Electronic Supplementary Material (ESI) for RSC Advances.

A novel magnetic nano particles with ionic liquids tags as a reusable catalyst in the synthesis of polyhydroquinolines

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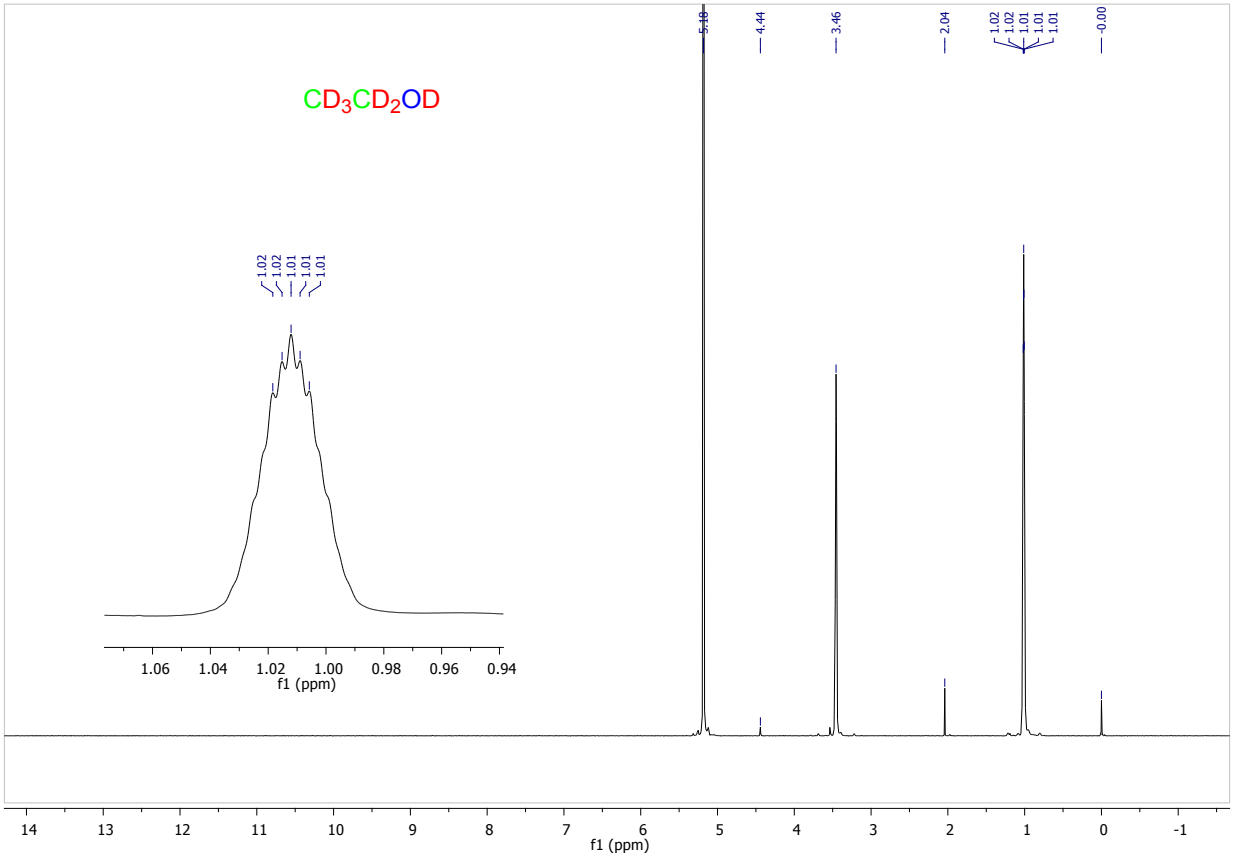
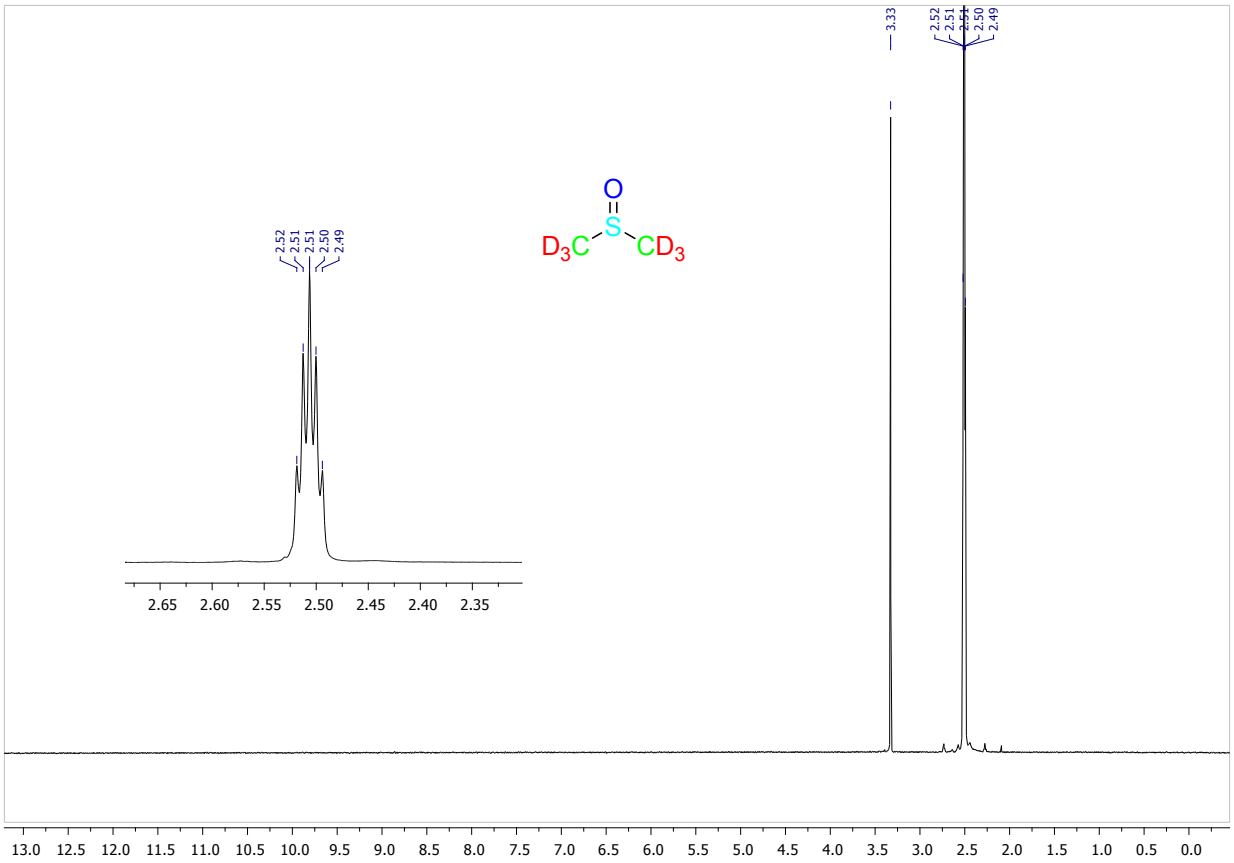
PART 1

