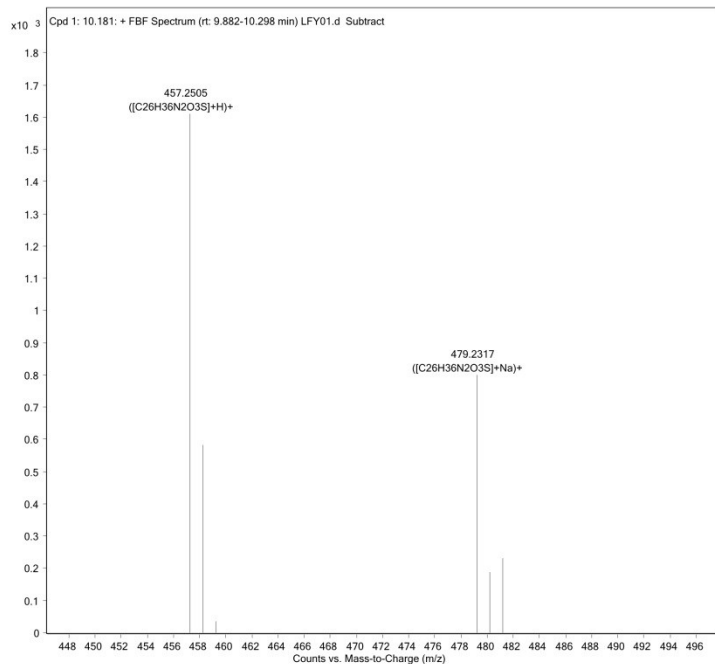


Figure S4. HR-MS spectrum of the target compound (**3a**)

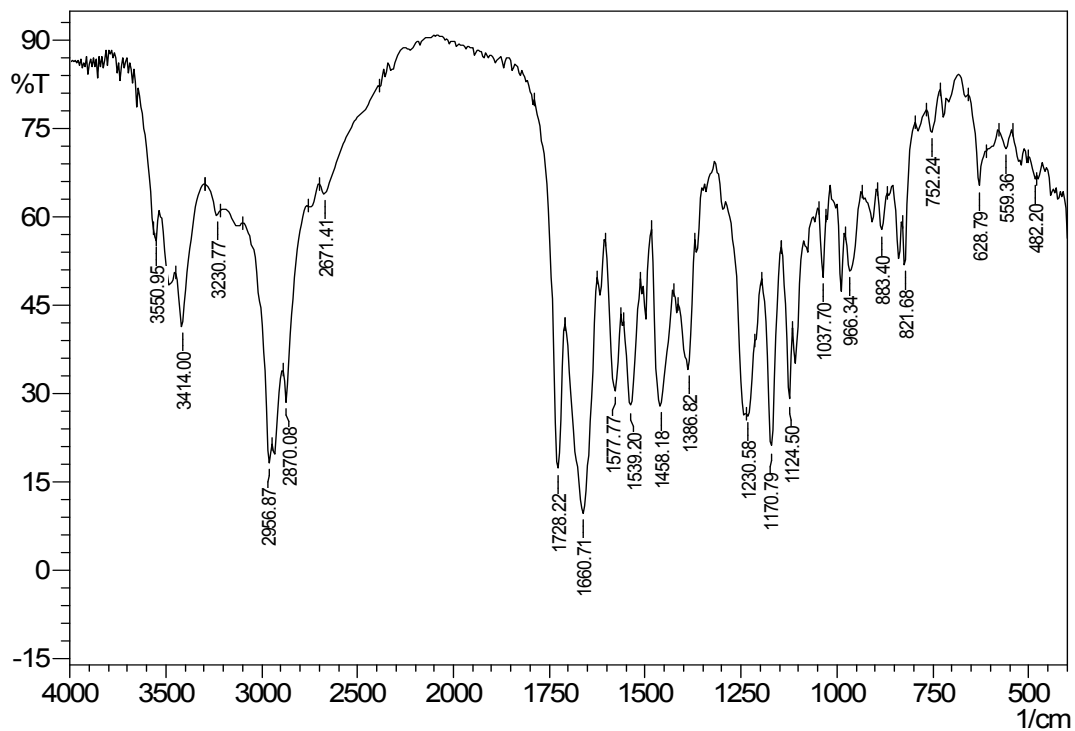


Figure S5. FTIR spectrum of the target compound (**3b**)

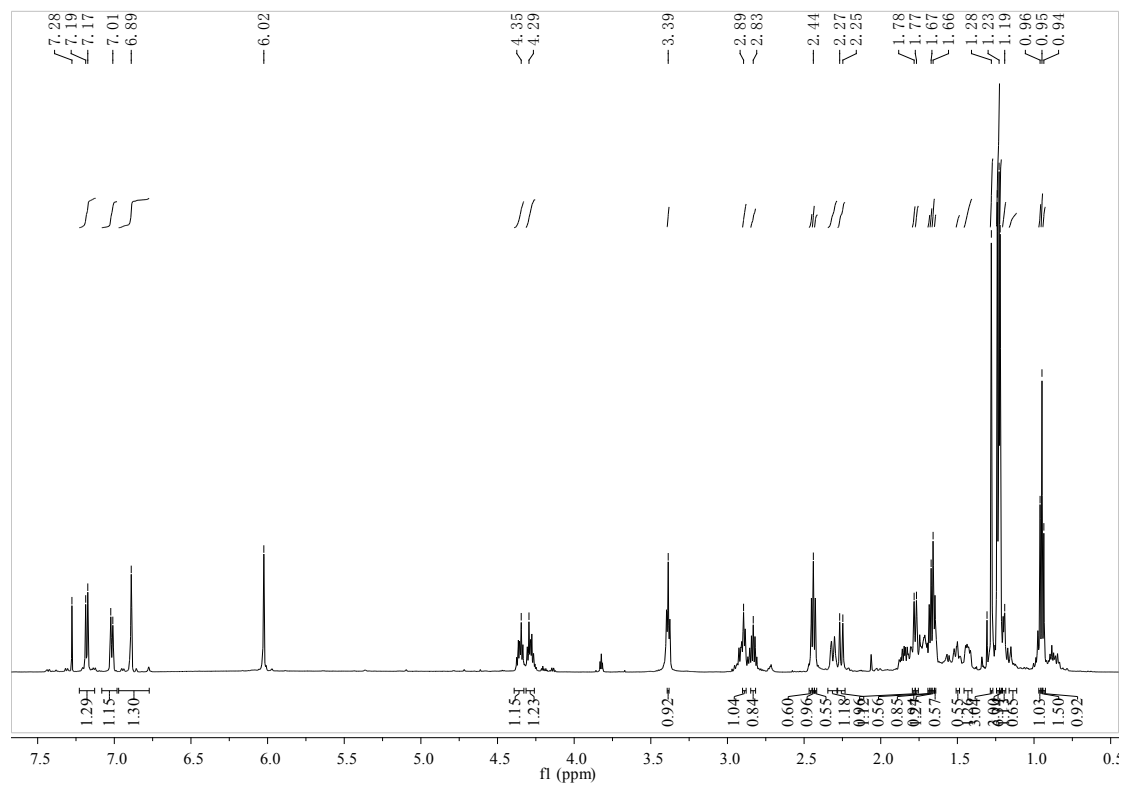


Figure S6. ^1H -NMR spectrum of the target compound (**3b**) in CDCl_3

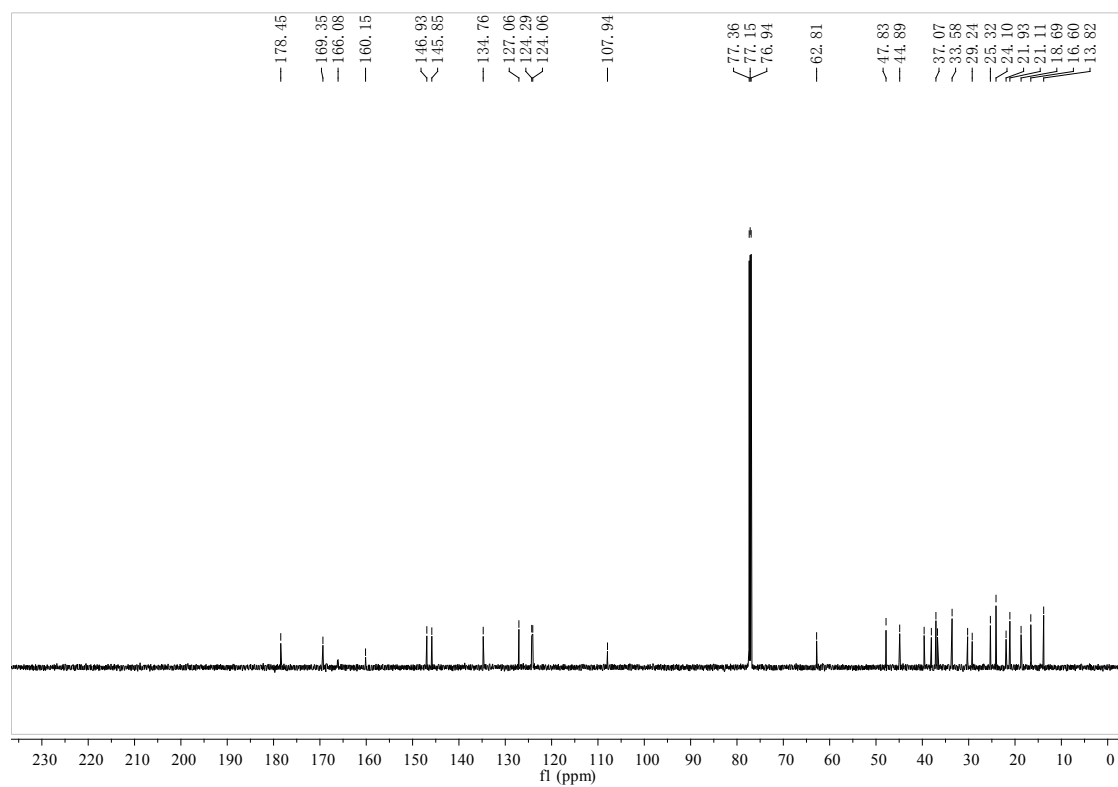


Figure S7. ^{13}C -NMR spectrum of the target compound (**3b**) in CDCl_3

Sample Name	LFY02	Position	P1-A2	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY02.d
ACQ Method	yijing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 3:20:44 PM

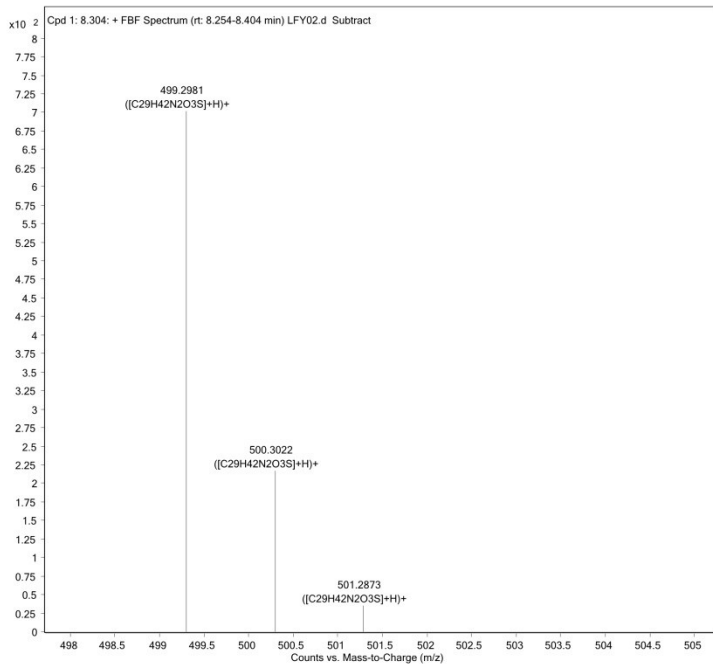


Figure S8. HR-MS spectrum of the target compound (**3b**)

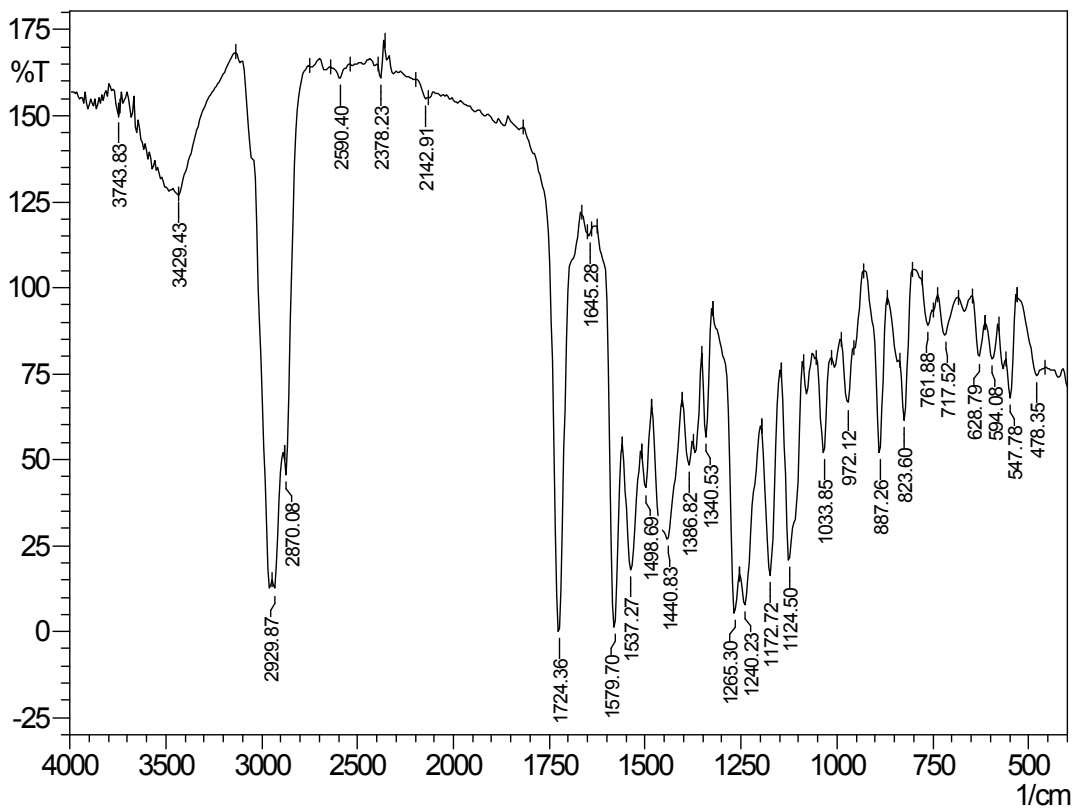


Figure S9. FTIR spectrum of the target compound (**3c**)

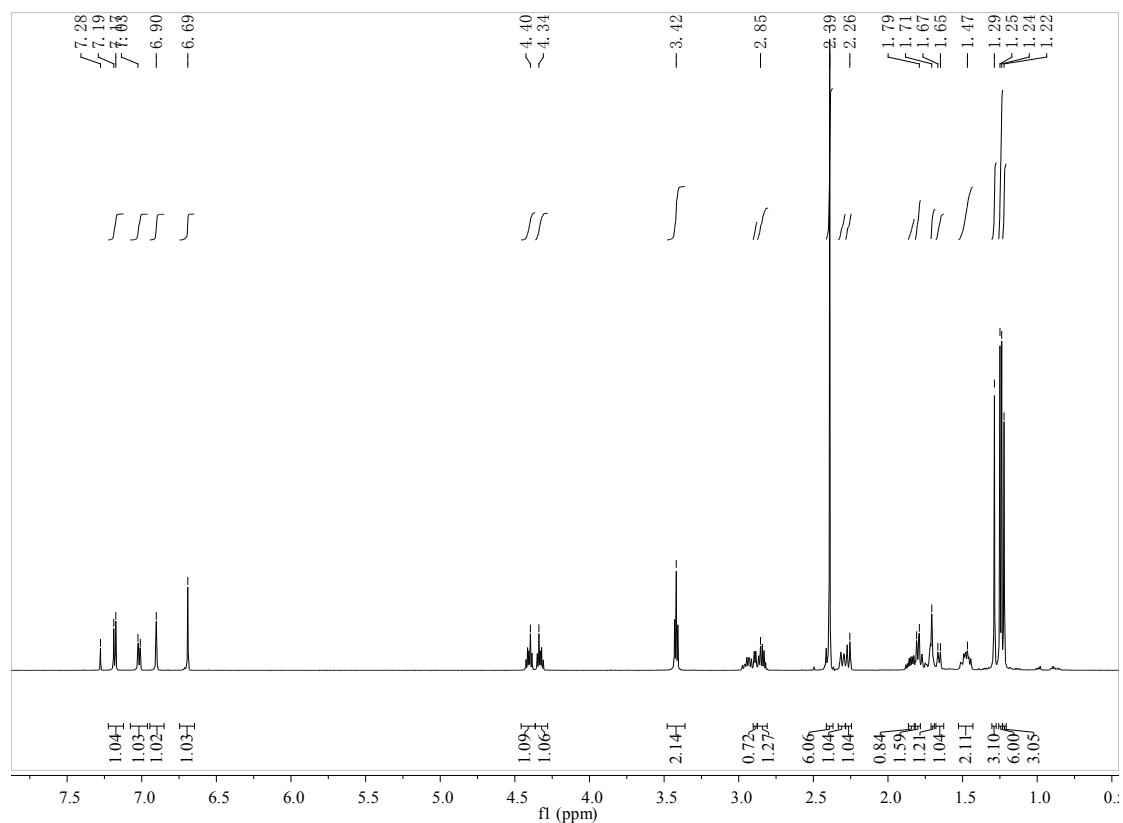


Figure S11. $^{13}\text{C-NMR}$ spectrum of the target compound (**3c**) in CDCl_3