^{1}H, ^{13}C, ^{19}F NMR

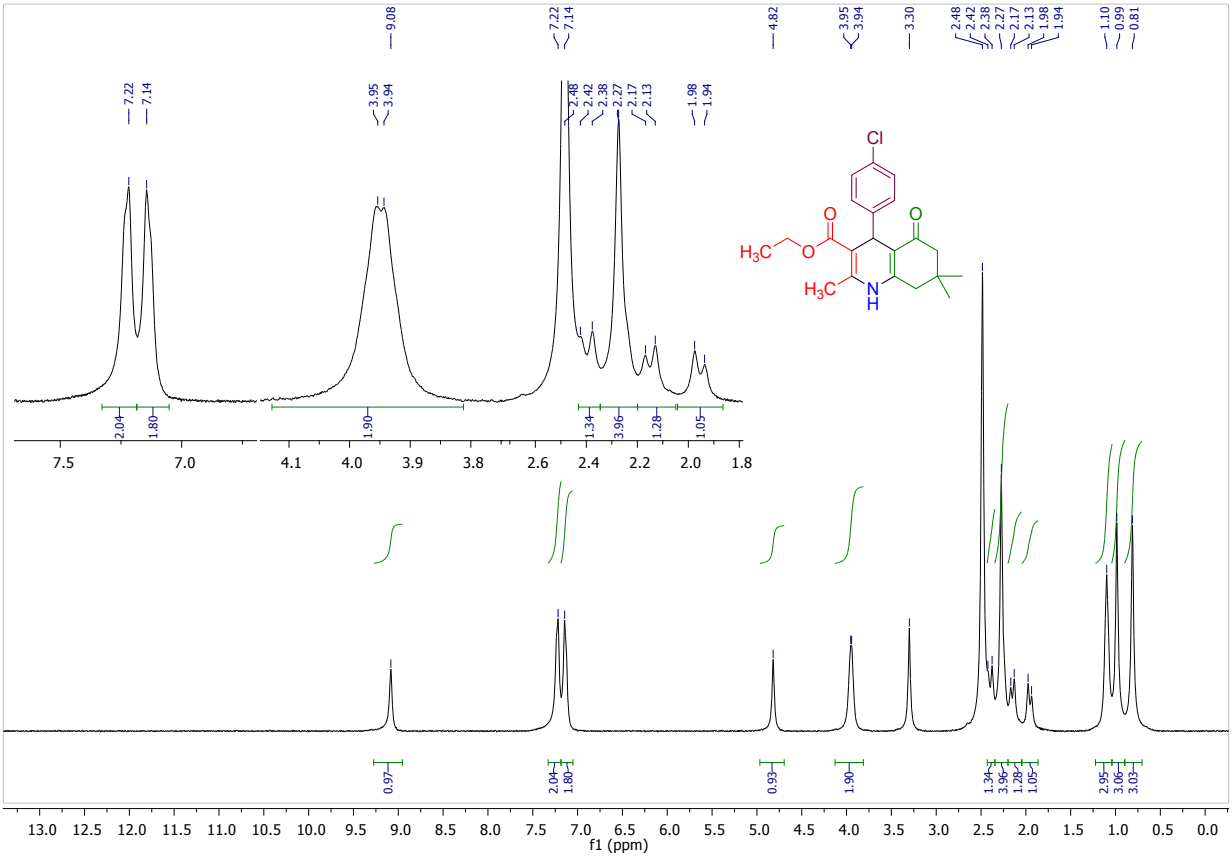
1. ^{1}H NMR spectrum of ethanol-d_6



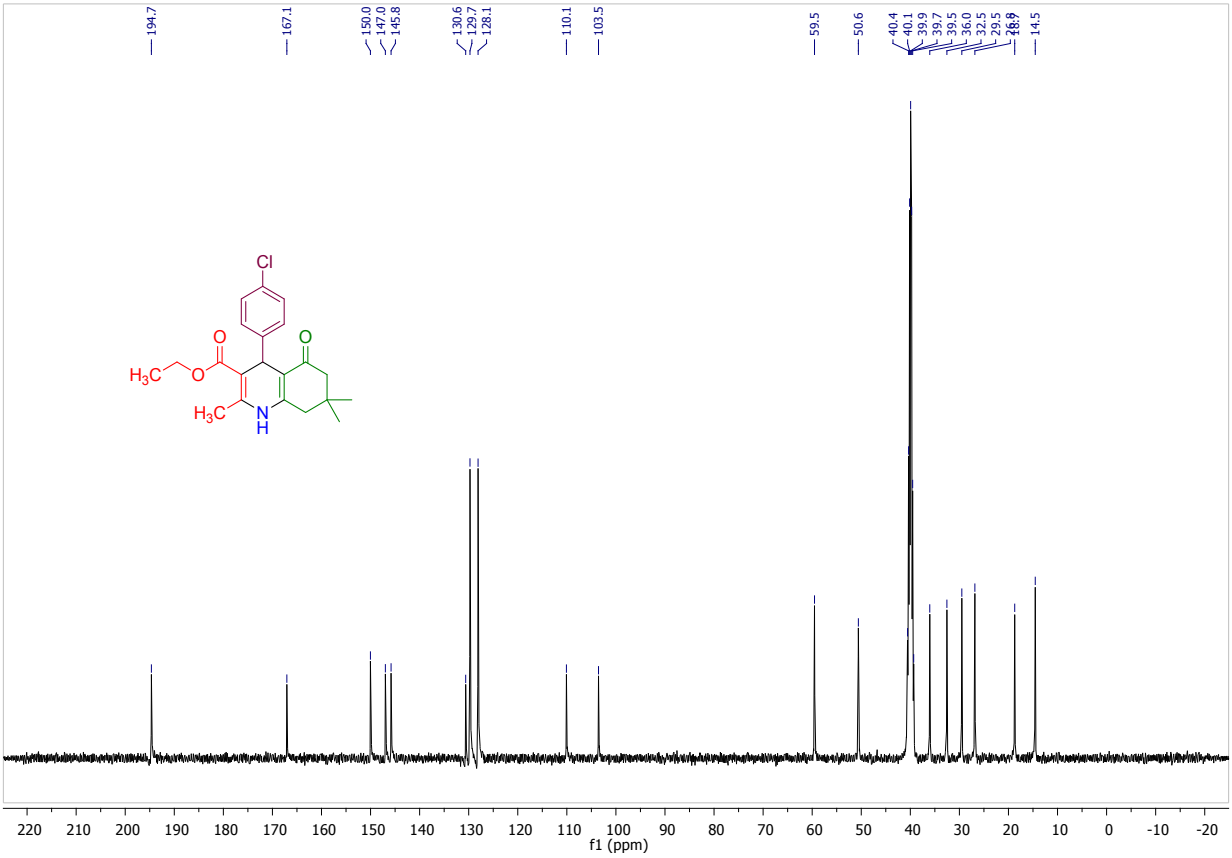
2. ^{1}H NMR spectrum of DMSO-d_6



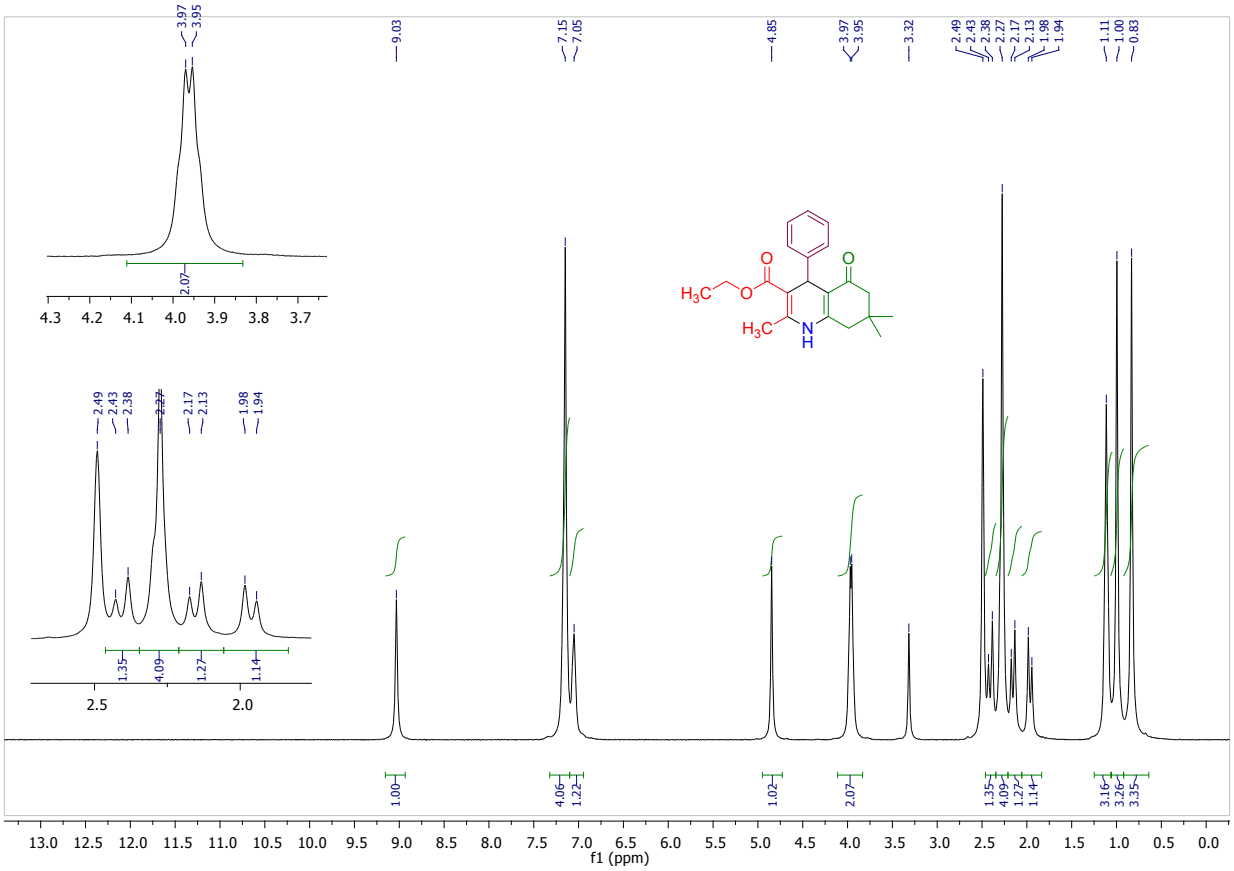
3. ^{1}H NMR spectrum of ethyl 4-(4-chlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1a**)



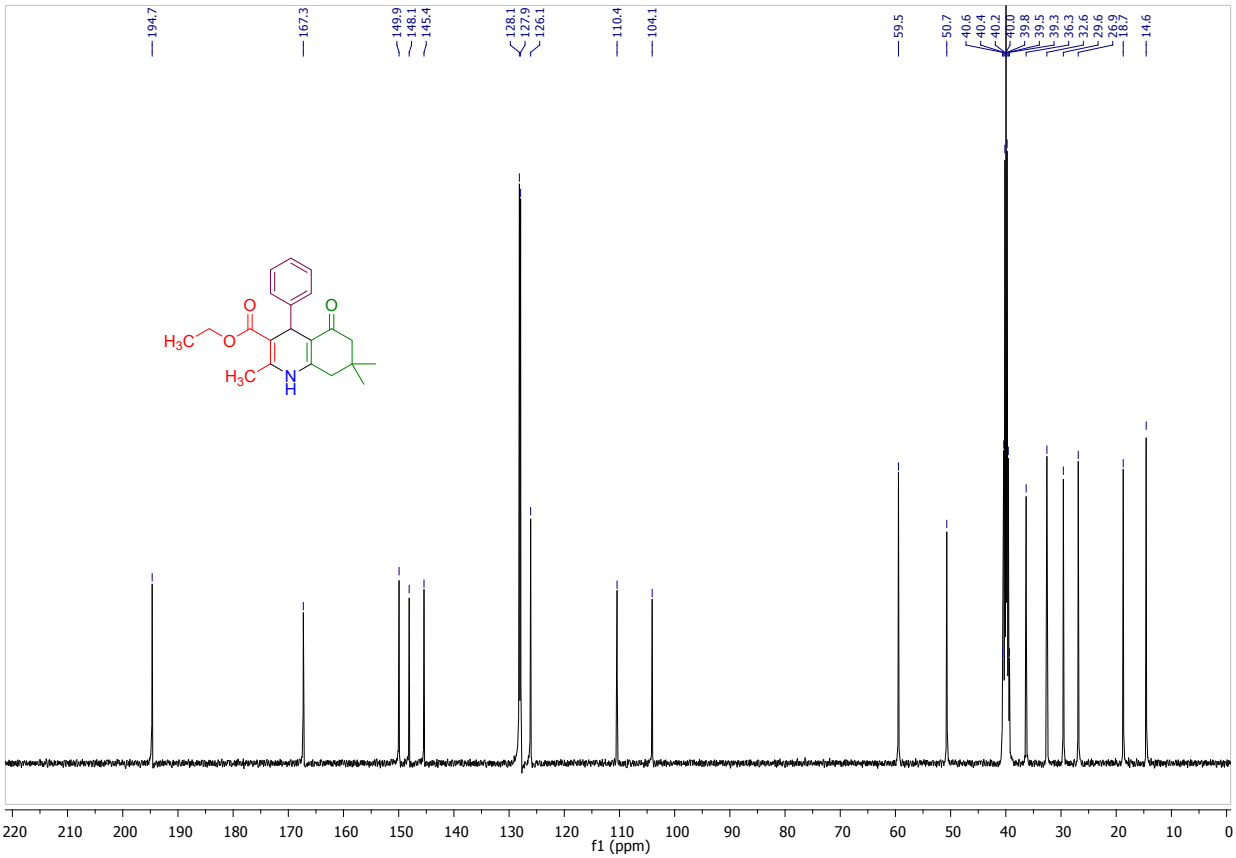
4. ^{13}C NMR spectrum of ethyl 4-(4-chlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1a**)



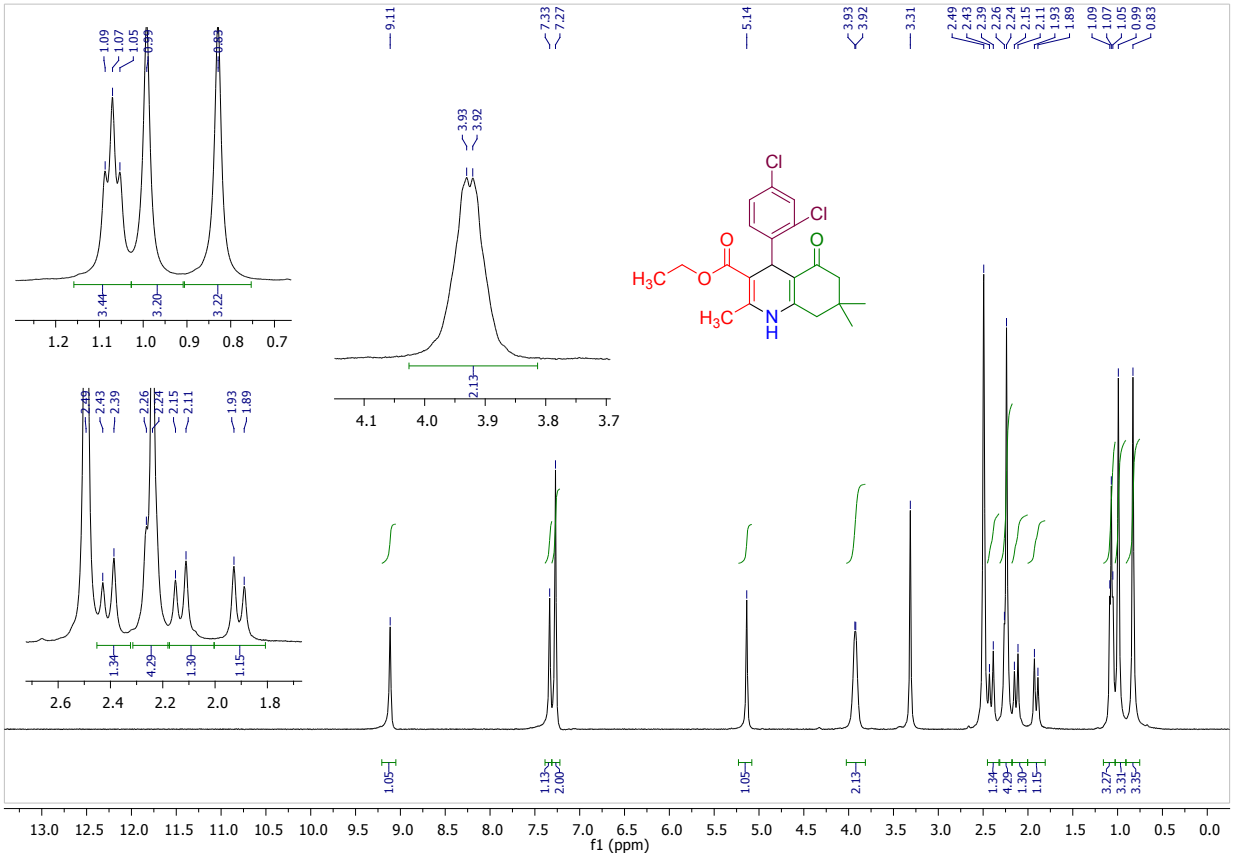
5. ^{1}H NMR spectrum of ethyl 2,7,7-trimethyl-5-oxo-4-phenyl-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1b**)