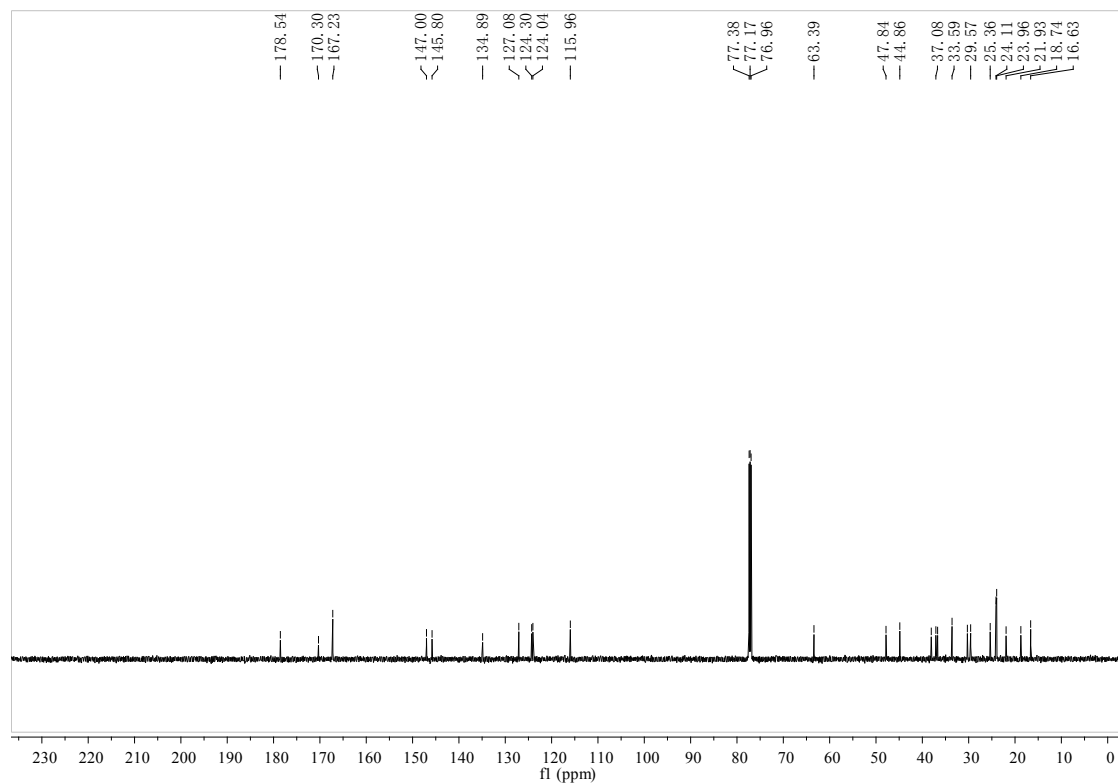


Figure S11. $^{13}\text{C-NMR}$ spectrum of the target compound (**3c**) in CDCl_3

Sample Name	LFY04	Position	P1-A4	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY04.d
ACQ Method	yijing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 3:50:11 PM (UTC+08:00)

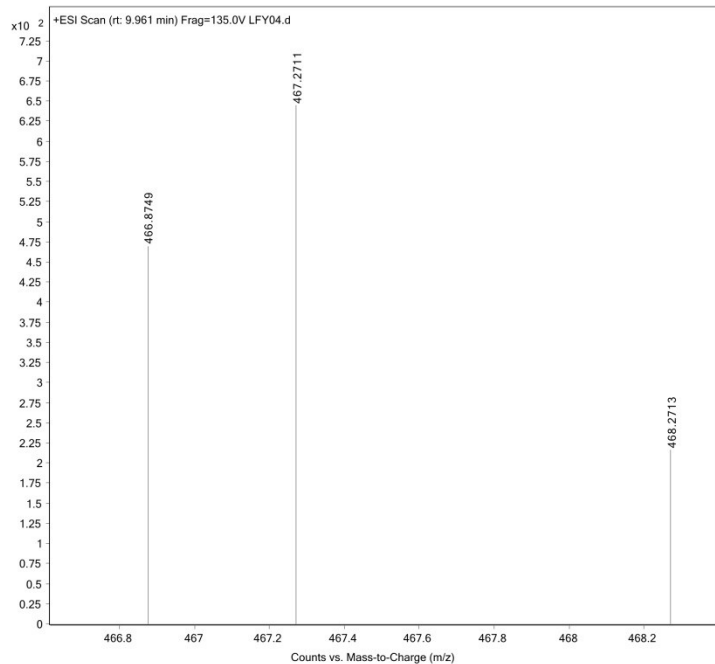


Figure S12. HR-MS spectrum of the target compound (3c)

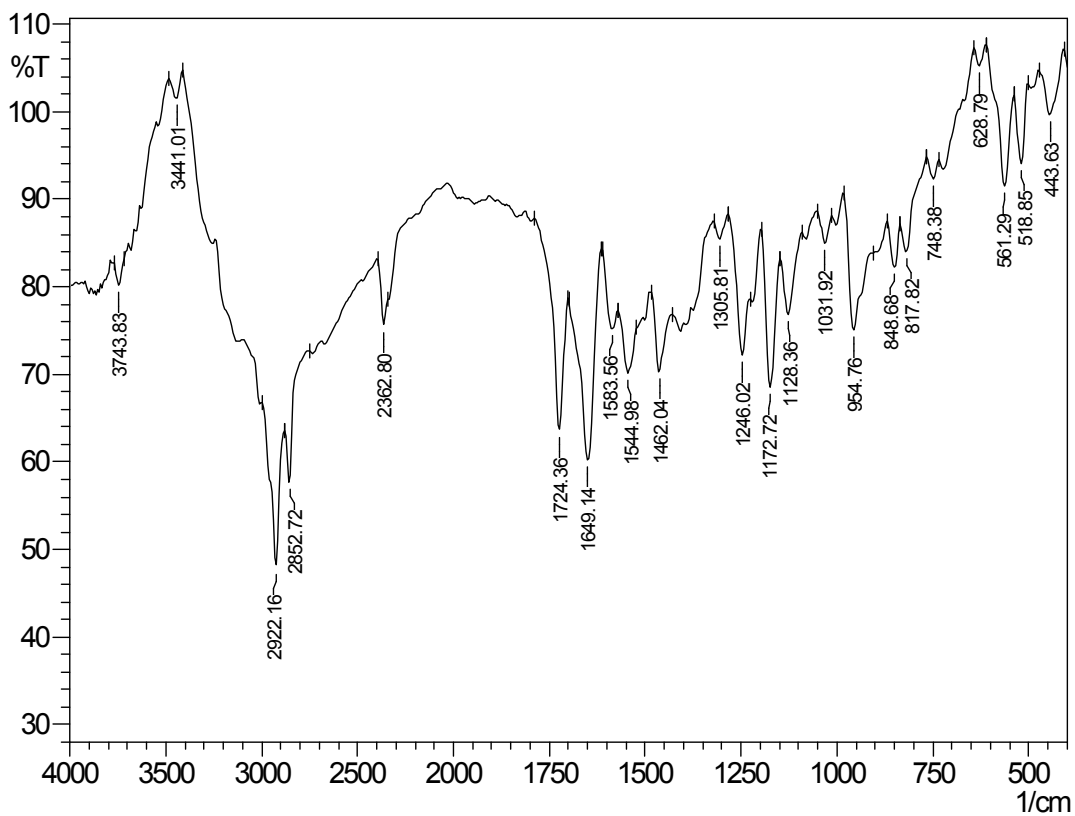


Figure S13. FTIR spectrum of the target compound (3d)

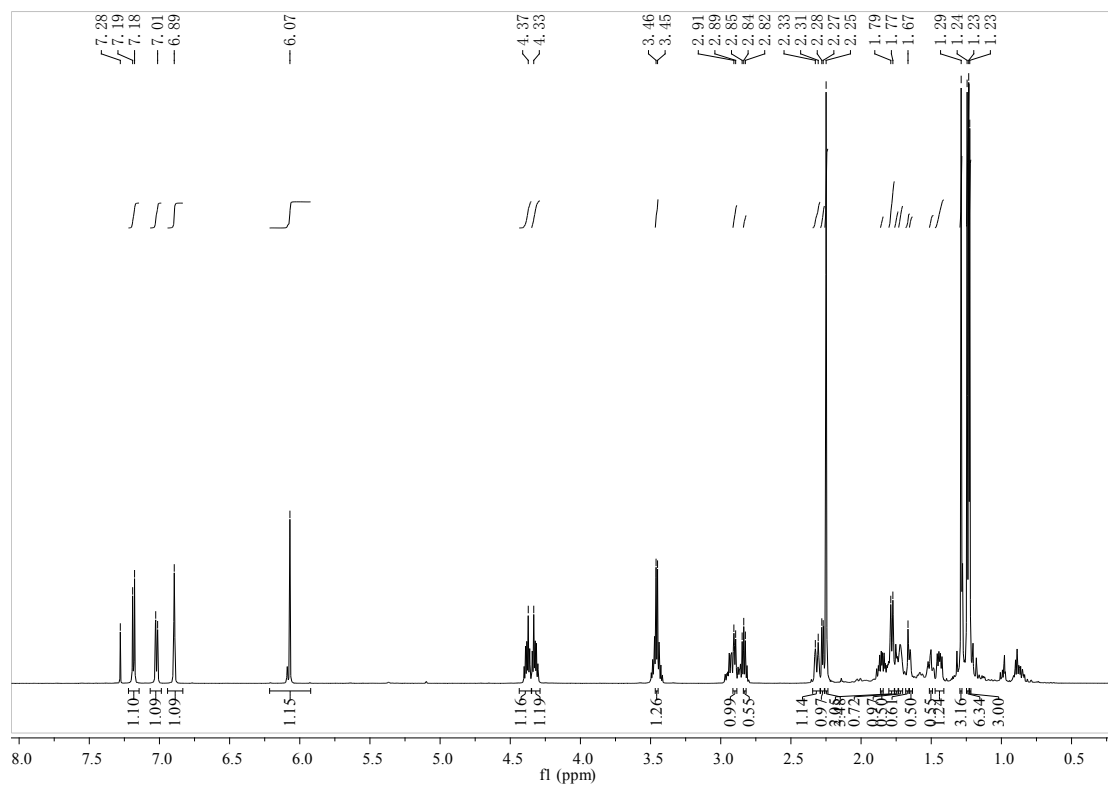


Figure S14. ¹H-NMR spectrum of the target compound (3d) in CDCl₃

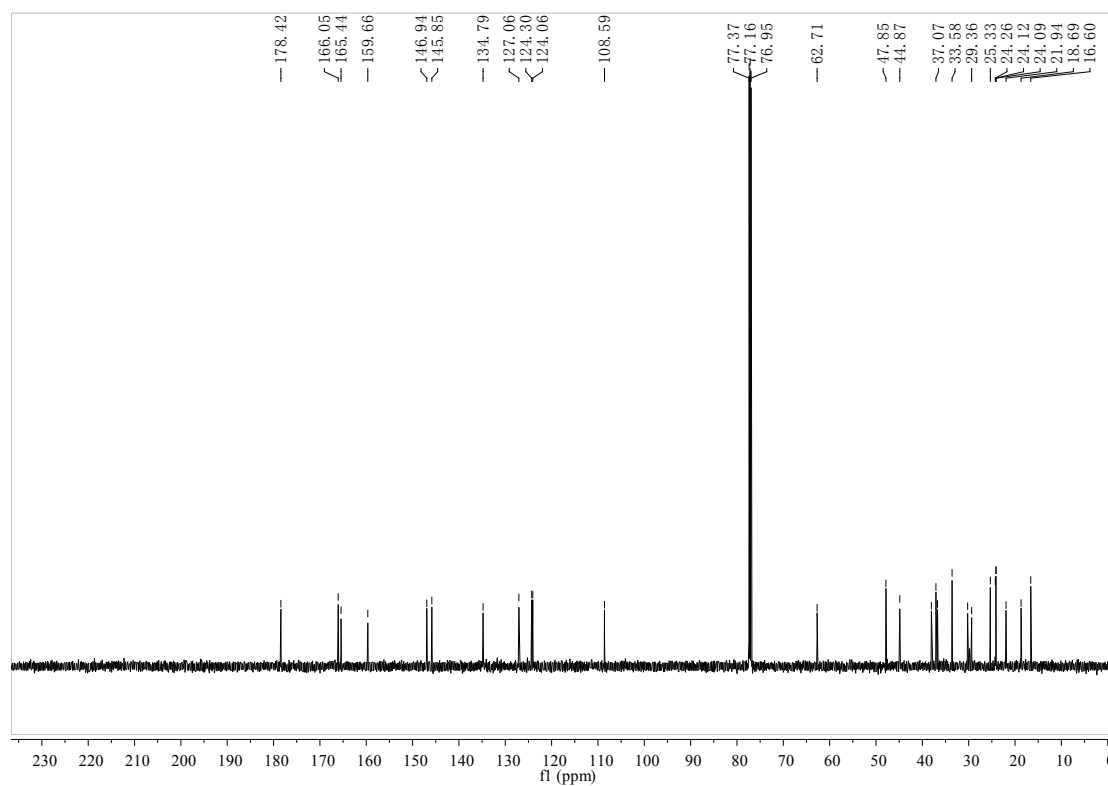


Figure S15. ¹³C-NMR spectrum of the target compound (3d) in CDCl₃

Sample Name	LFY03	Position	P1-A3	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY03.d
ACQ Method	yijing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 3:35:26 PM (UTC+08:00)

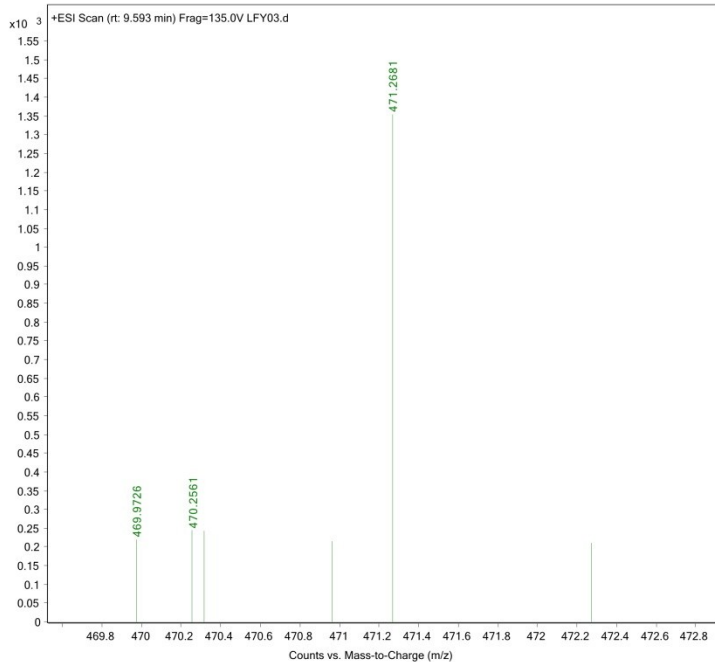


Figure S16. HR-MS spectrum of the target compound (**3d**)

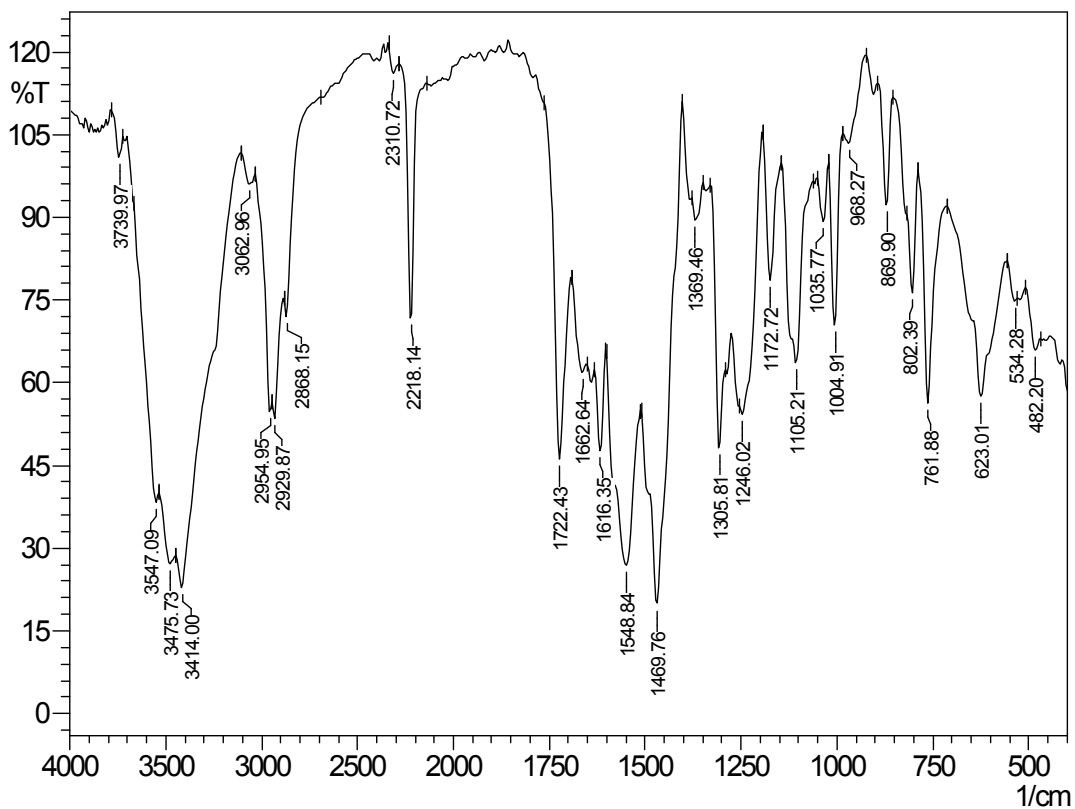


Figure S17. FTIR spectrum of the target compound (**3e**)