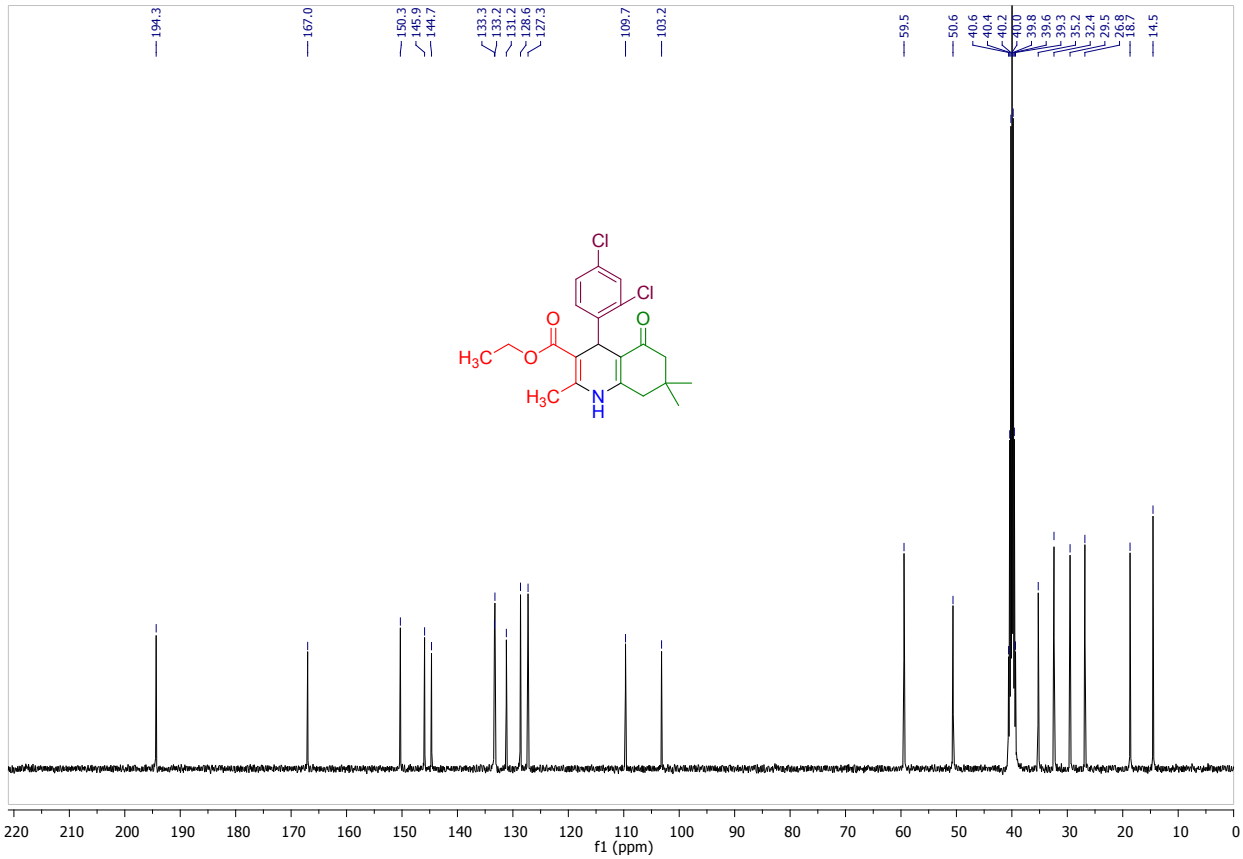
6. ^{13}C NMR spectrum of ethyl 2,7,7-trimethyl-5-oxo-4-phenyl-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1b**)



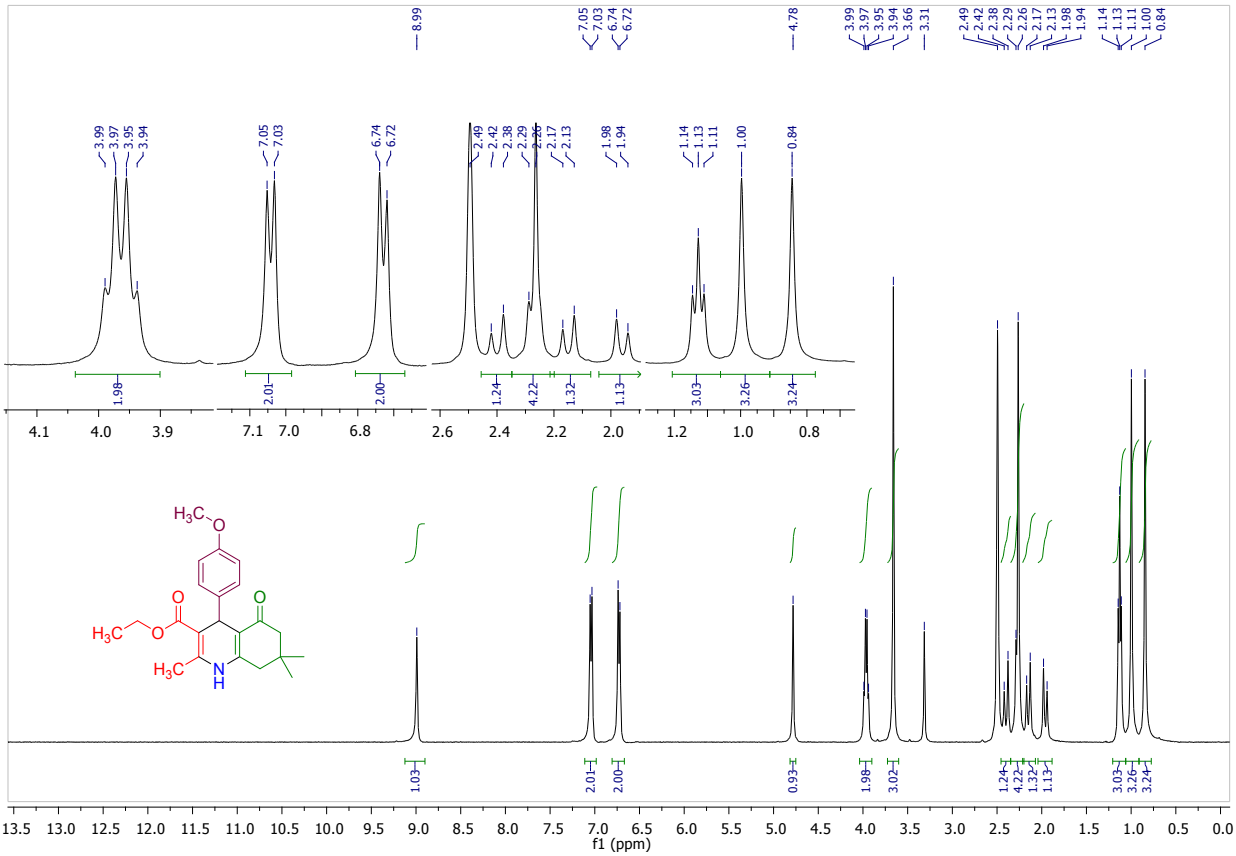
7. ^{1}H NMR spectrum of ethyl 4-(2,4-dichlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1c**)



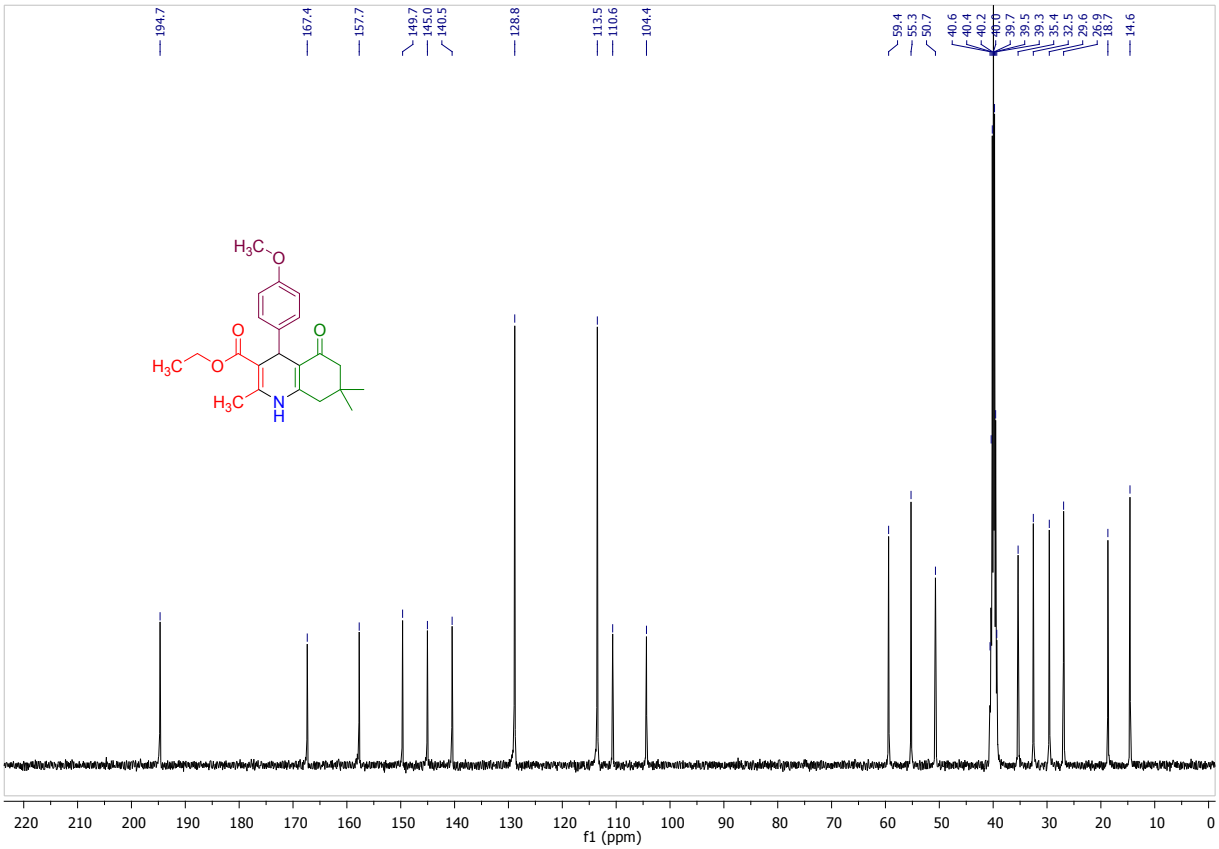
8. ^{13}C NMR spectrum of ethyl 4-(2,4-dichlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1c**)



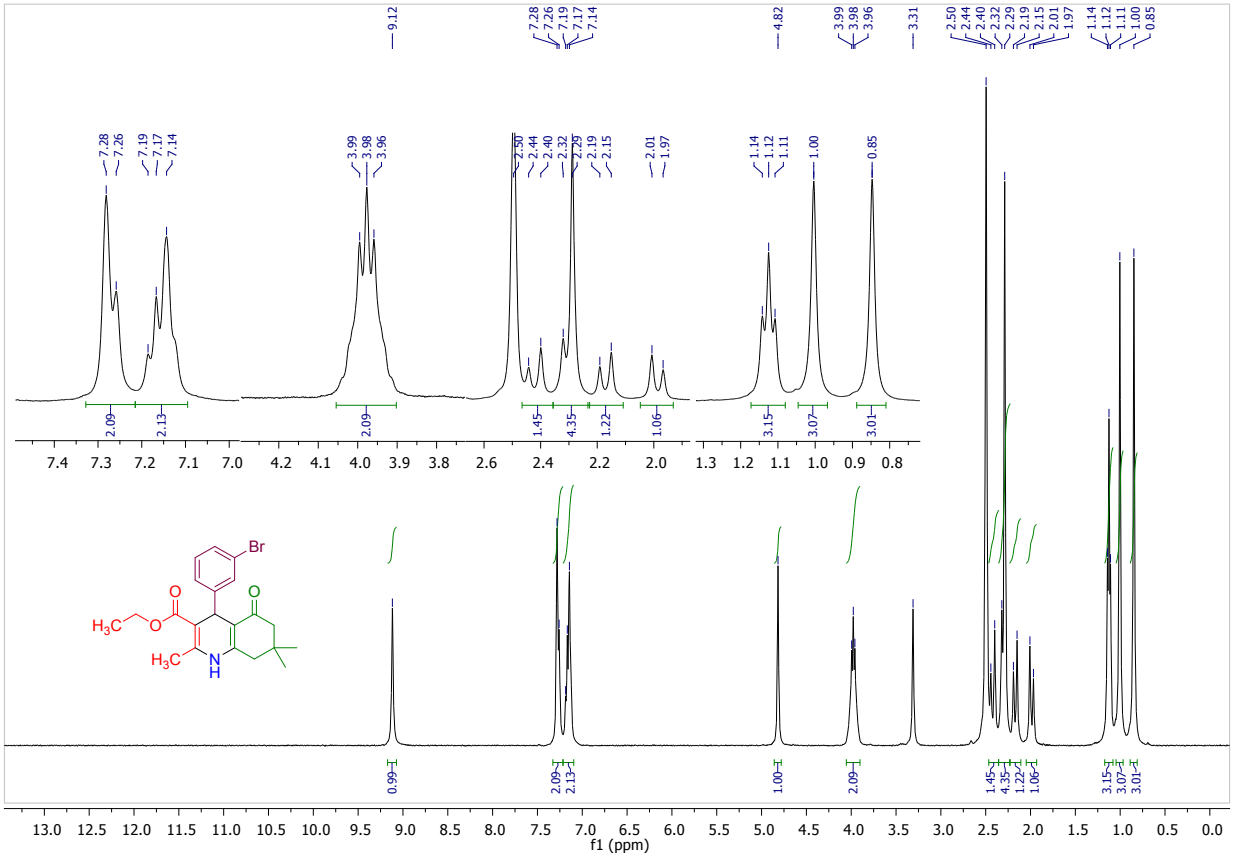
9. ^{1}H NMR spectrum of ethyl 4-(4-methoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1d**)