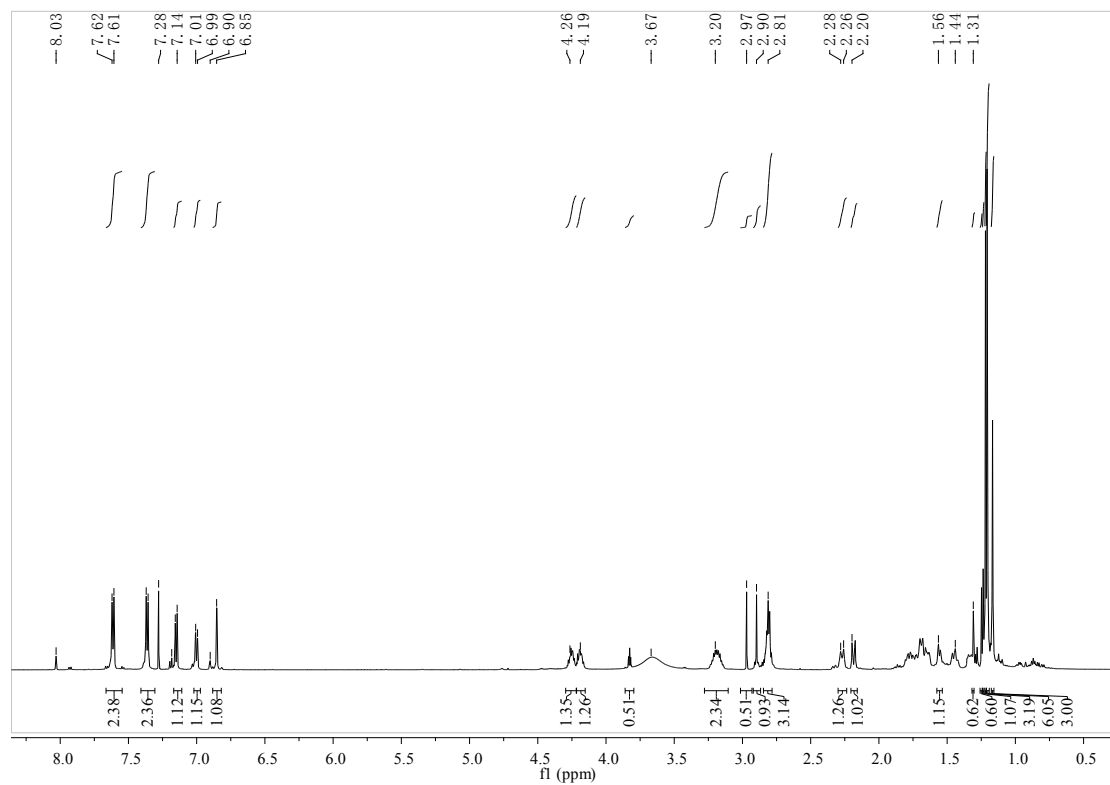


Figure S18. ^1H -NMR spectrum of the target compound (**3e**) in CDCl_3

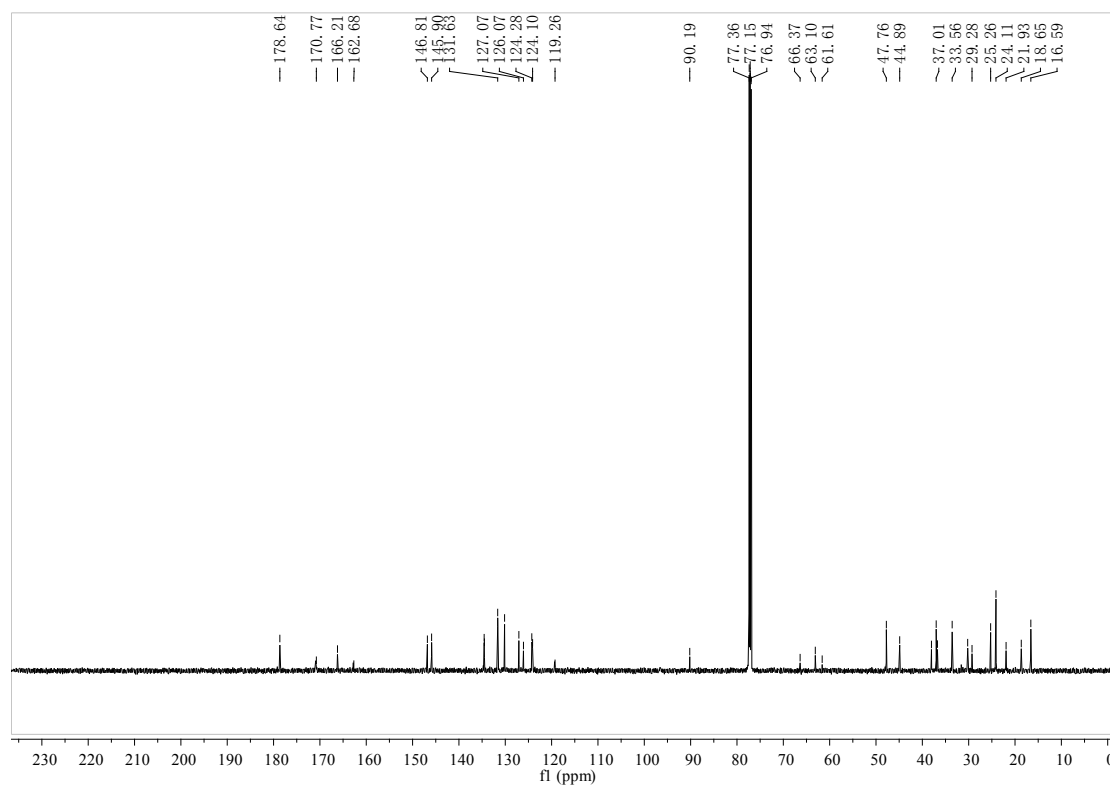


Figure S19. ^{13}C -NMR spectrum of the target compound (**3e**) in CDCl_3

Sample Name	LFY05	Position	P1-A5	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY05.d
ACQ Method	yijing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 4:04:52 PM

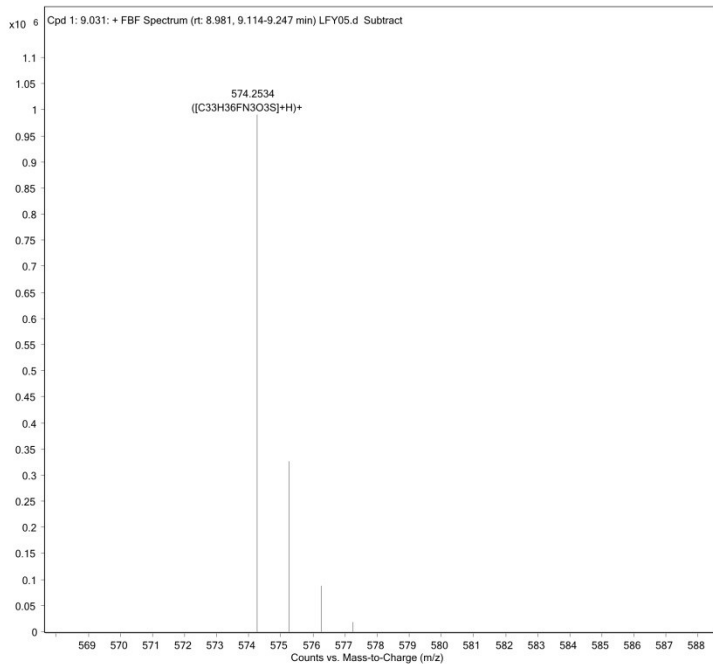


Figure S20.HR-MS spectrum of the target compound (**3e**)

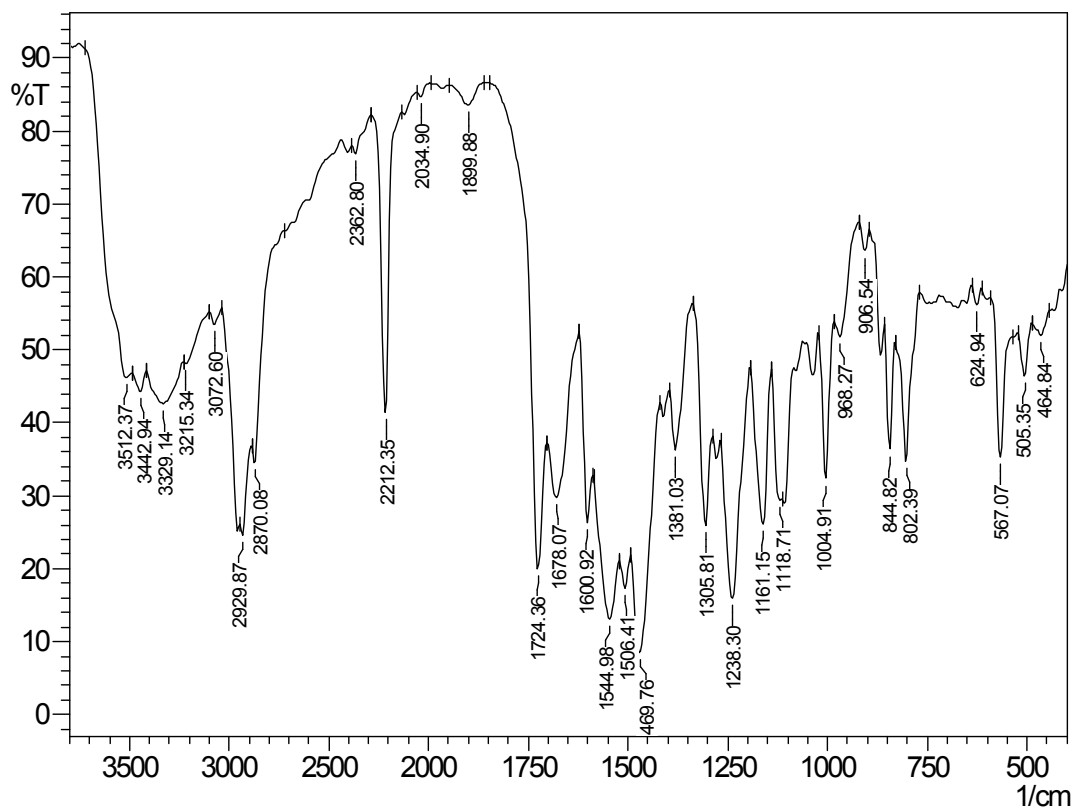


Figure S21. FTIR spectrum of the target compound (**3f**)

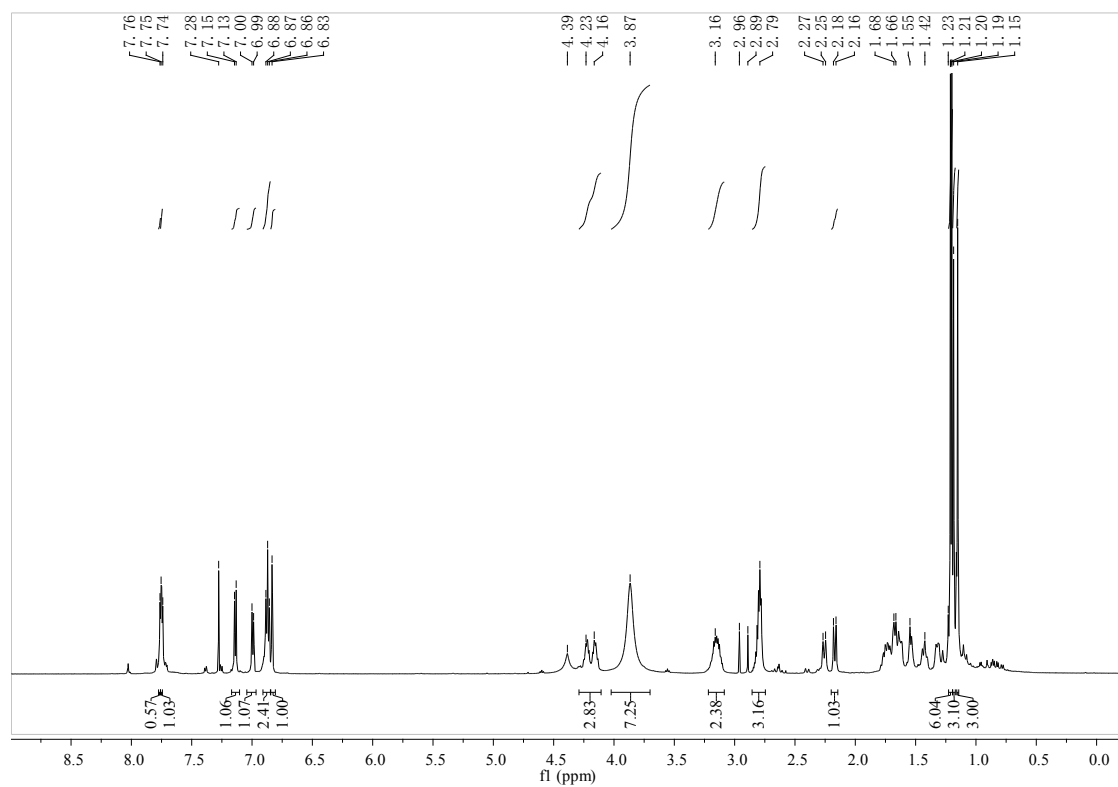


Figure S22. $^1\text{H-NMR}$ spectrum of the target compound (**3f**) in CDCl_3

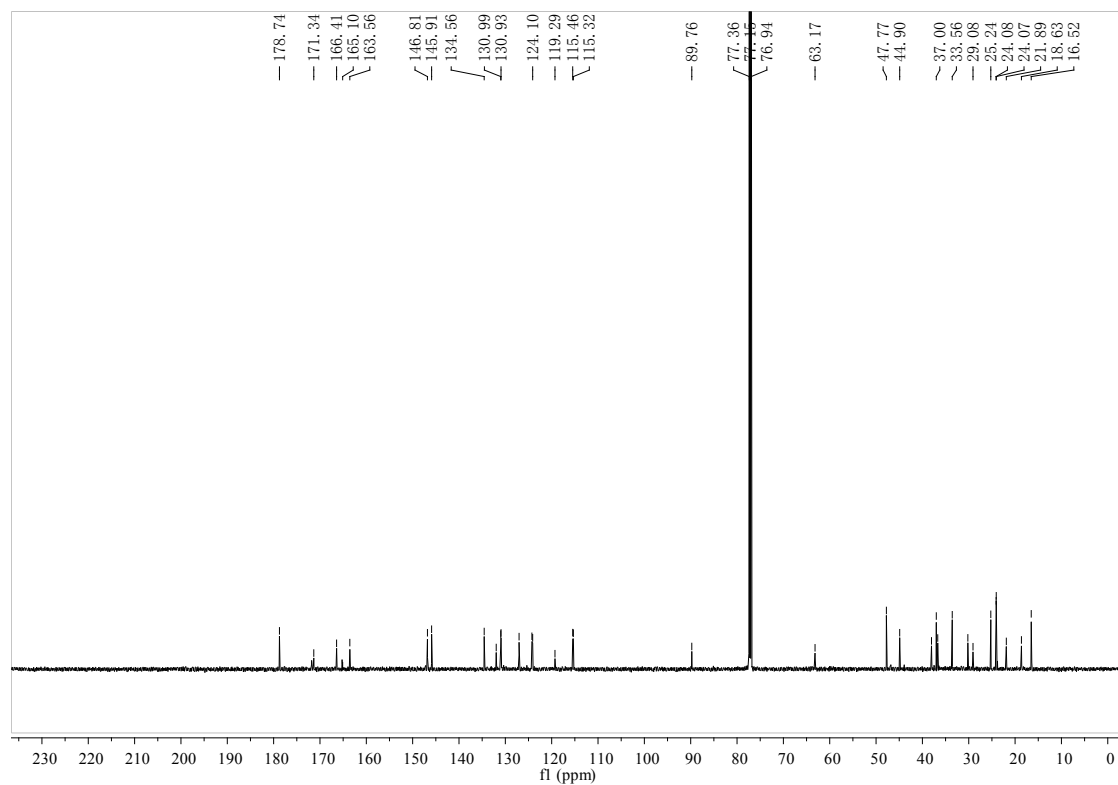


Figure S23. $^{13}\text{C-NMR}$ spectrum of the target compound (**3f**) in CDCl_3

Sample Name	LFY06	Position	P1-A6	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY06.d
ACQ Method	yijing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 4:19:37 PM

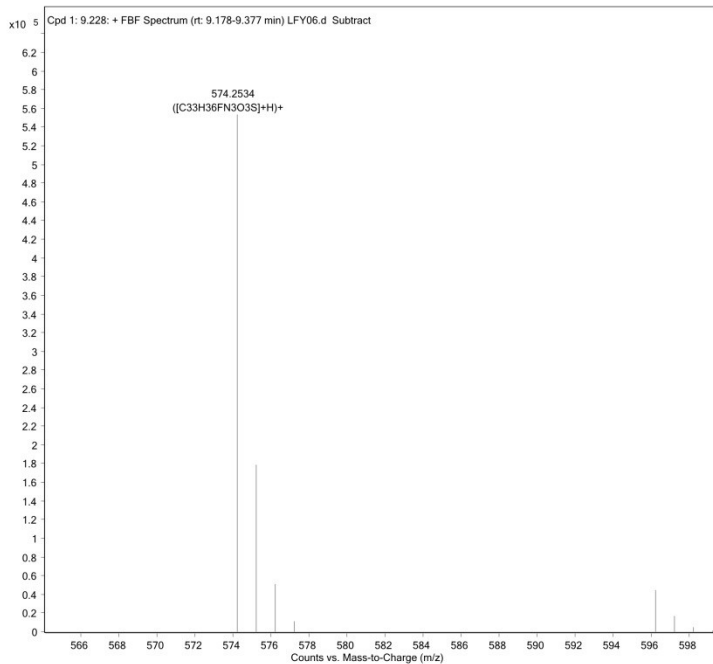


Figure S24. HR-MS spectrum of the target compound (3f)

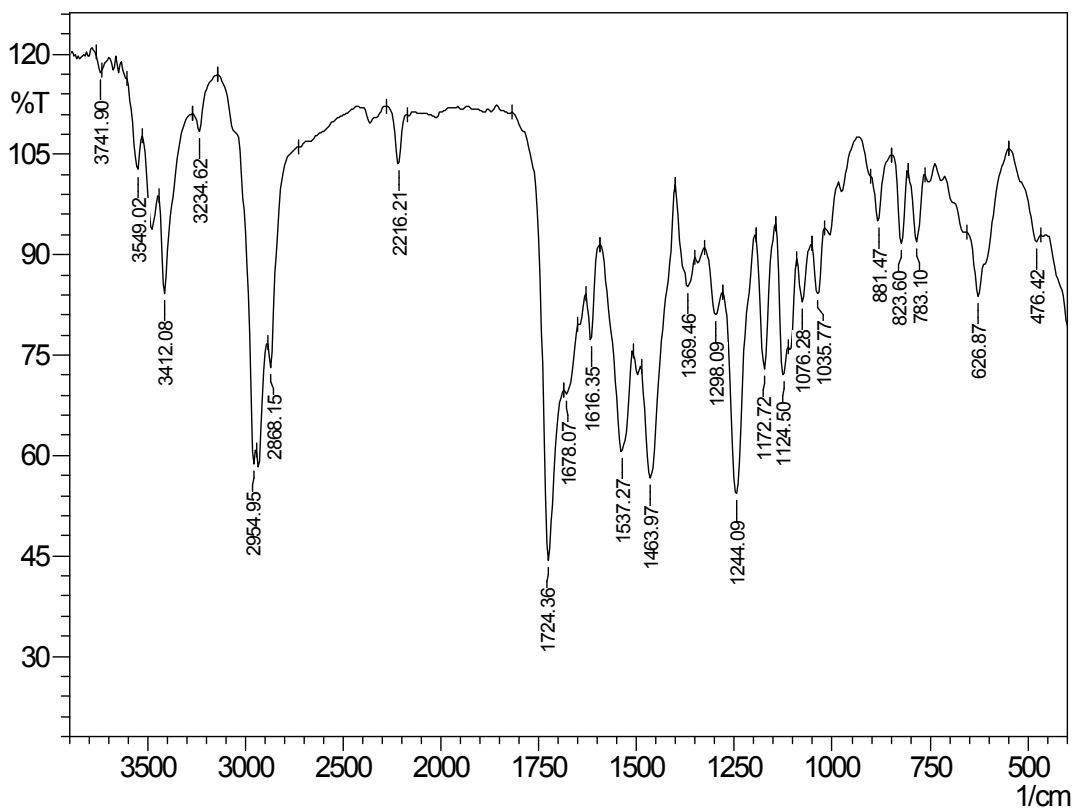


Figure S25. FTIR spectrum of the target compound (3g)

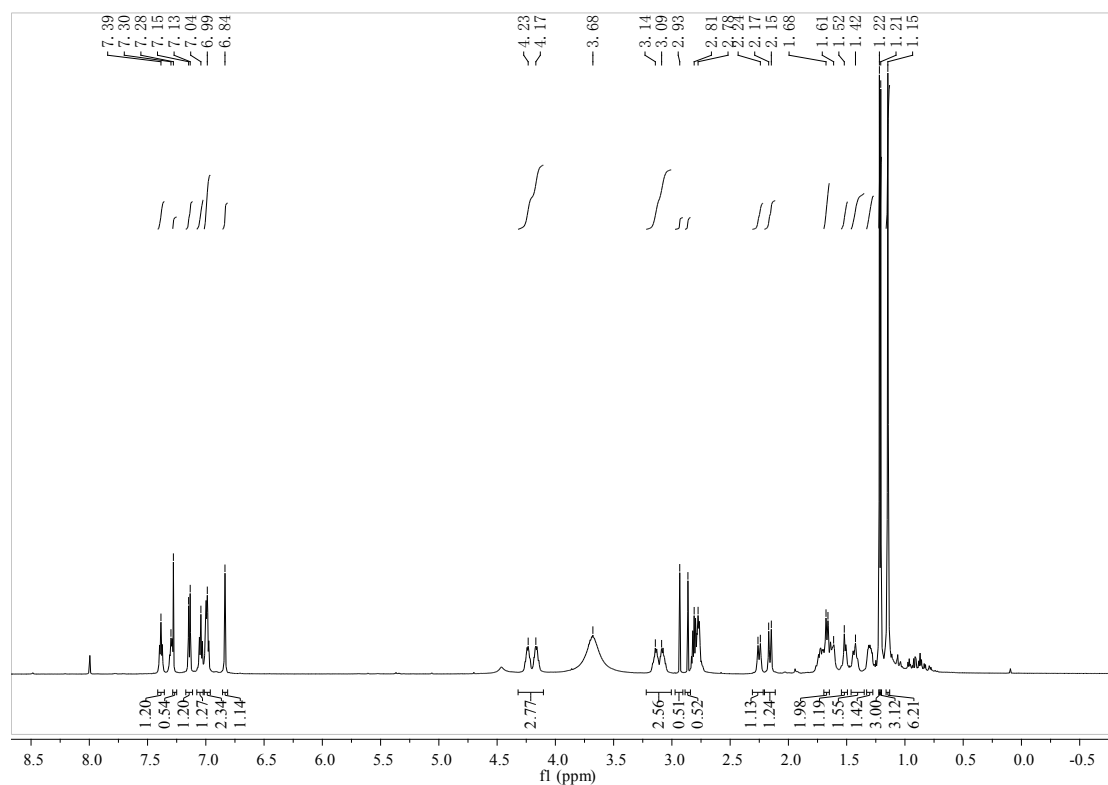


Figure S26. $^1\text{H-NMR}$ spectrum of the target compound (**3g**) in CDCl_3

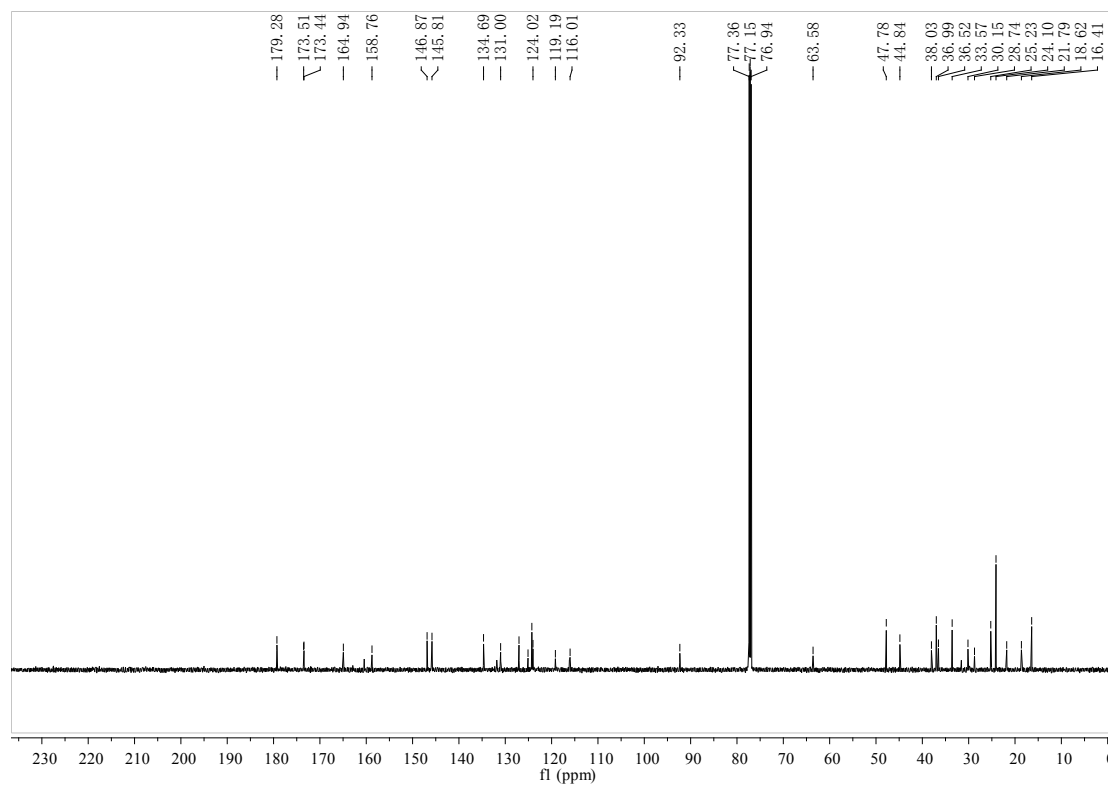


Figure S27. $^{13}\text{C-NMR}$ spectrum of the target compound (**3g**) in CDCl_3

Sample Name	LFY07	Position	P1-A7	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY07.d
ACQ Method	yijing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 4:34:19 PM

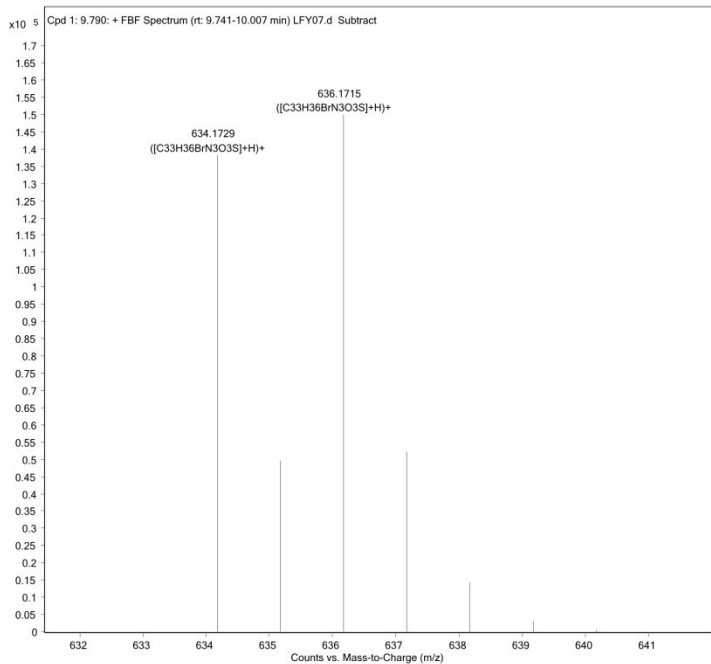


Figure S28. HR-MS spectrum of the target compound (**3g**)

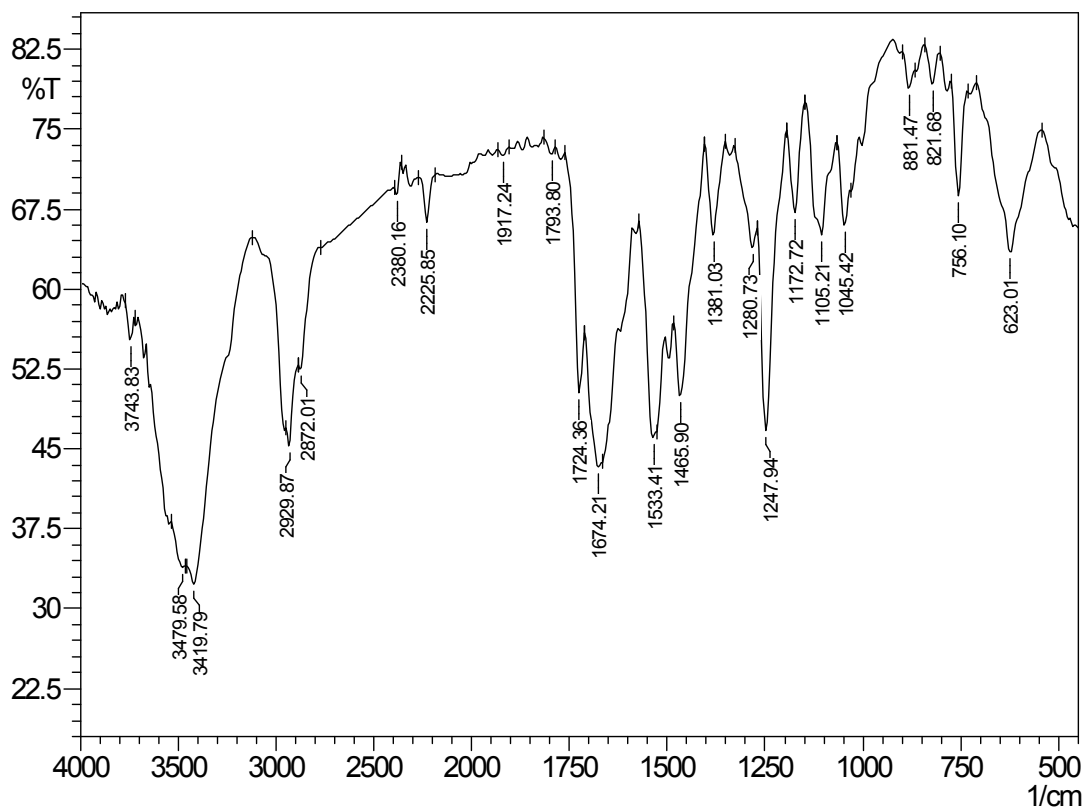


Figure S29. FTIR spectrum of the target compound (**3h**)

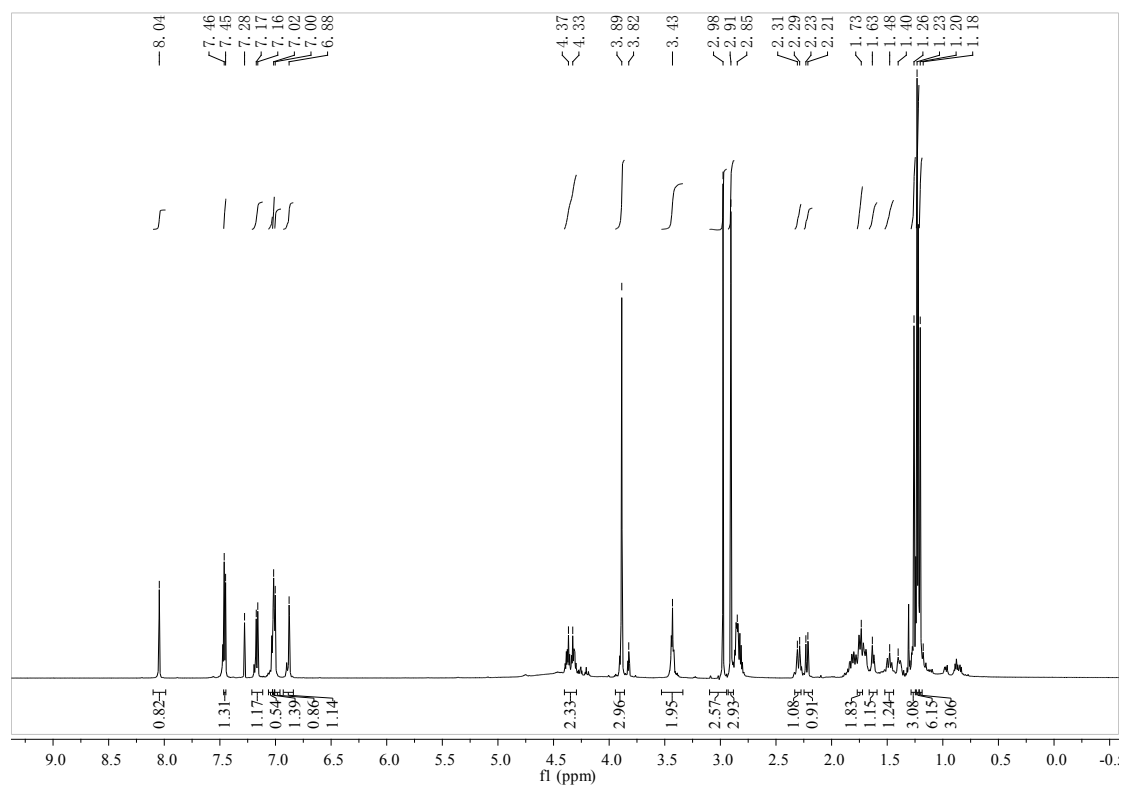


Figure S30. $^1\text{H-NMR}$ spectrum of the target compound (**3h**) in CDCl_3

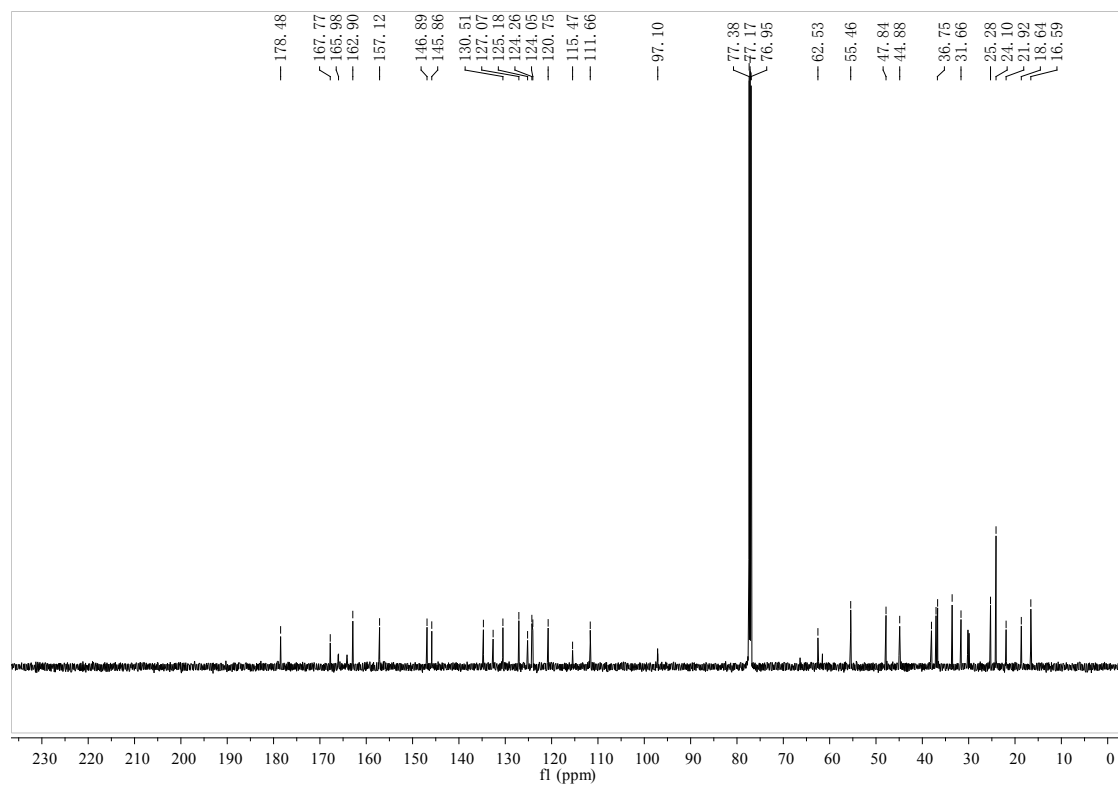


Figure S31. $^{13}\text{C-NMR}$ spectrum of the target compound (**3h**) in CDCl_3

Sample Name	LFY08	Position	P1-A8	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY08.d
ACQ Method	yijing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 4:49:04 PM

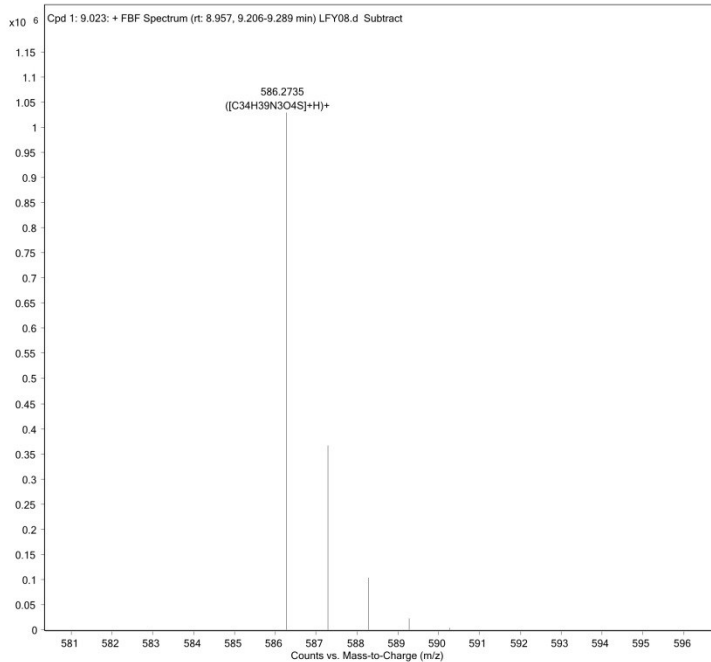


Figure S32. HR-MS spectrum of the target compound (**3h**)