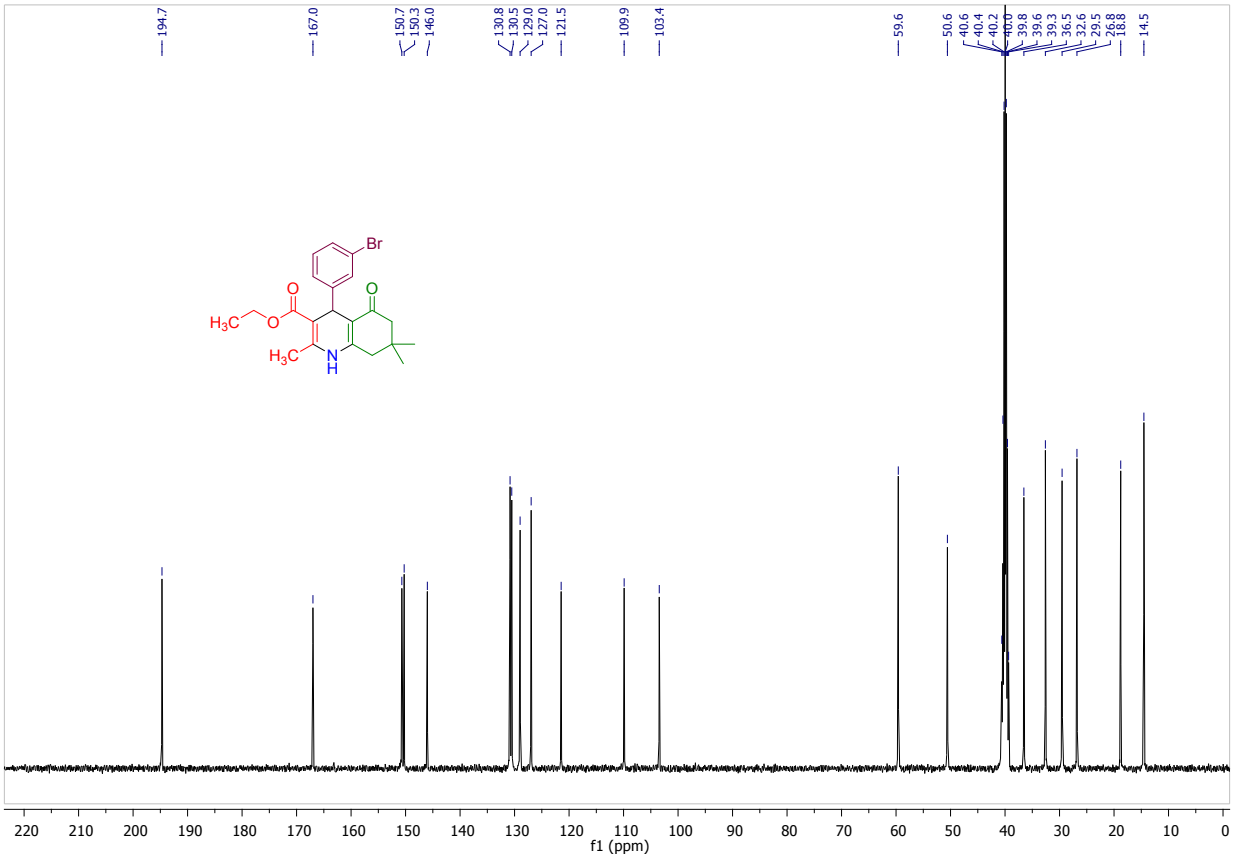
10. ^{13}C NMR spectrum of ethyl 4-(4-methoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1d**)



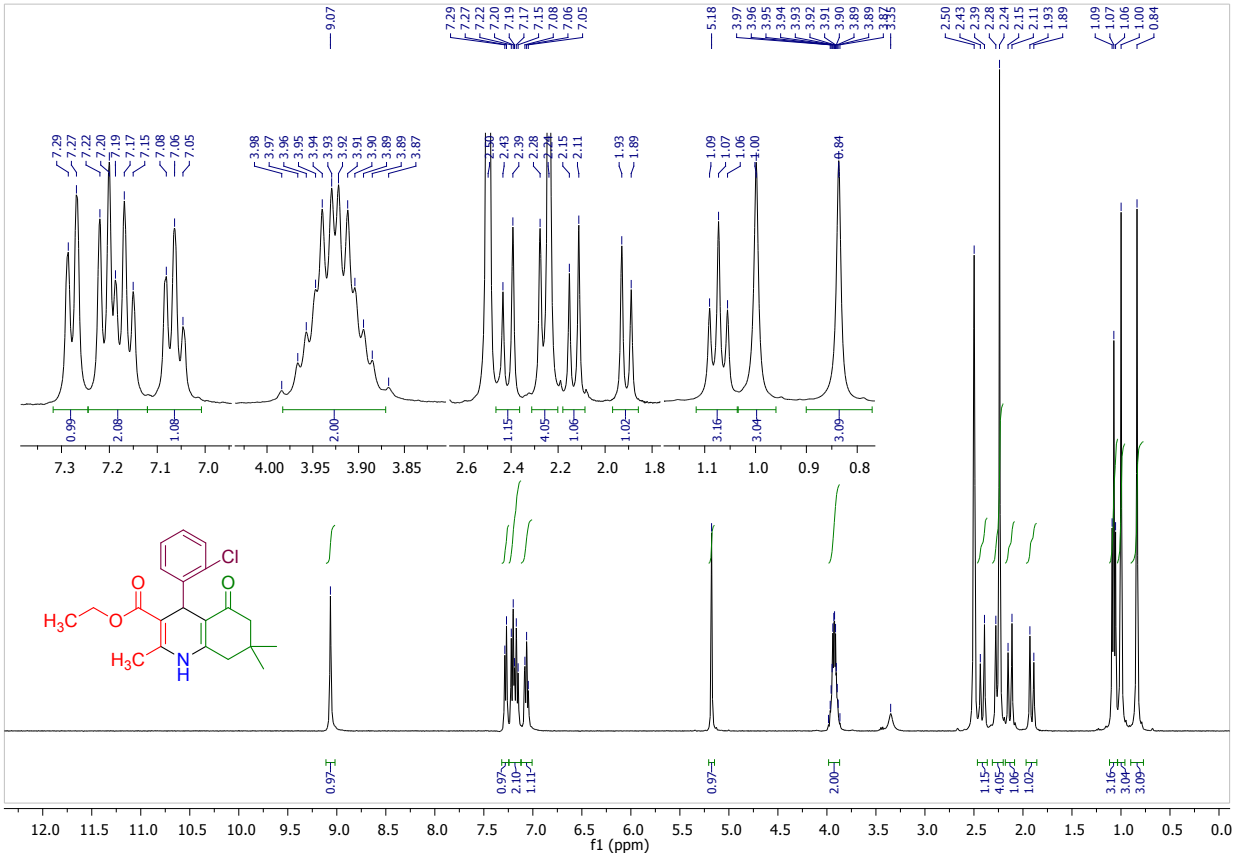
11. ^{1}H NMR spectrum of ethyl 4-(3-bromophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1e**)



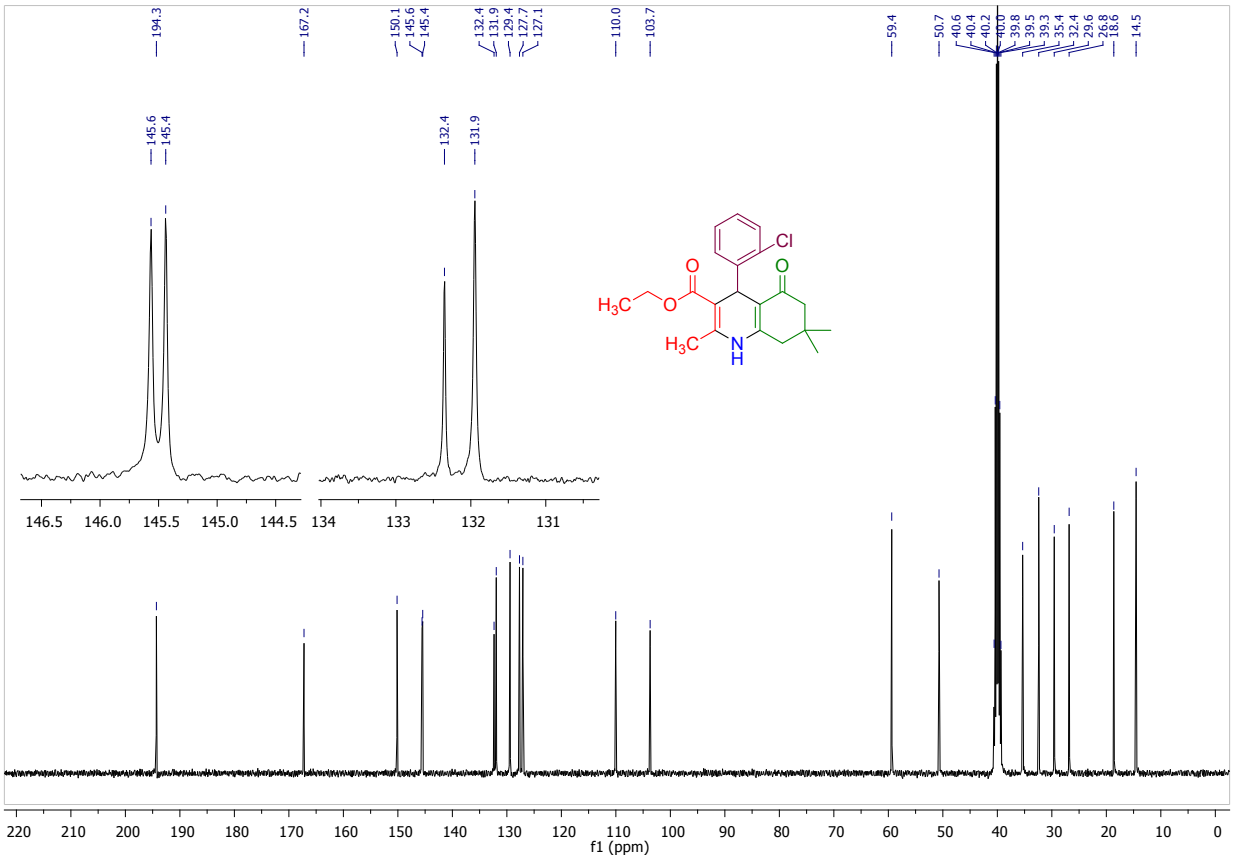
12. ^{13}C NMR spectrum of ethyl 4-(3-bromophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1e**)



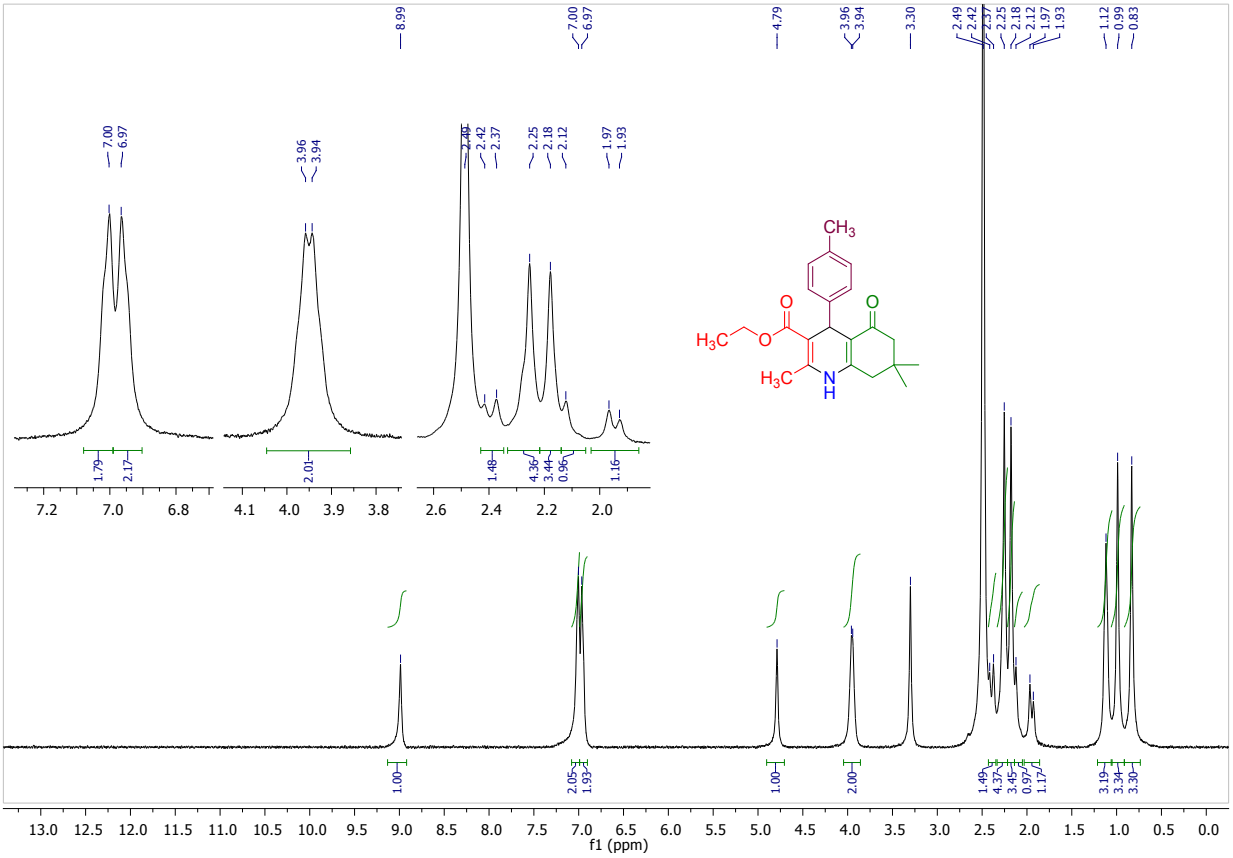
13. ^{1}H NMR spectrum of ethyl 4-(2-chlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1f**)