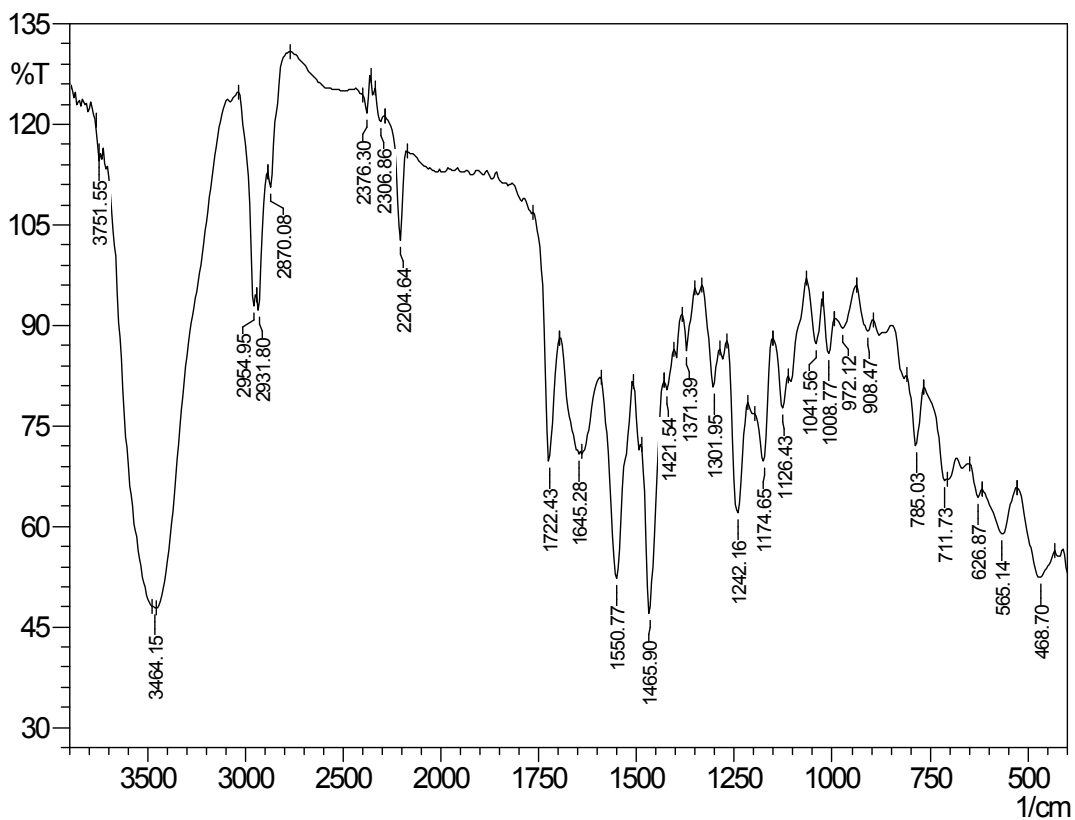


Figure S33. FTIR spectrum of the target compound (**3i**)

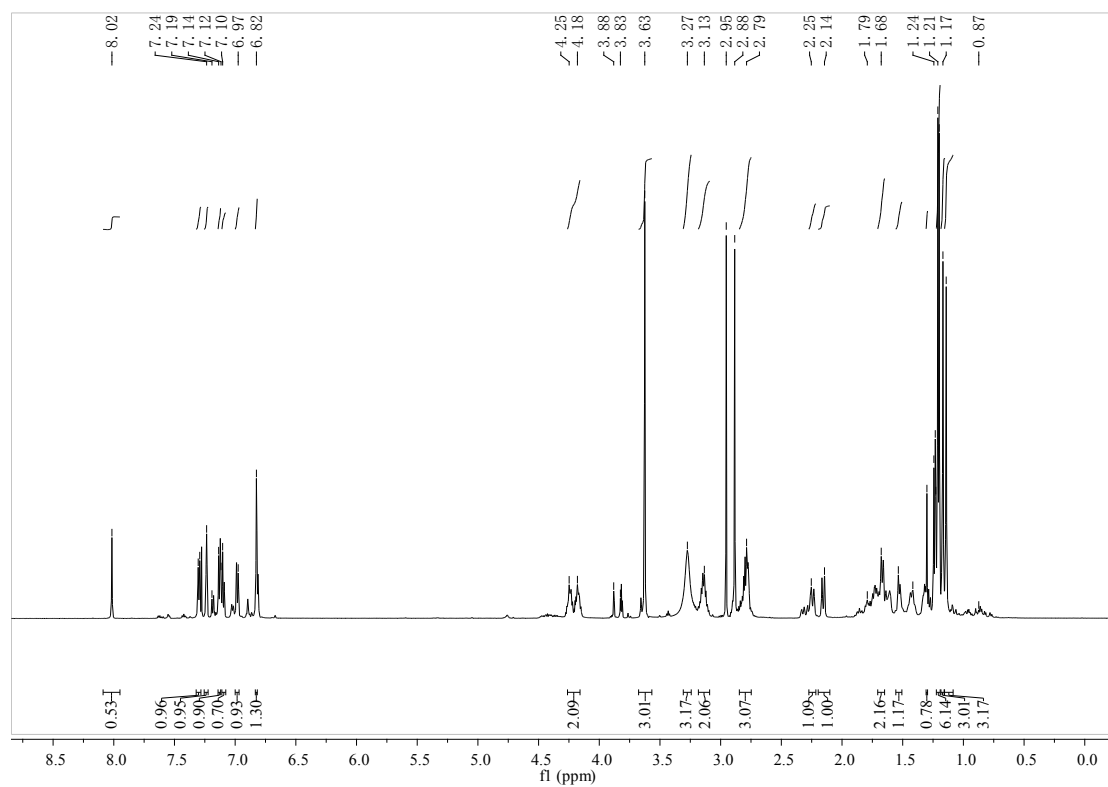


Figure S34. $^1\text{H-NMR}$ spectrum of the target compound (**3i**) in CDCl_3

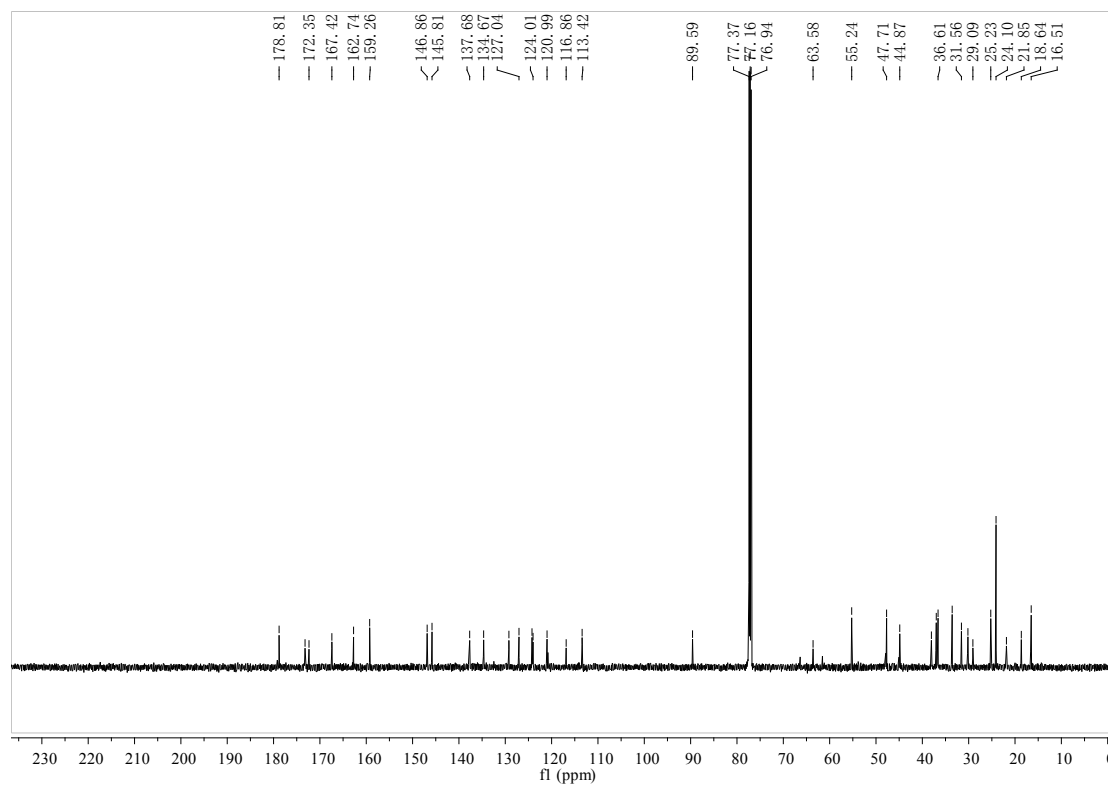


Figure S35. $^{13}\text{C-NMR}$ spectrum of the target compound (**3i**) in CDCl_3

Sample Name	LFY09	Position	P1-A9	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY09.d
ACQ Method	yijing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 5:03:46 PM

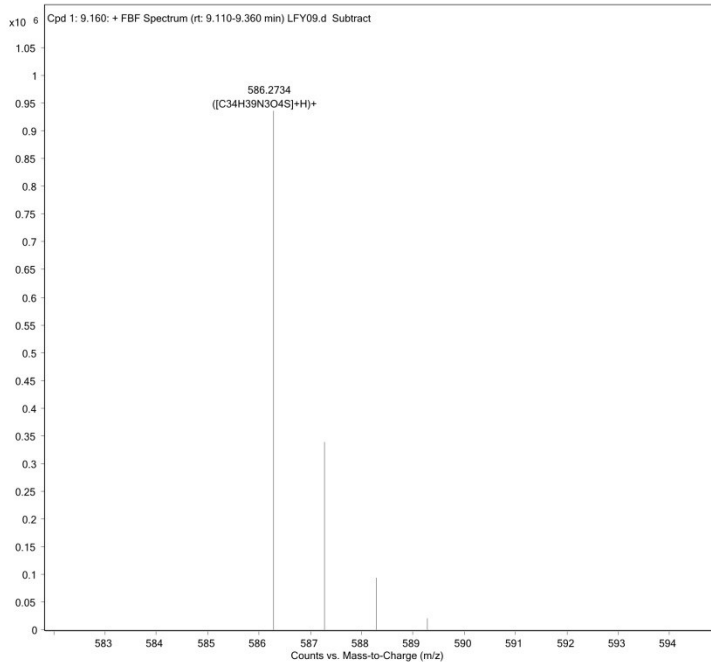


Figure S36. HR-MS spectrum of the target compound (**3i**)

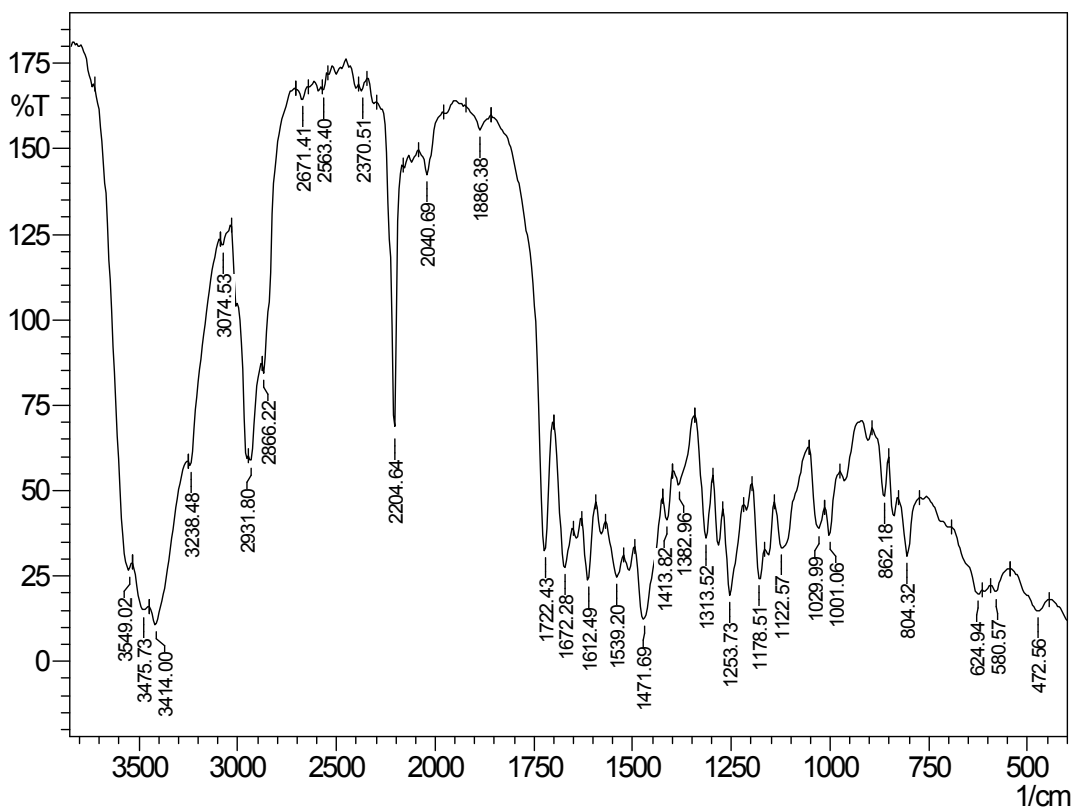


Figure S37. FTIR spectrum of the target compound (**3j**)

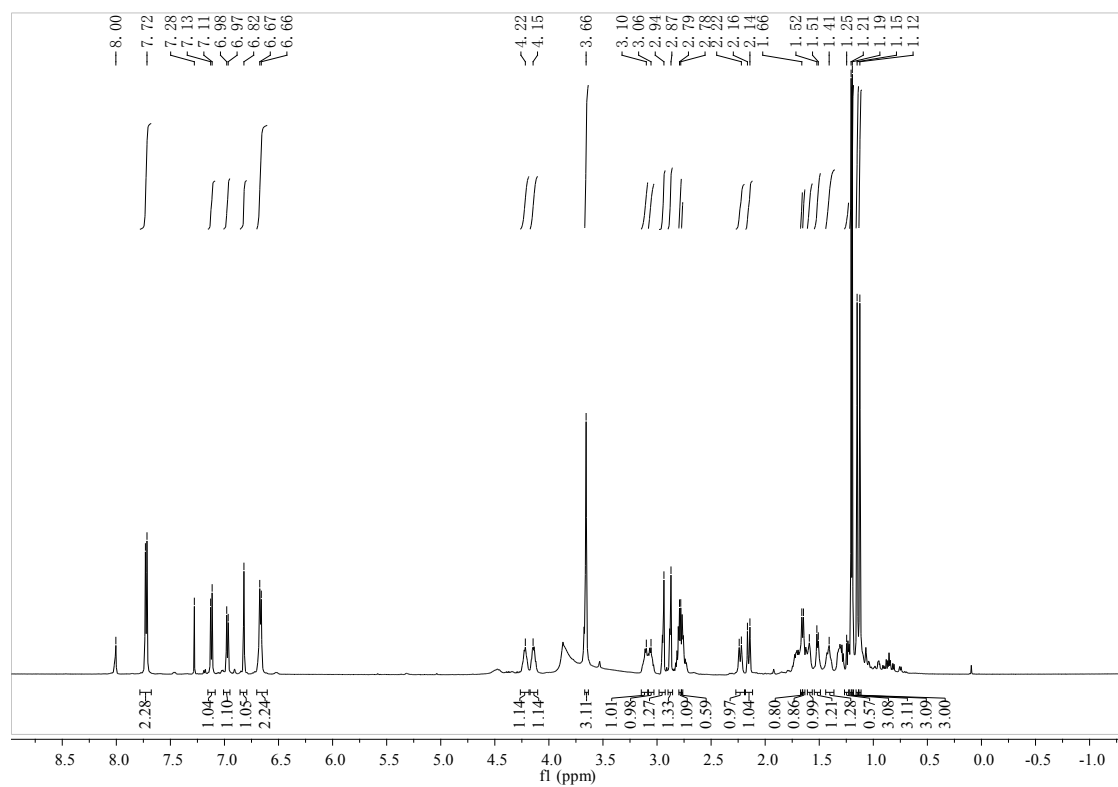


Figure S38. $^1\text{H-NMR}$ spectrum of the target compound (**3j**) in CDCl_3

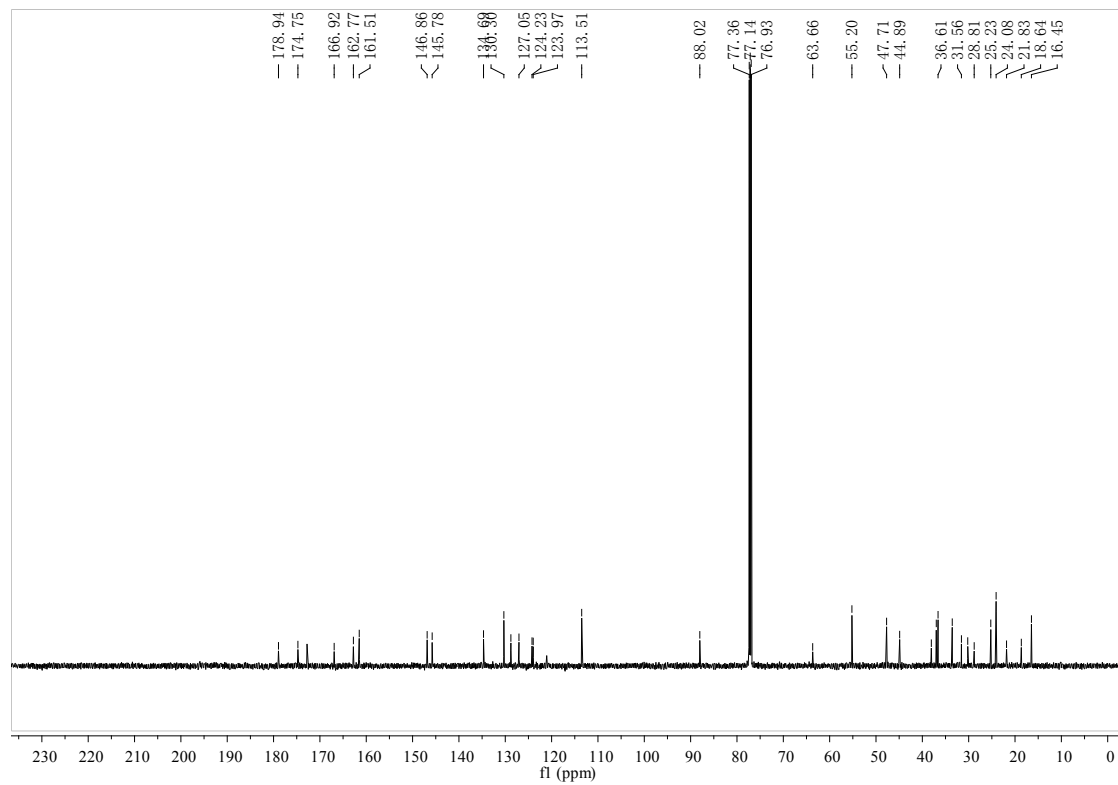


Figure S39. $^{13}\text{C-NMR}$ spectrum of the target compound (**3j**) in CDCl_3

Sample Name	LFY10	Position	P1-B1	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY10.d
ACQ Method	yijing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 5:18:29 PM

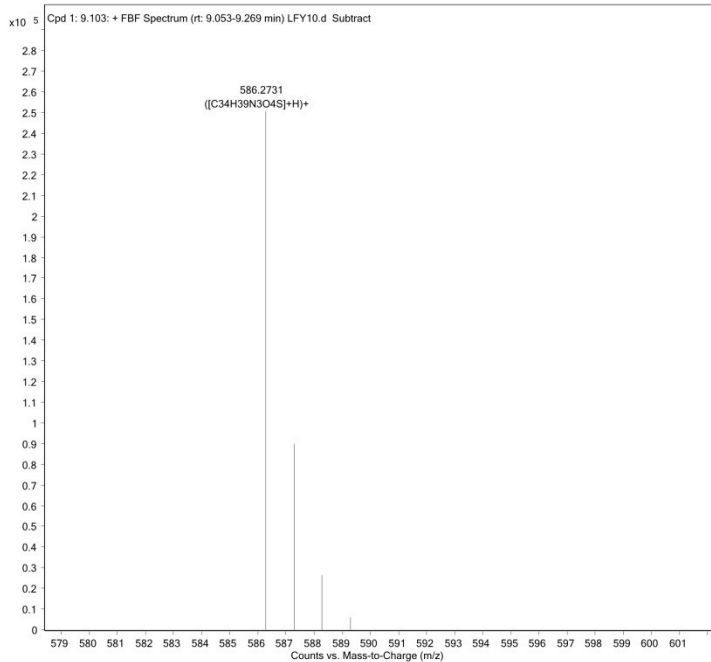


Figure S40. HR-MS spectrum of the target compound (3j)

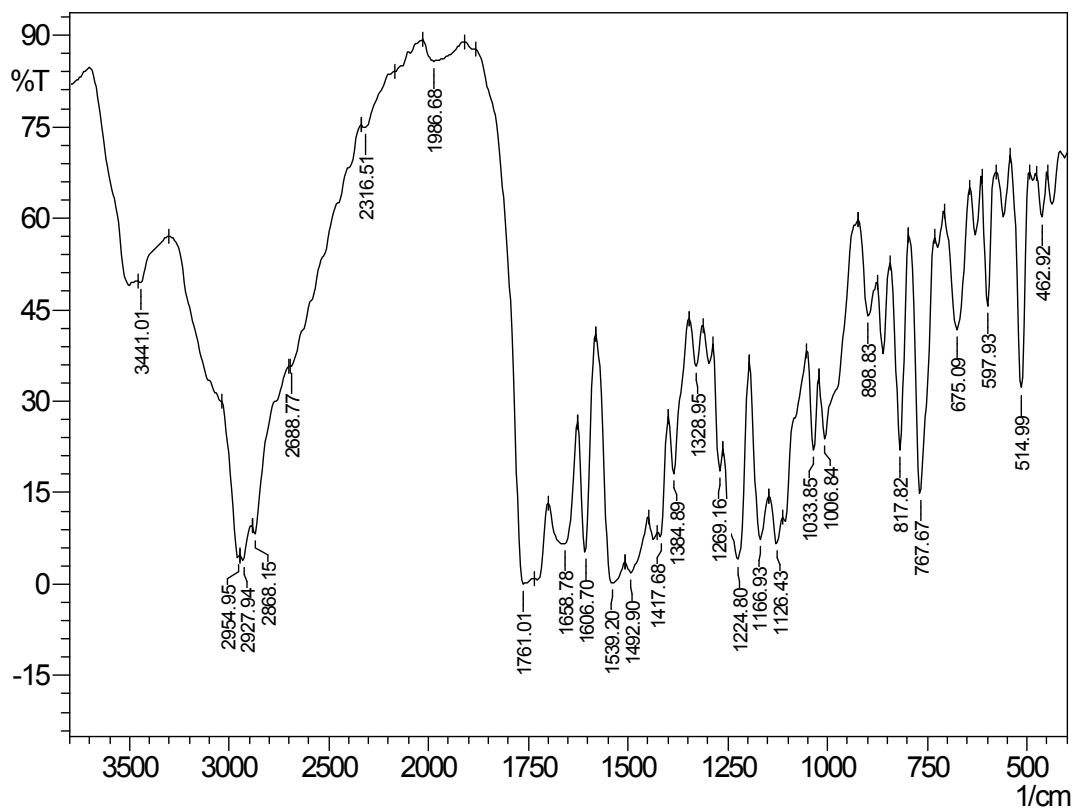


Figure S41. FTIR spectrum of the target compound (3k)

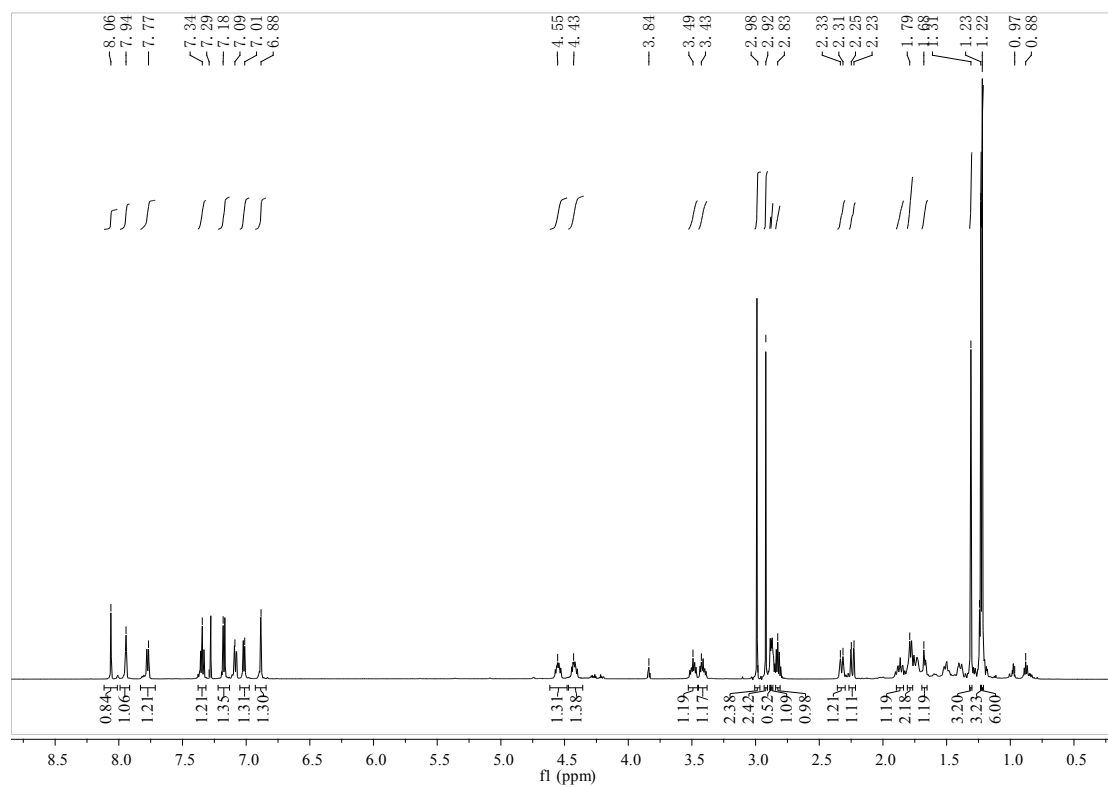


Figure S42. $^1\text{H-NMR}$ spectrum of the target compound (**3k**) in CDCl_3

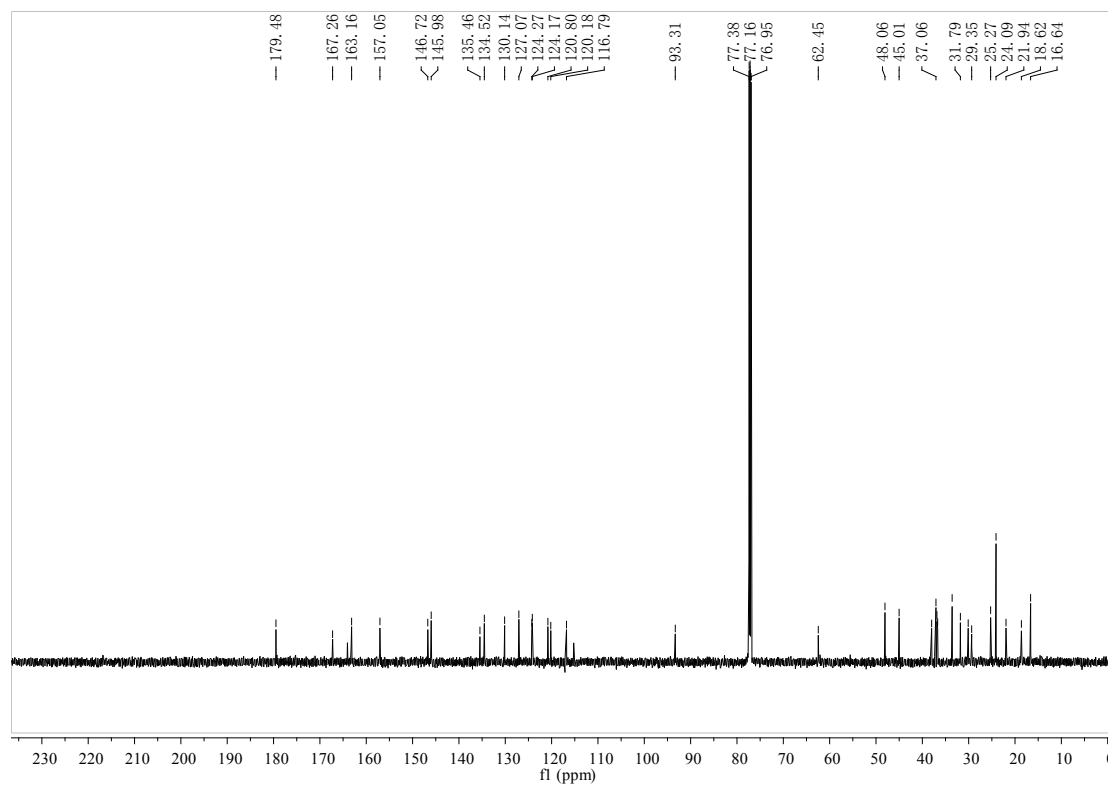


Figure S43. $^{13}\text{C-NMR}$ spectrum of the target compound (**3k**) in CDCl_3

Sample Name	LFY11	Position	P1-B2	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY11.d
ACQ Method	yijing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 5:33:14 PM

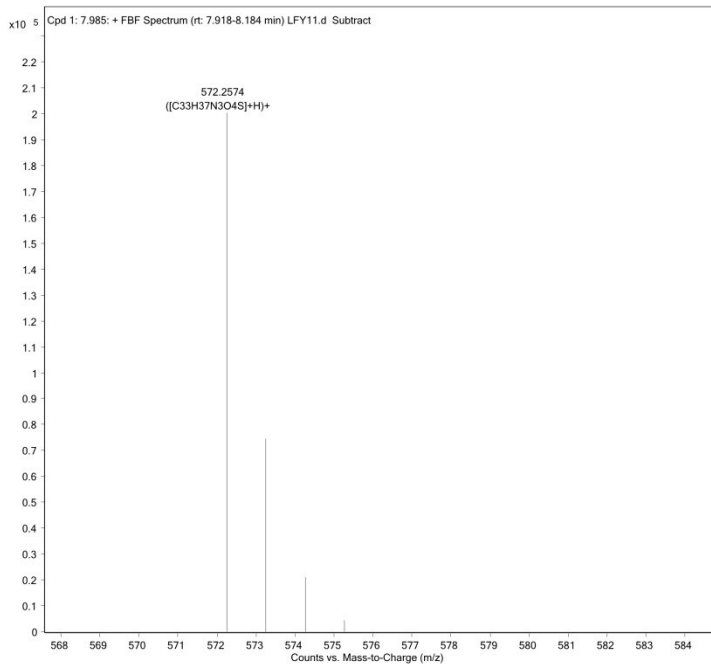


Figure S44. HR-MS spectrum of the target compound (**3k**)

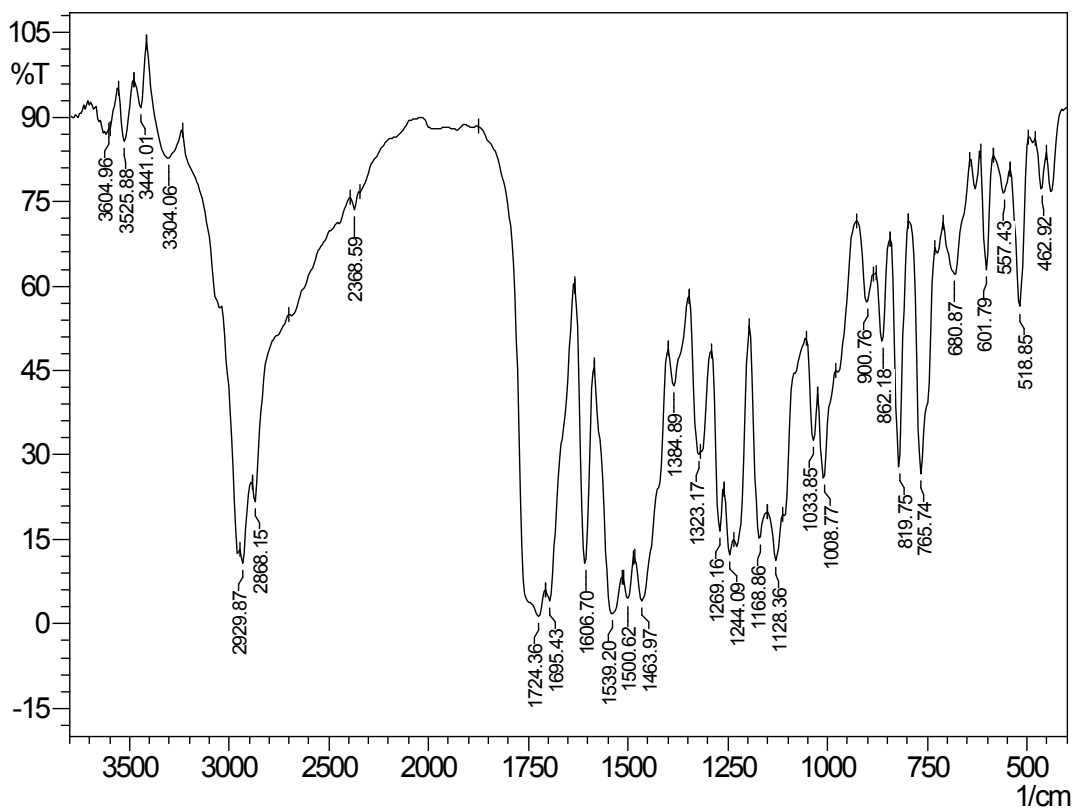


Figure S45. FTIR spectrum of the target compound (**3l**)