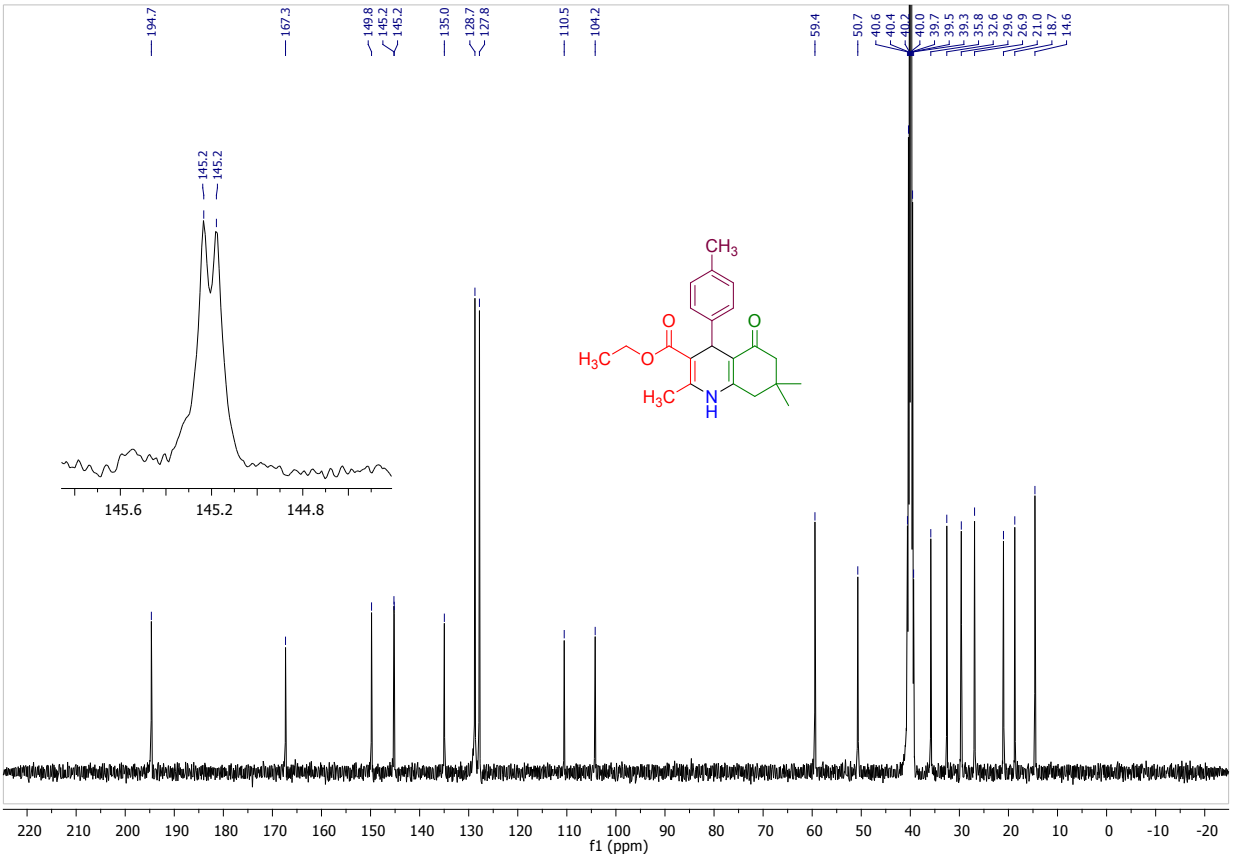
14. ^{13}C NMR spectrum of ethyl 4-(2-chlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1f**)



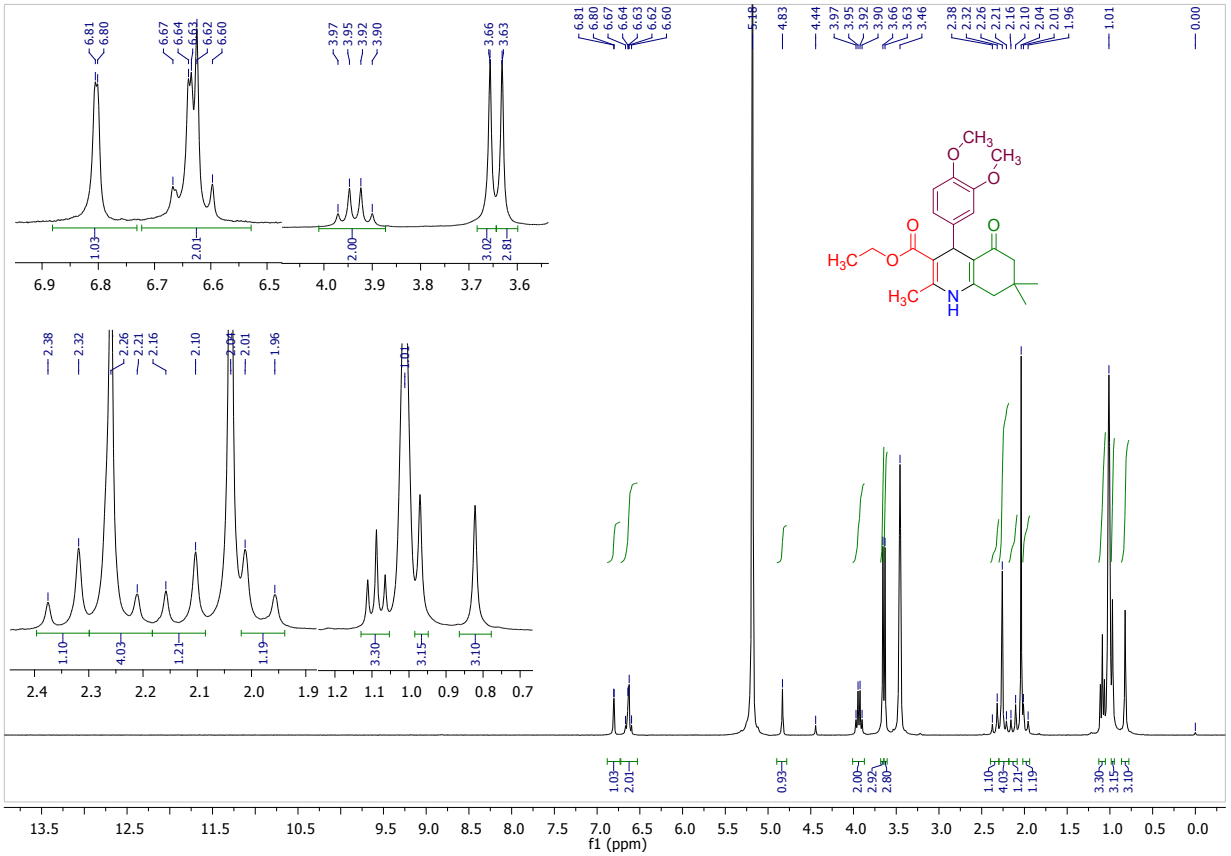
15. ^{1}H NMR spectrum of ethyl 2,7,7-trimethyl-5-oxo-4-(p-tolyl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1g**)



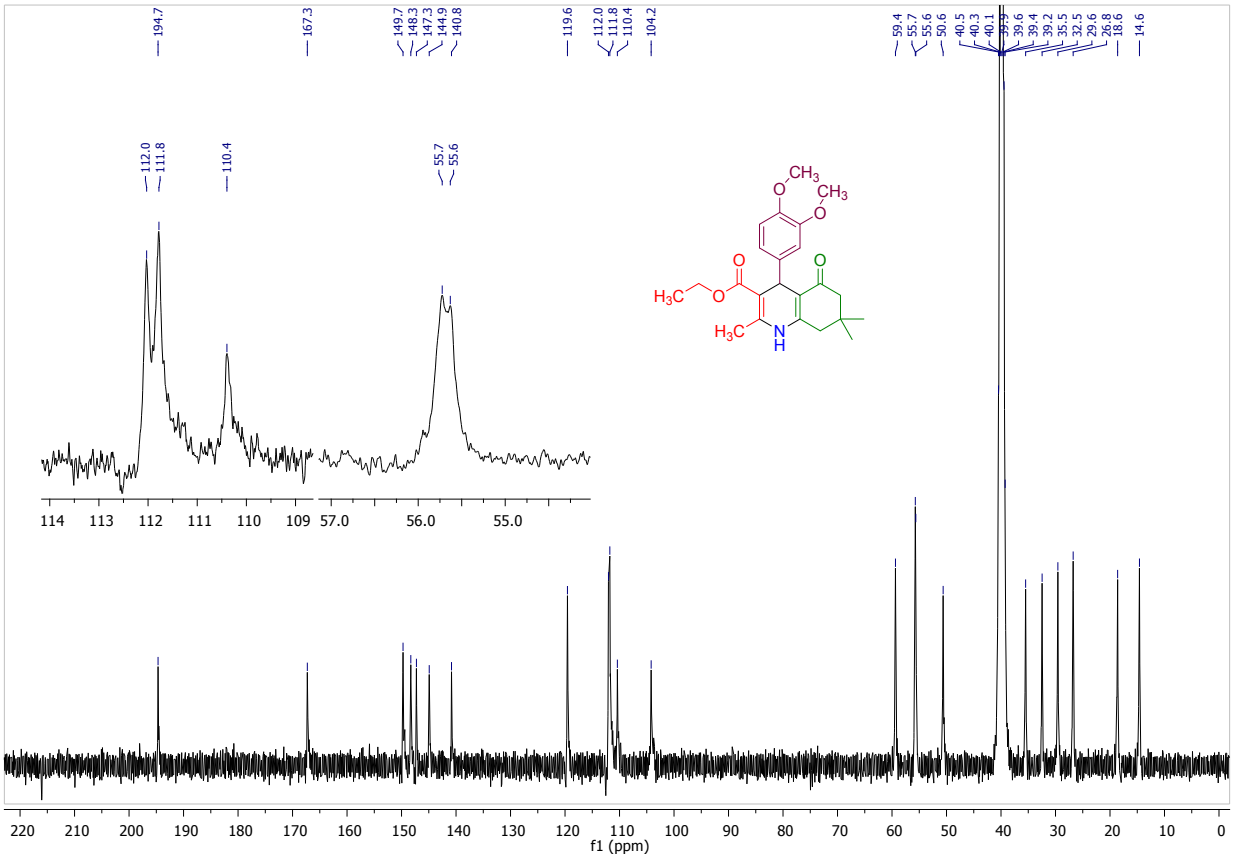
16. ^{13}C NMR spectrum of ethyl 2,7,7-trimethyl-5-oxo-4-(p-tolyl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1g**)



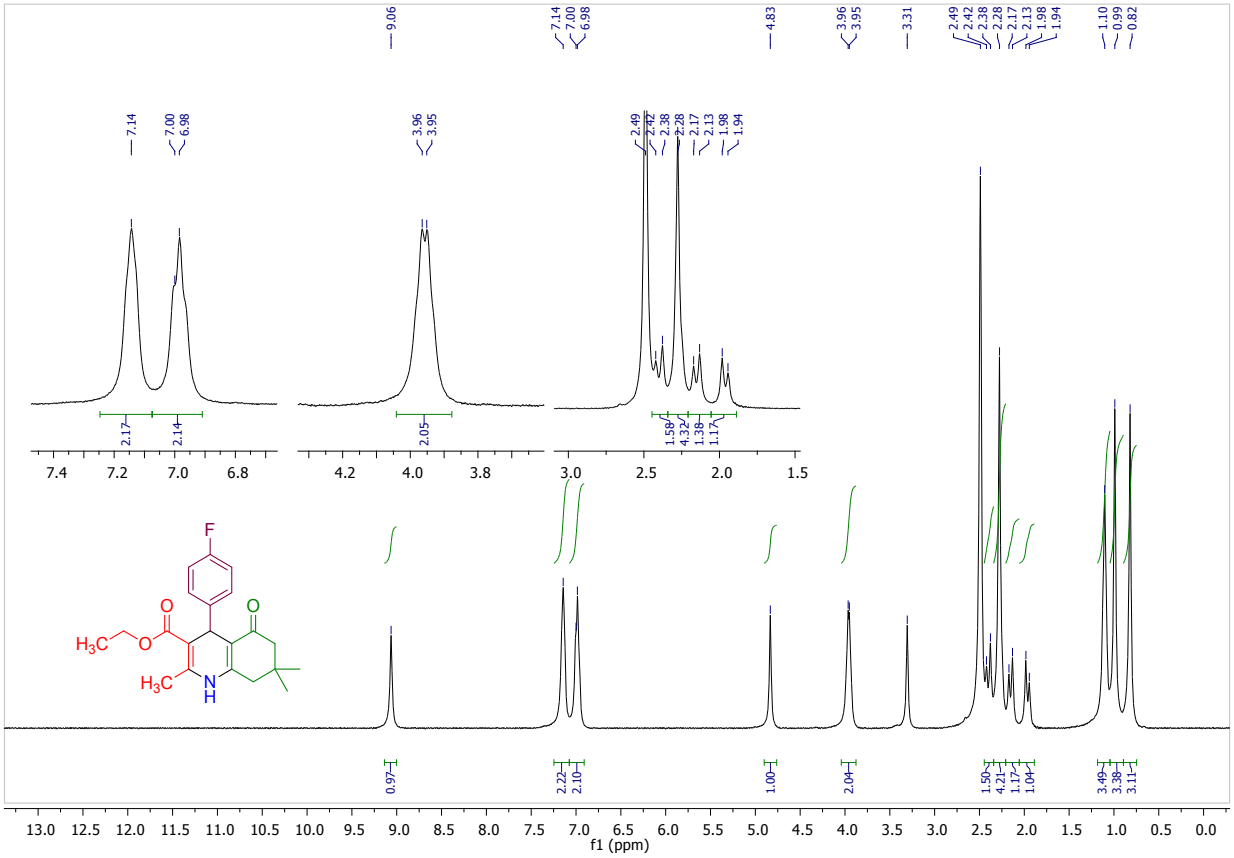
17. ^{1}H NMR spectrum of ethyl 4-(3,4-dimethoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate in Ethanol-d_6: (**1h**)



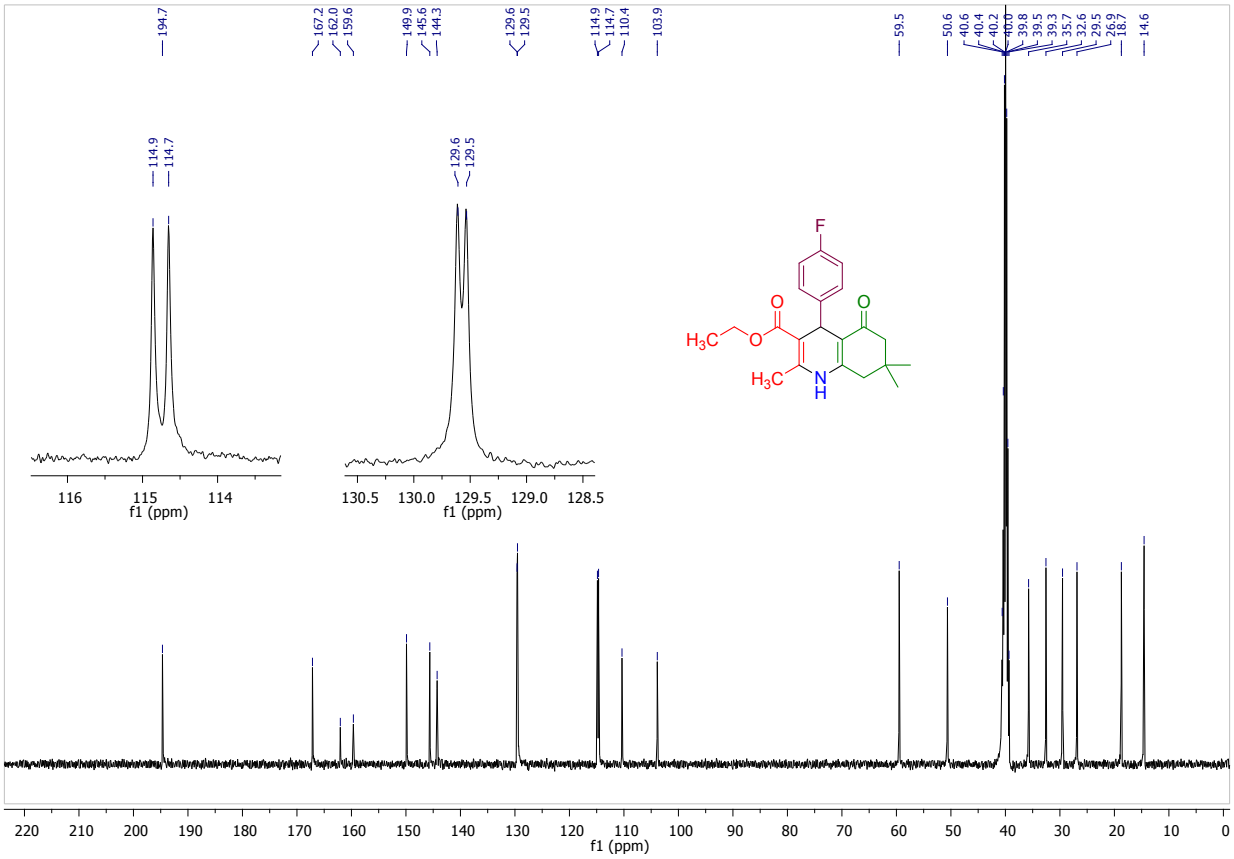
18. ^{13}C NMR spectra of ethyl 4-(3,4-dimethoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1h**)



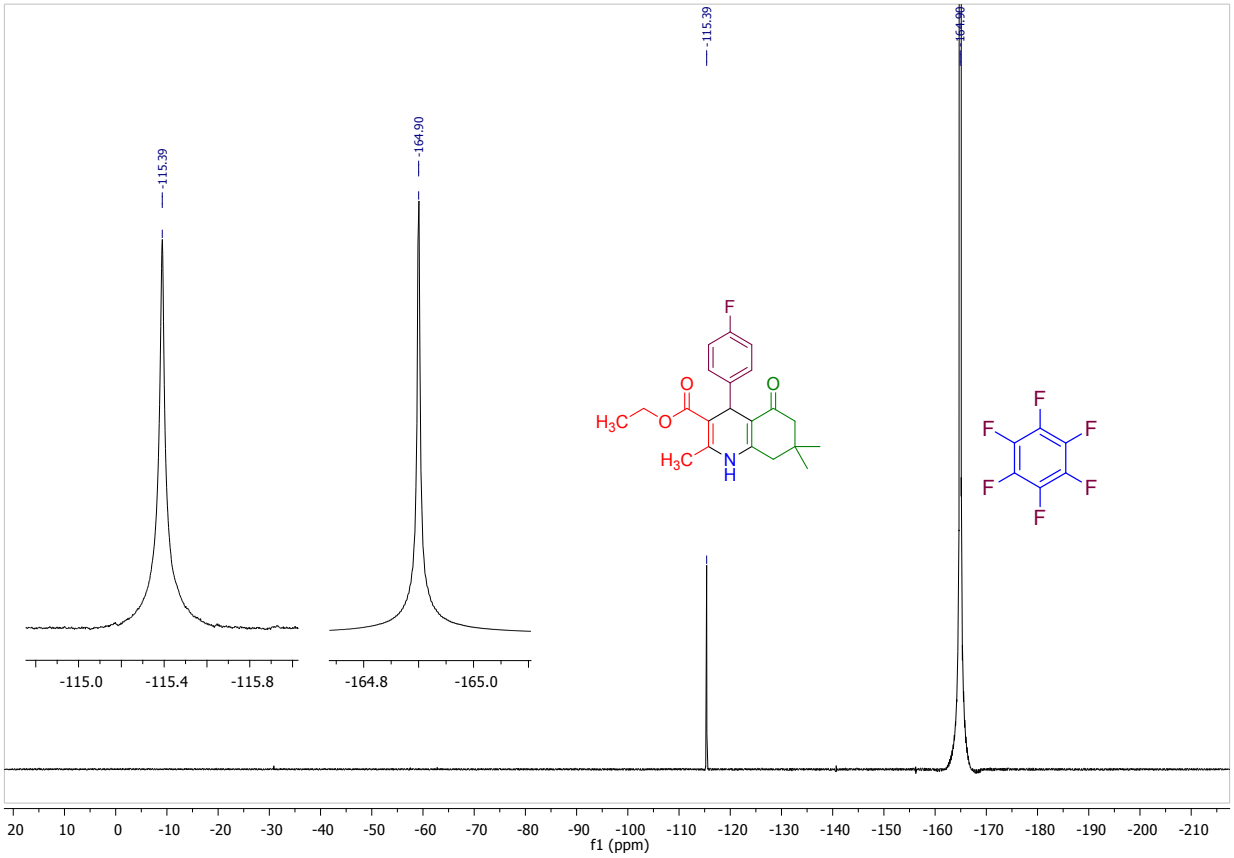
19. ^{1}H NMR spectrum of ethyl 4-(4-fluorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1i**)



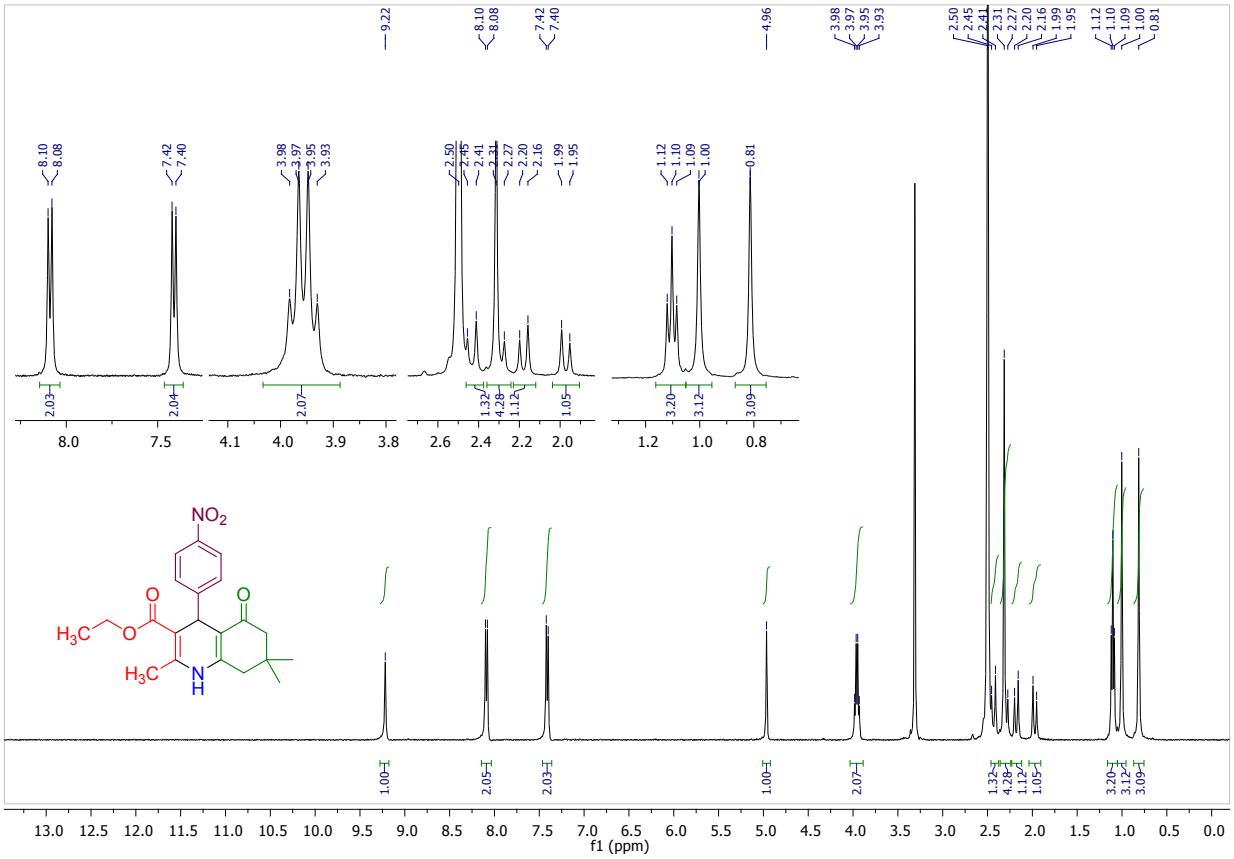
20. ^{13}C NMR spectrum of ethyl 4-(4-fluorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1i**)