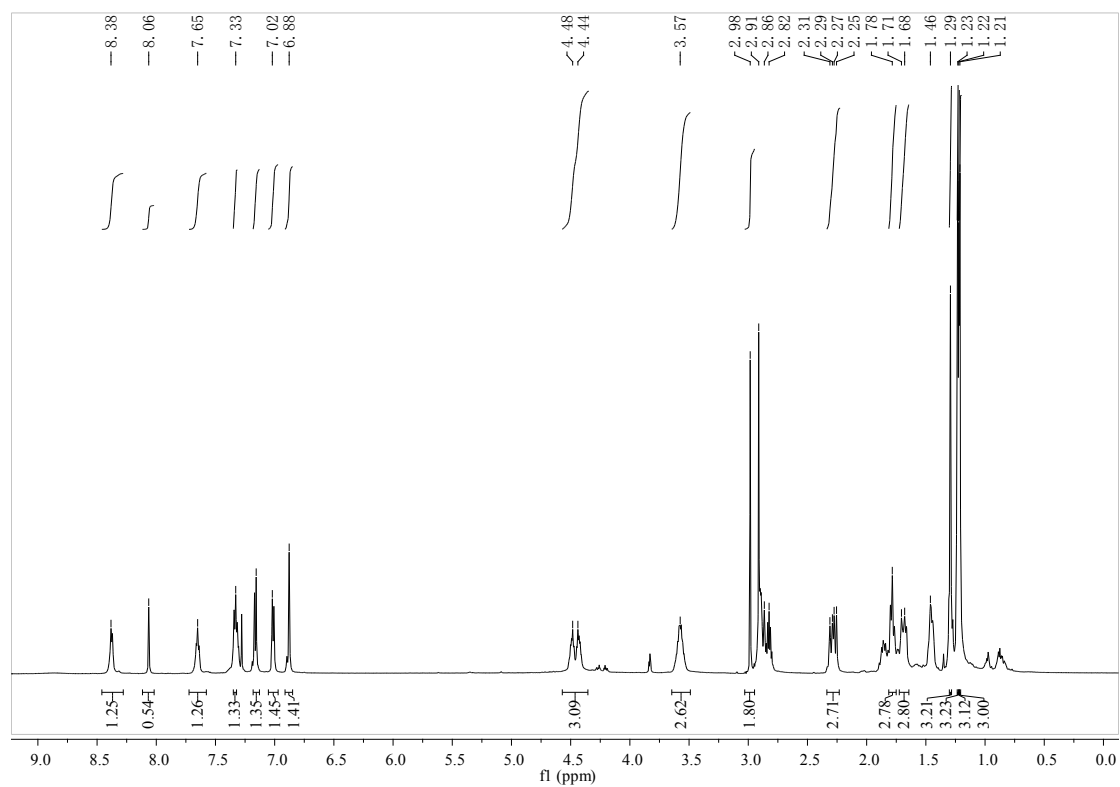


Figure S46. $^1\text{H-NMR}$ spectrum of the target compound (**31**) in CDCl_3

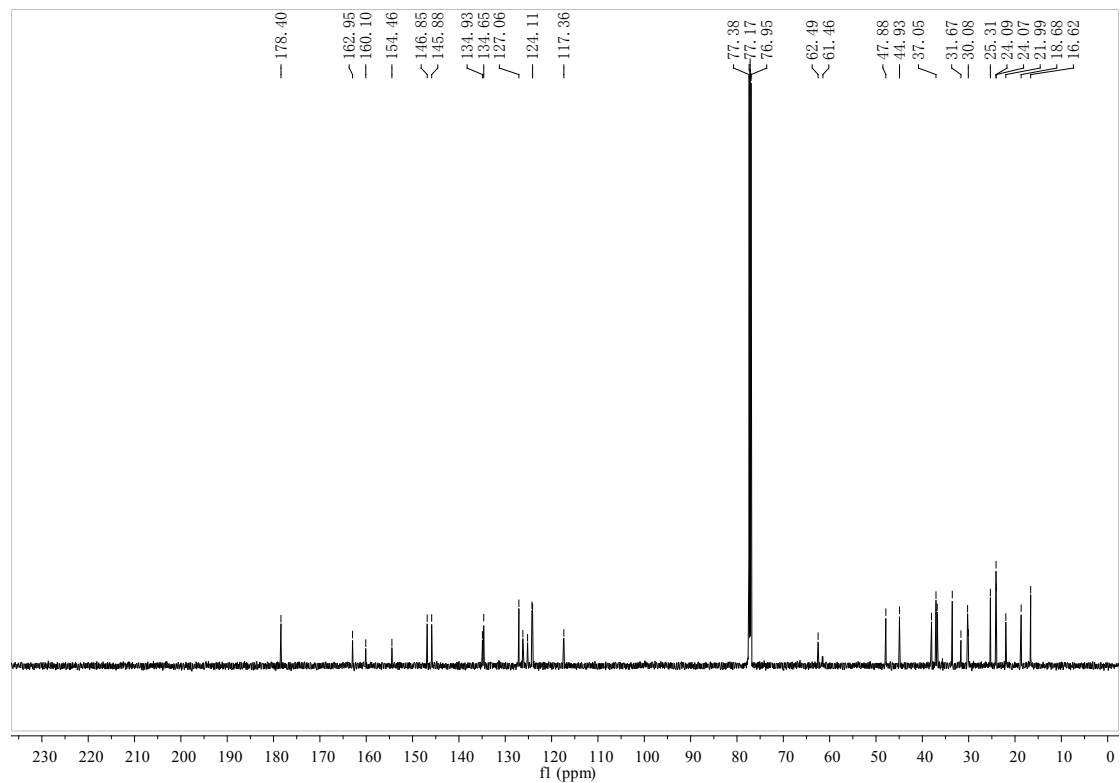


Figure S47. $^{13}\text{C-NMR}$ spectrum of the target compound (**31**) in CDCl_3

Sample Name	LFY12	Position	P1-B3	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY12.d
ACQ Method	yijing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 5:47:56 PM

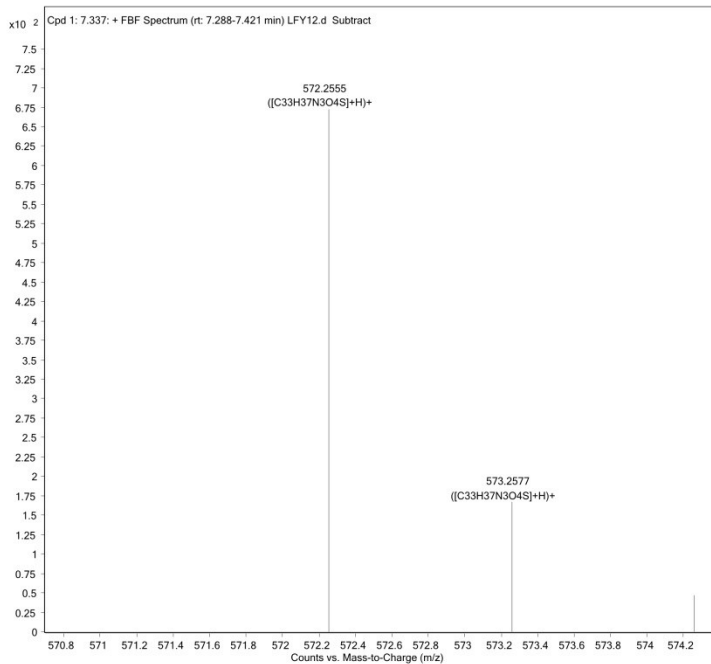


Figure S48. HR-MS spectrum of the target compound (**3I**)

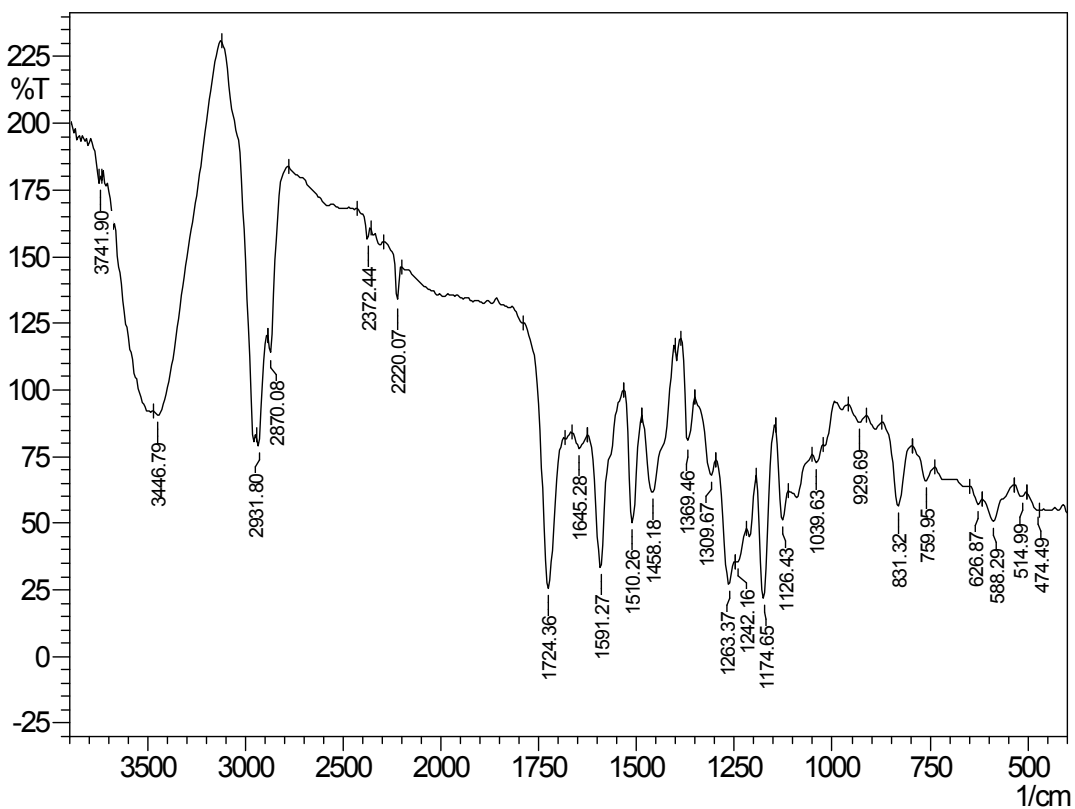


Figure S49. FTIR spectrum of the target compound (**3m**)

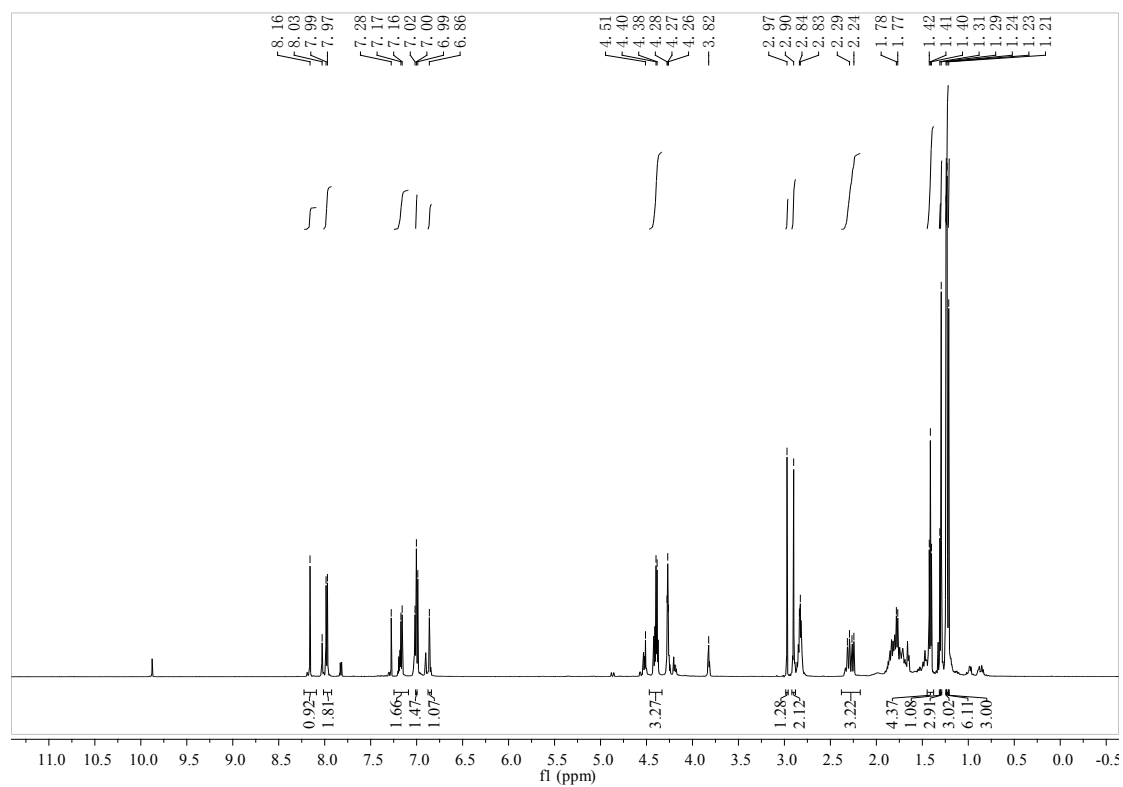


Figure S50. $^1\text{H-NMR}$ spectrum of the target compound (**3m**) in CDCl_3

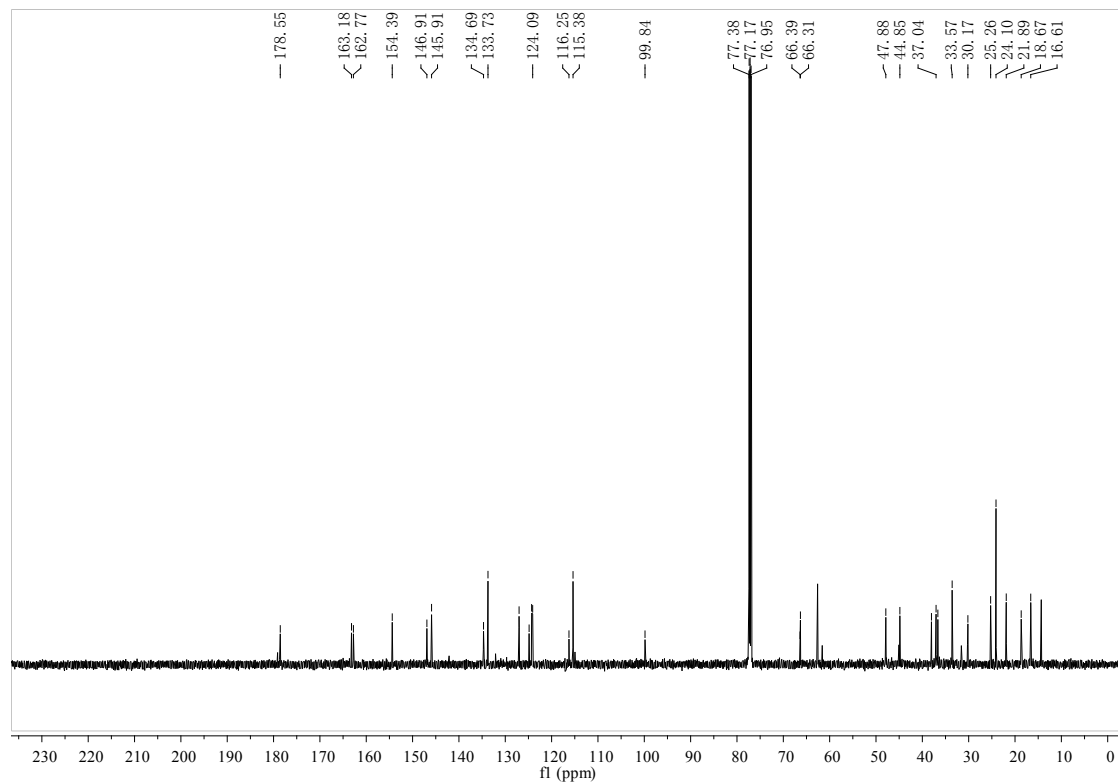


Figure S51. $^{13}\text{C-NMR}$ spectrum of the target compound (**3m**) in CDCl_3

Sample Name	LFY16	Position	P1-B7	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY16.d
ACQ Method	yijing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 6:46:49 PM

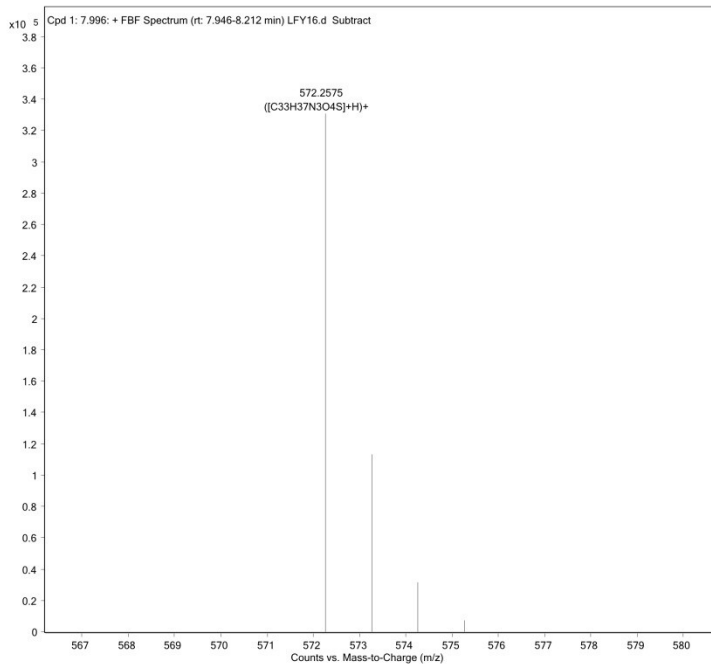


Figure S52. HR-MS spectrum of the target compound (**3m**)

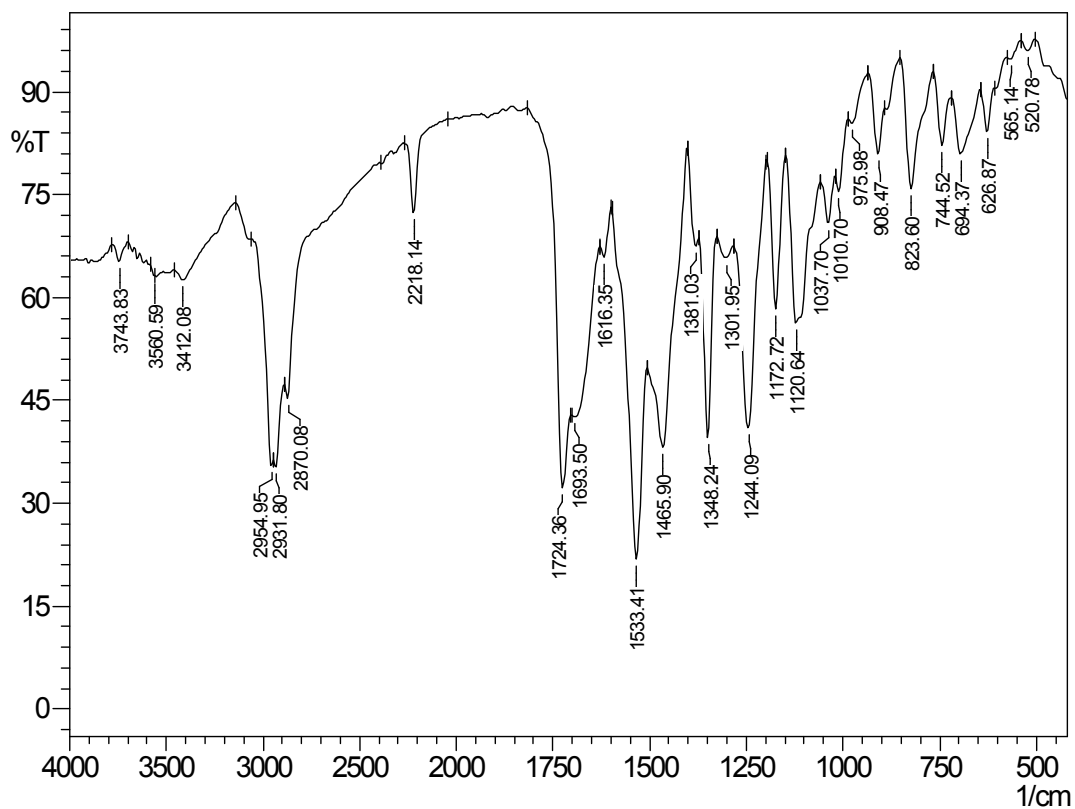


Figure S53. FTIR spectrum of the target compound (**3n**)