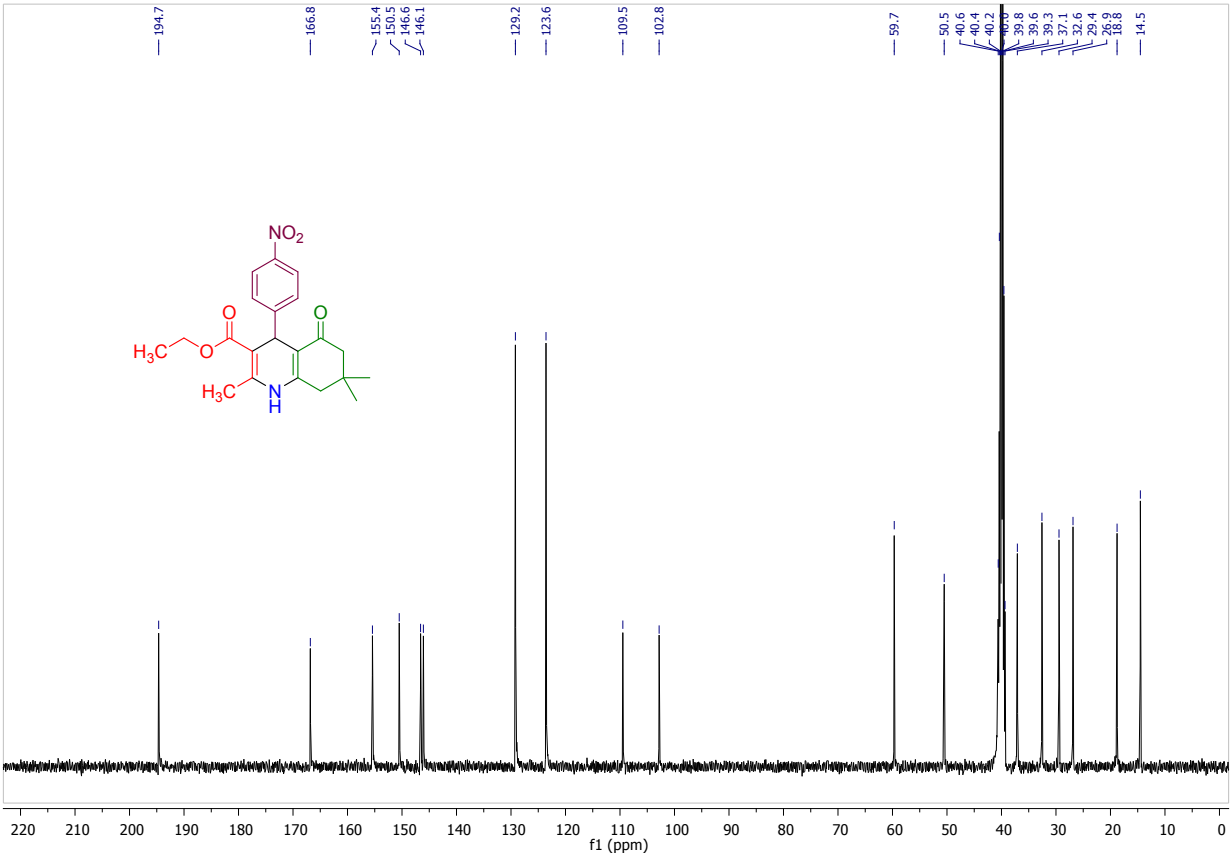
21. ^{19}F NMR spectrum of ethyl 4-(4-fluorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1i**)



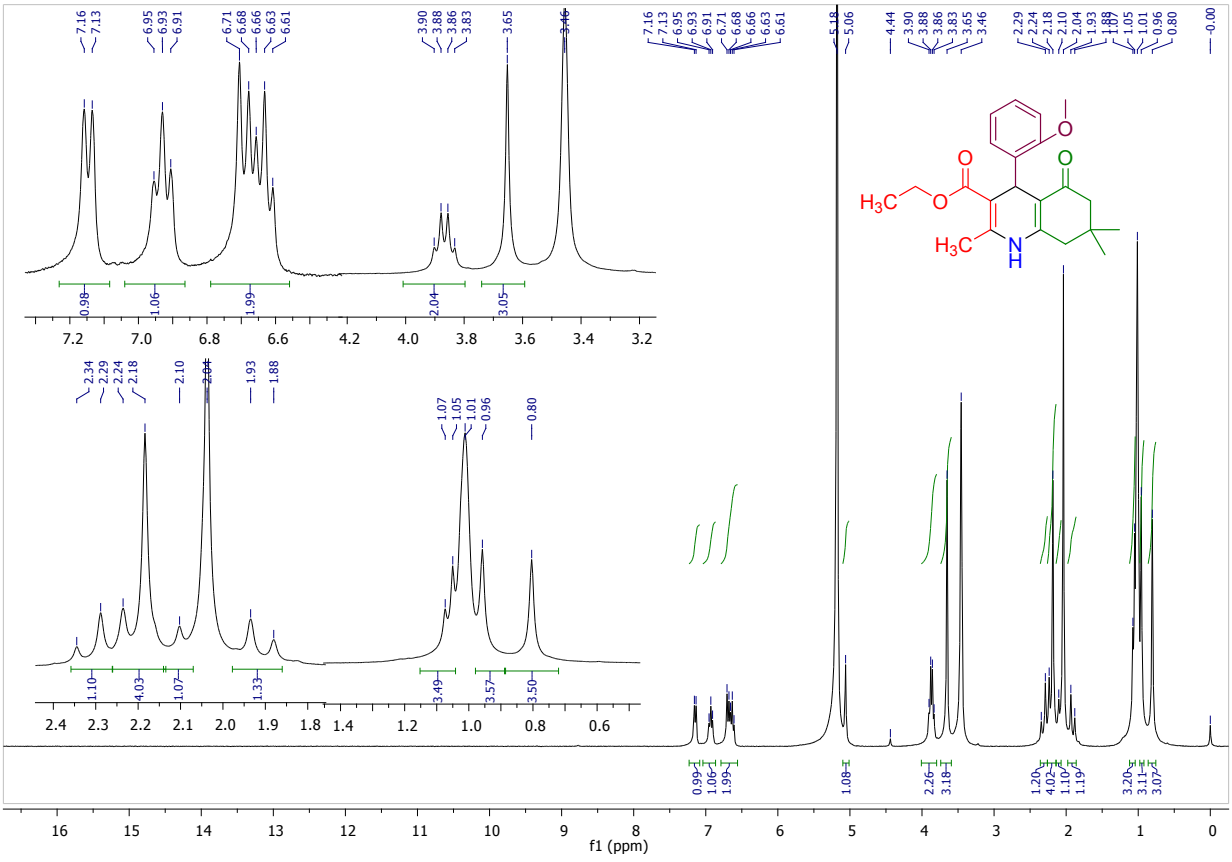
22. ^{1}H NMR spectrum of ethyl 2,7,7-trimethyl-4-(4-nitrophenyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1j**)



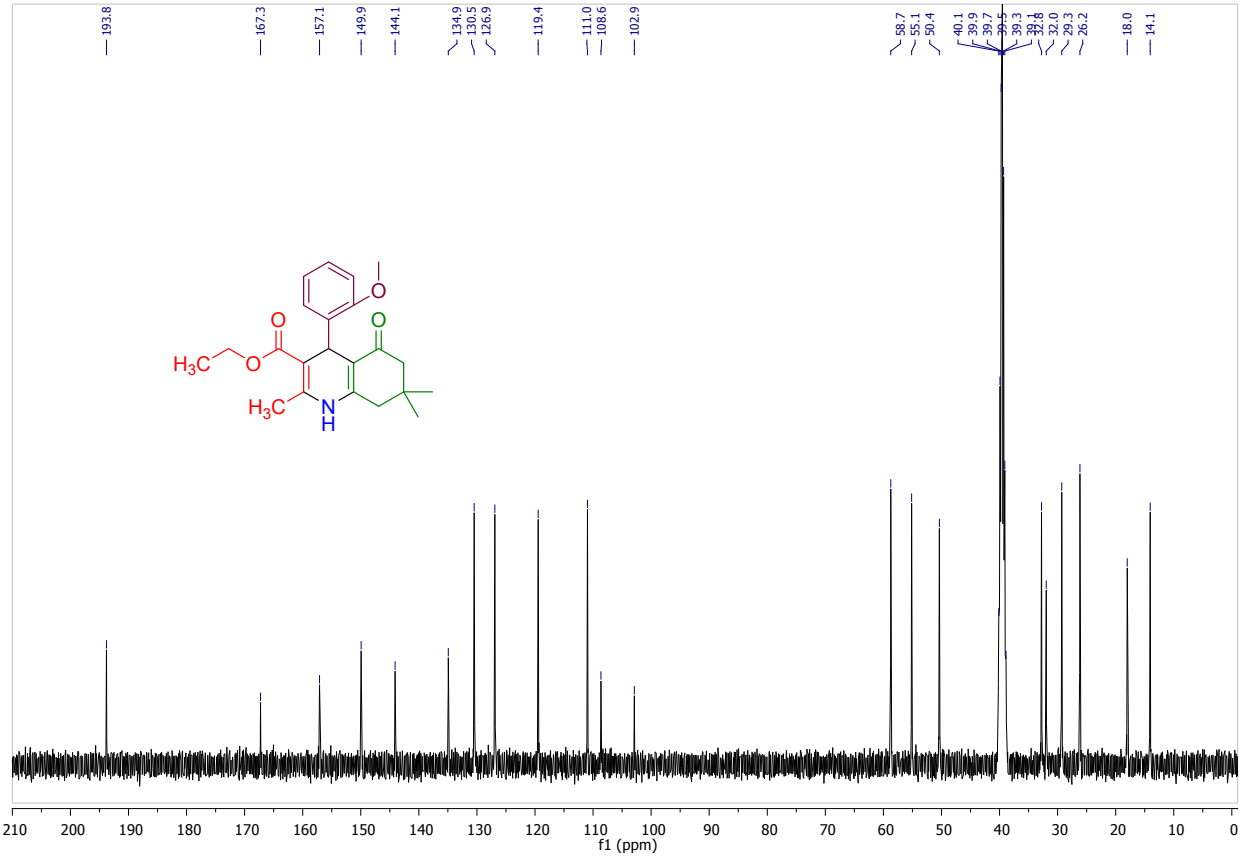
23. ^{13}C NMR spectrum of ethyl 2,7,7-trimethyl-4-(4-nitrophenyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1j**)



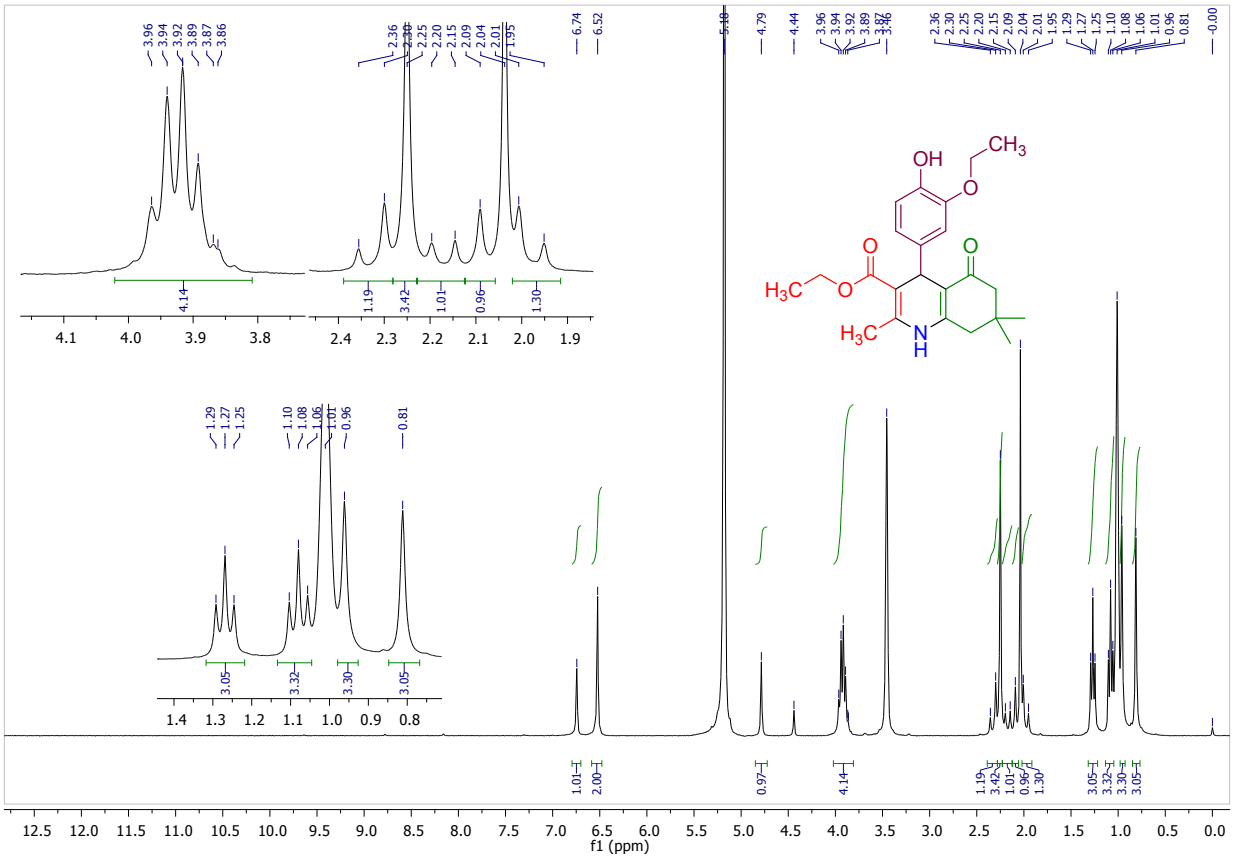
24. ^{1}H NMR spectrum of ethyl 4-(2-methoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate in EtOD-d_6: (**1k**)