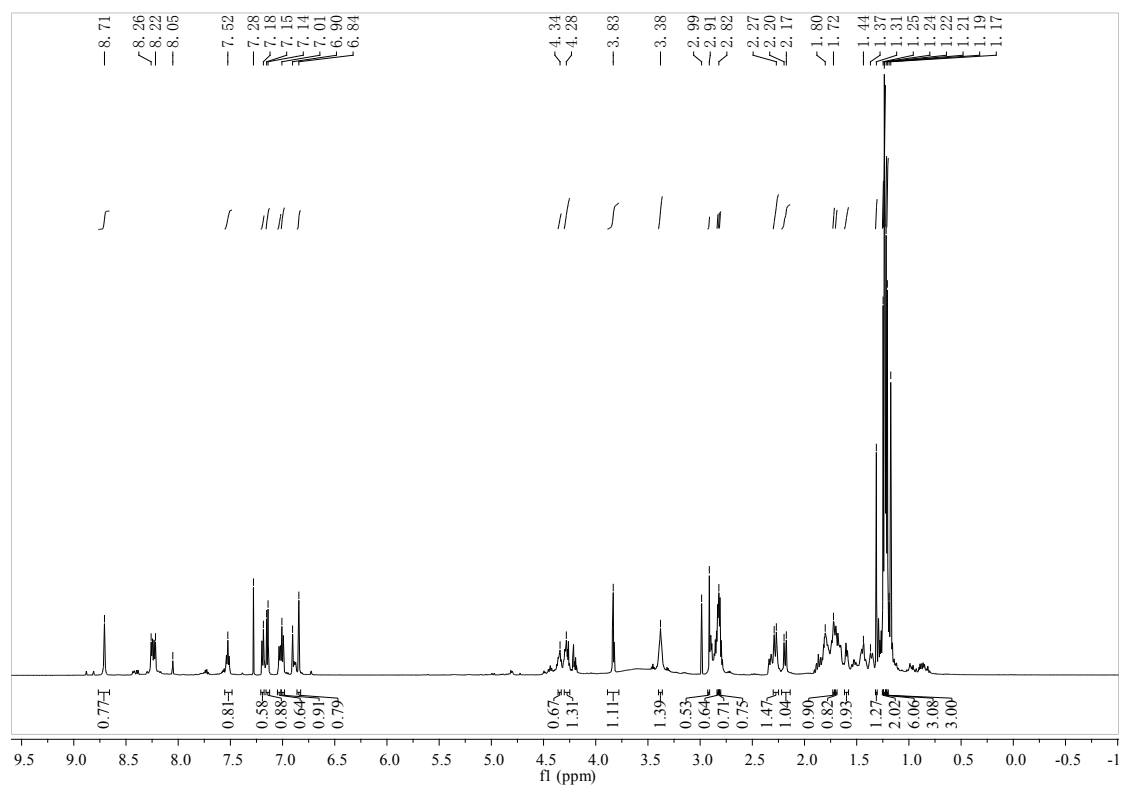


Figure S54. $^1\text{H-NMR}$ spectrum of the target compound (**3n**) in CDCl_3

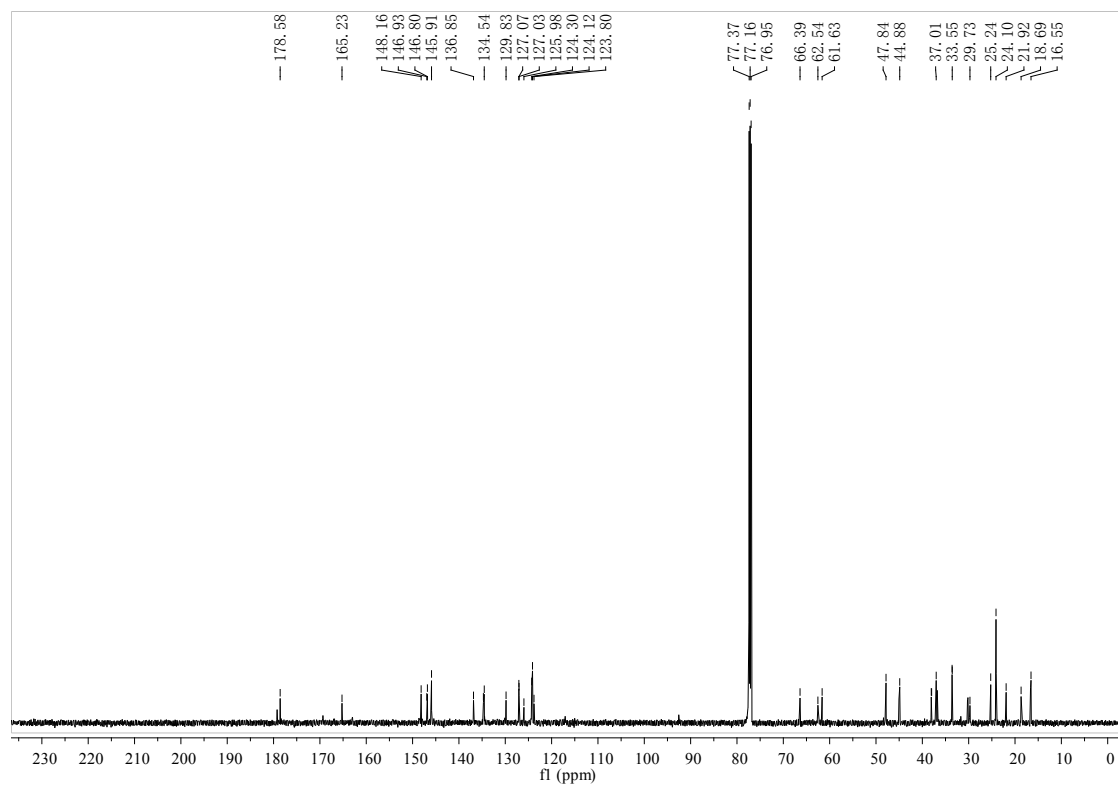


Figure S55. $^{13}\text{C-NMR}$ spectrum of the target compound (**3n**) in CDCl_3

Sample Name	LFY14	Position	P1-B5	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY14.d
ACQ Method	yijing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 6:17:23 PM

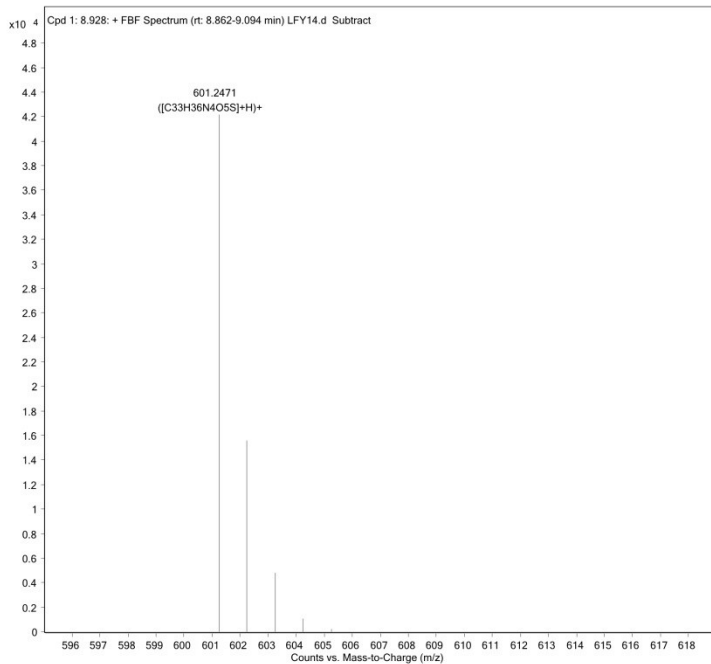


Figure S56. HR-MS spectrum of the target compound (**3n**)

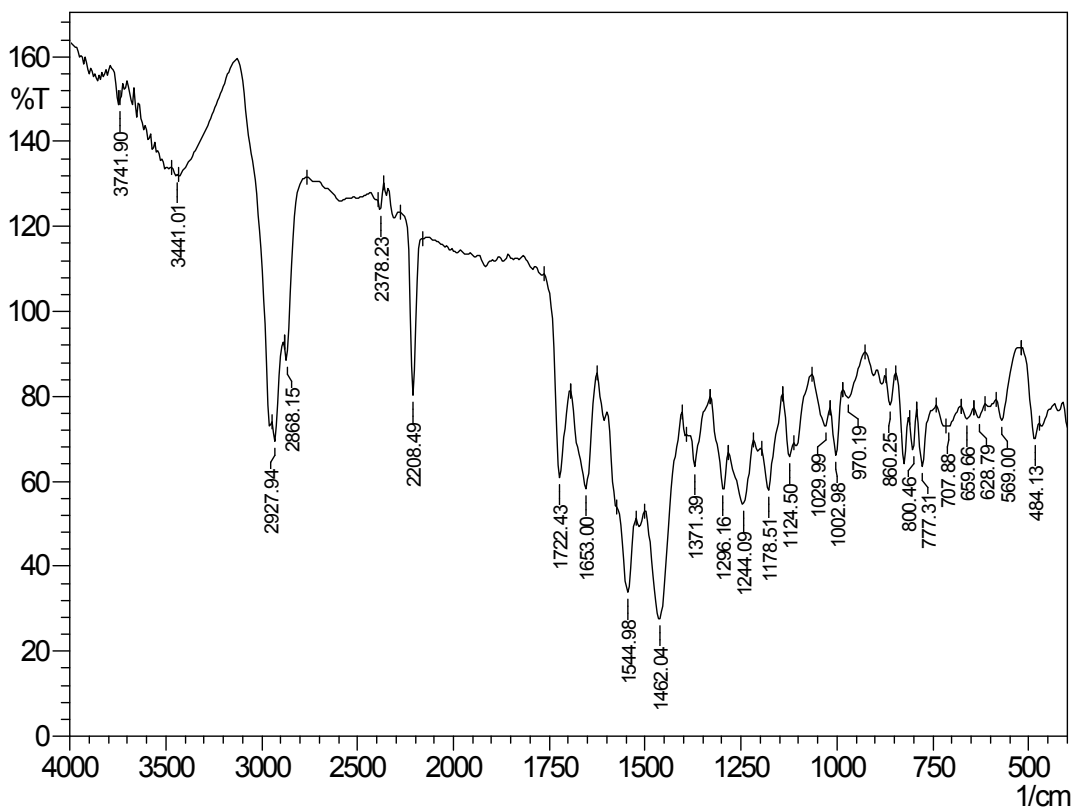


Figure S57. FTIR spectrum of the target compound (**3o**)

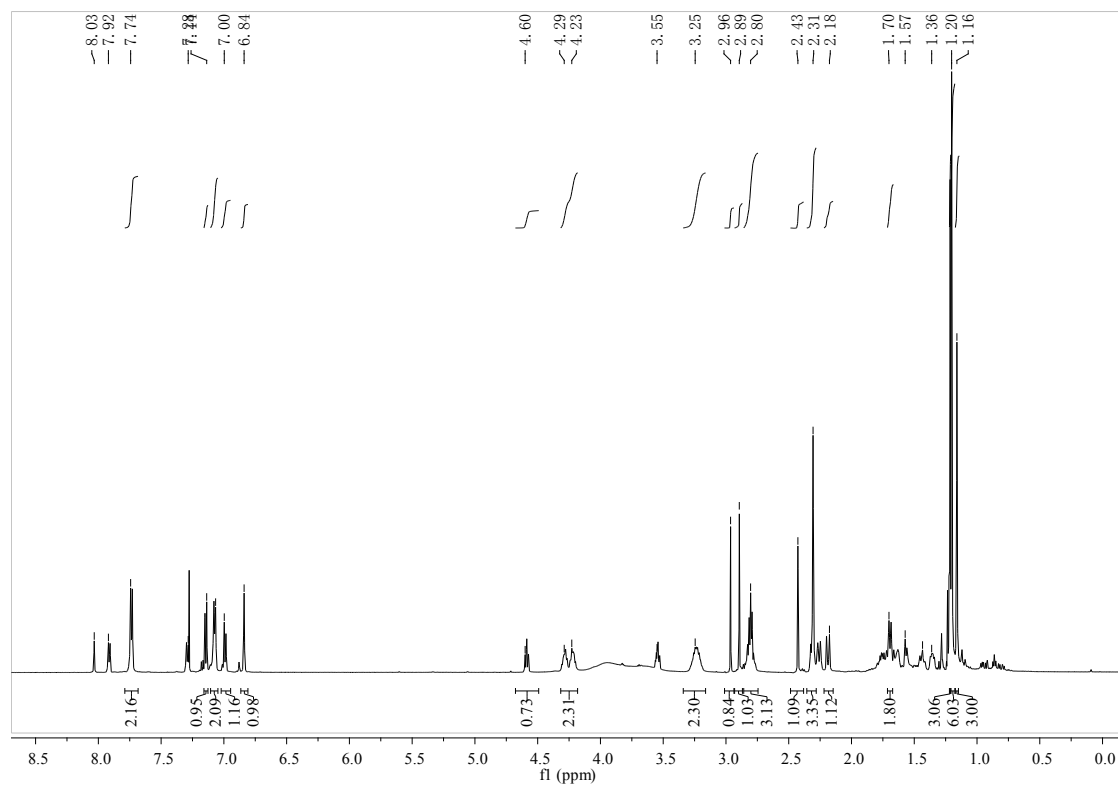


Figure S58. ¹H-NMR spectrum of the target compound (**3o**) in CDCl₃

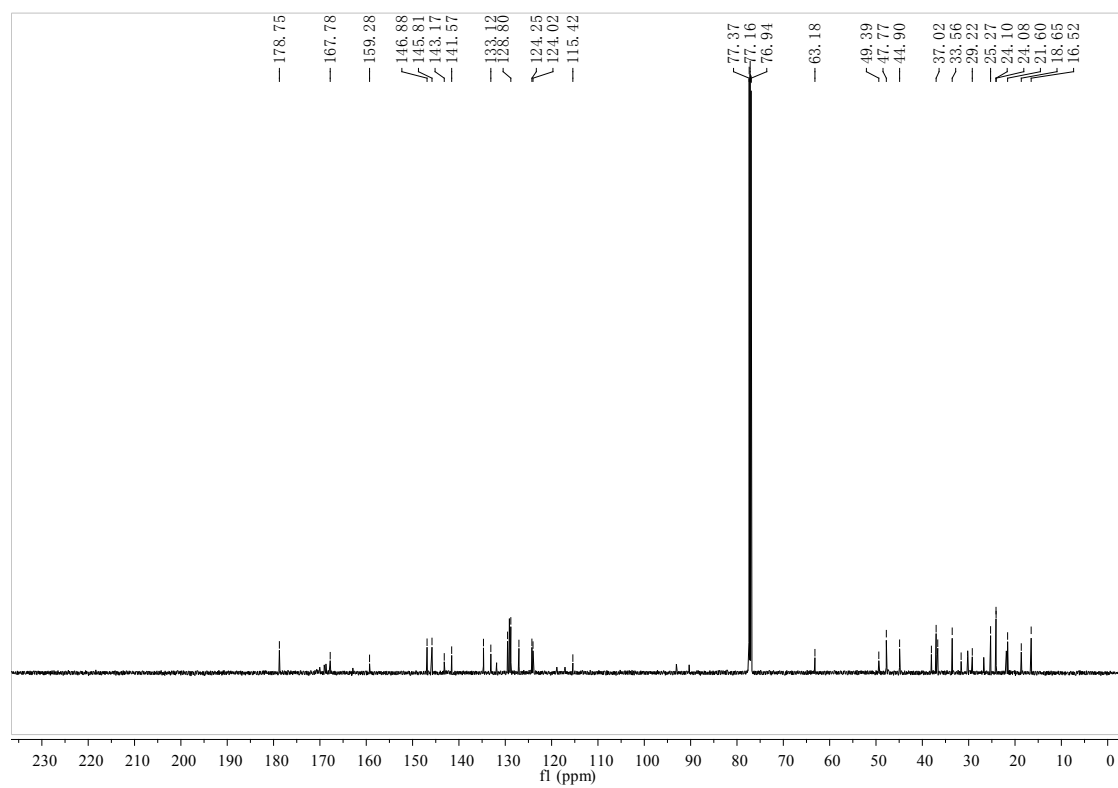


Figure S59. ¹³C-NMR spectrum of the target compound (**3o**) in CDCl₃

Sample Name	LFY15	Position	P1-B6	Instrument Name	Instrument 1
User Name		Inj Vol	0.05	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	LFY15.d
ACQ Method	yijing10-95% 8min Zheng.m	Comment		Acquired Time	4/20/2020 6:32:07 PM

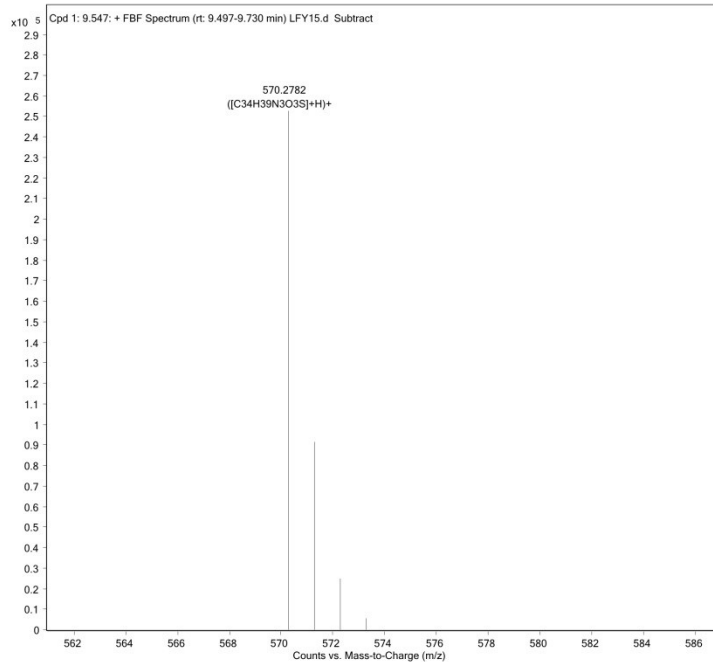


Figure S60. HR-MS spectrum of the target compound (**30**)