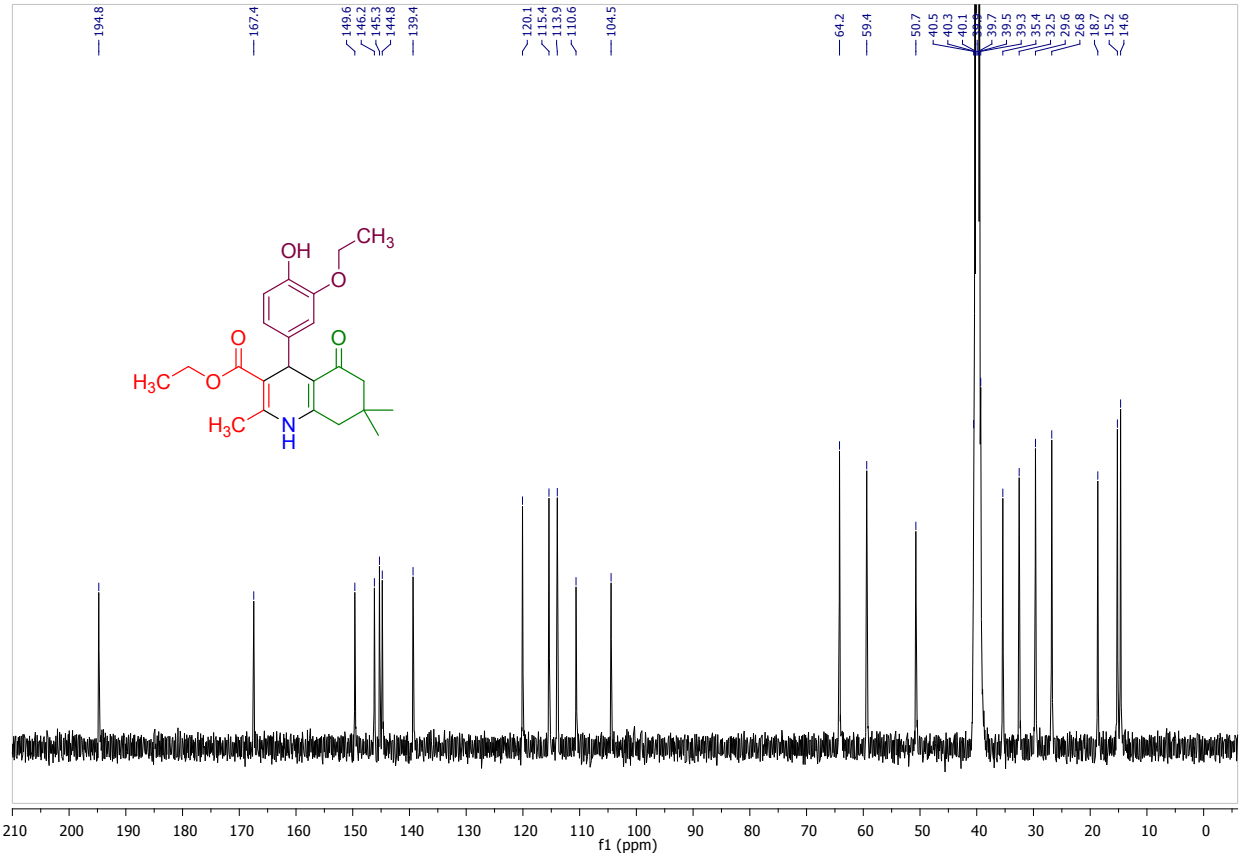
25. ^{13}C NMR spectrum of ethyl 4-(2-methoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1k**)



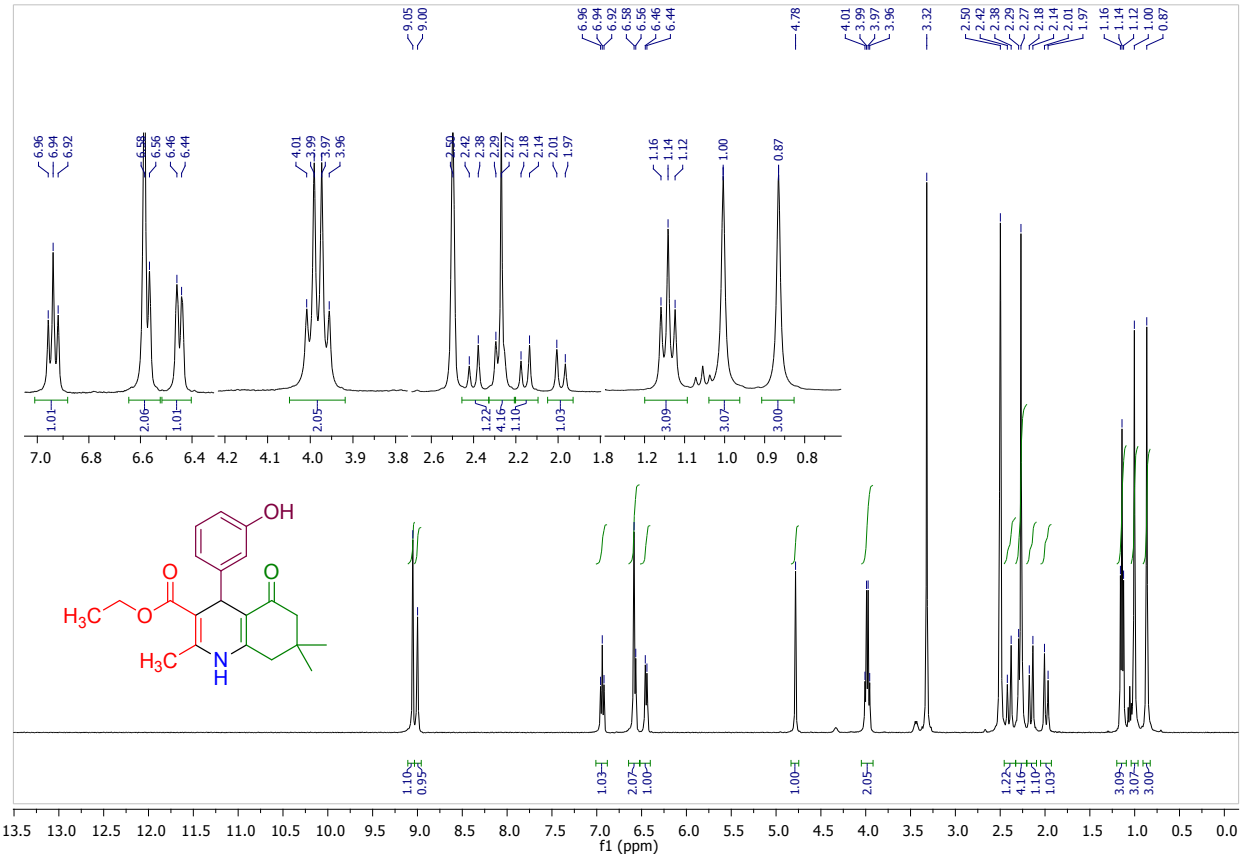
26. ^{1}H NMR spectrum ethyl 4-(3-ethoxy-4-hydroxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate in Ethanol-d_6: (**1l**)



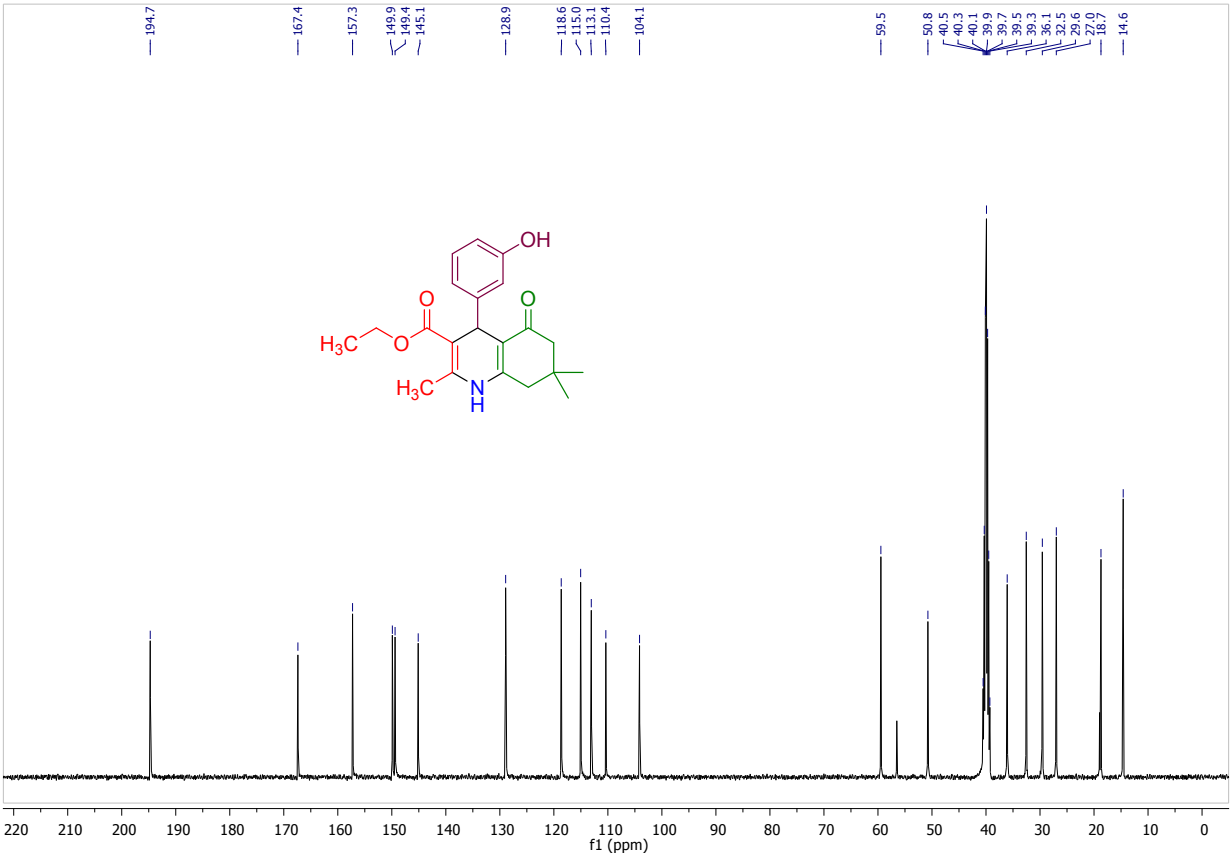
27. ^{13}C NMR spectrum ethyl 4-(3-ethoxy-4-hydroxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1l**)



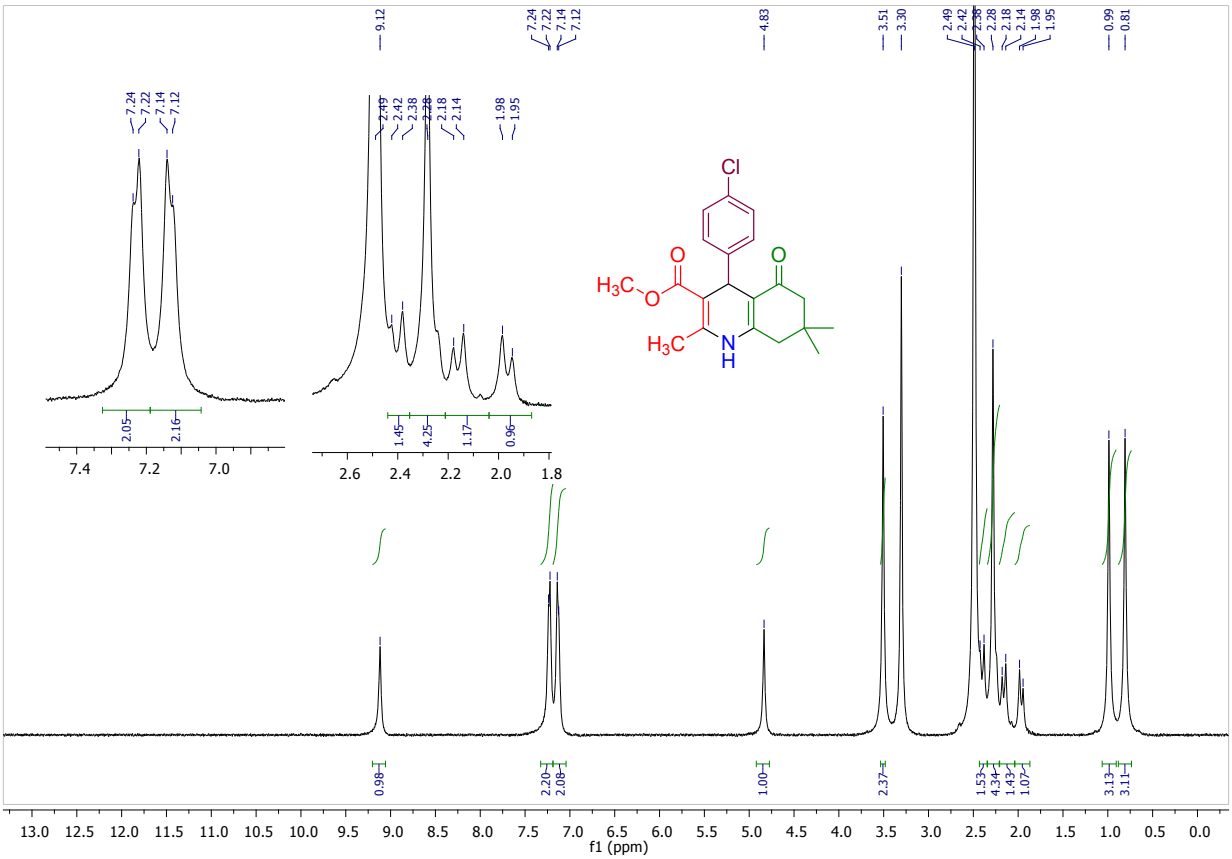
28. ^{1}H NMR spectrum of ethyl 4-(3-hydroxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1m**)



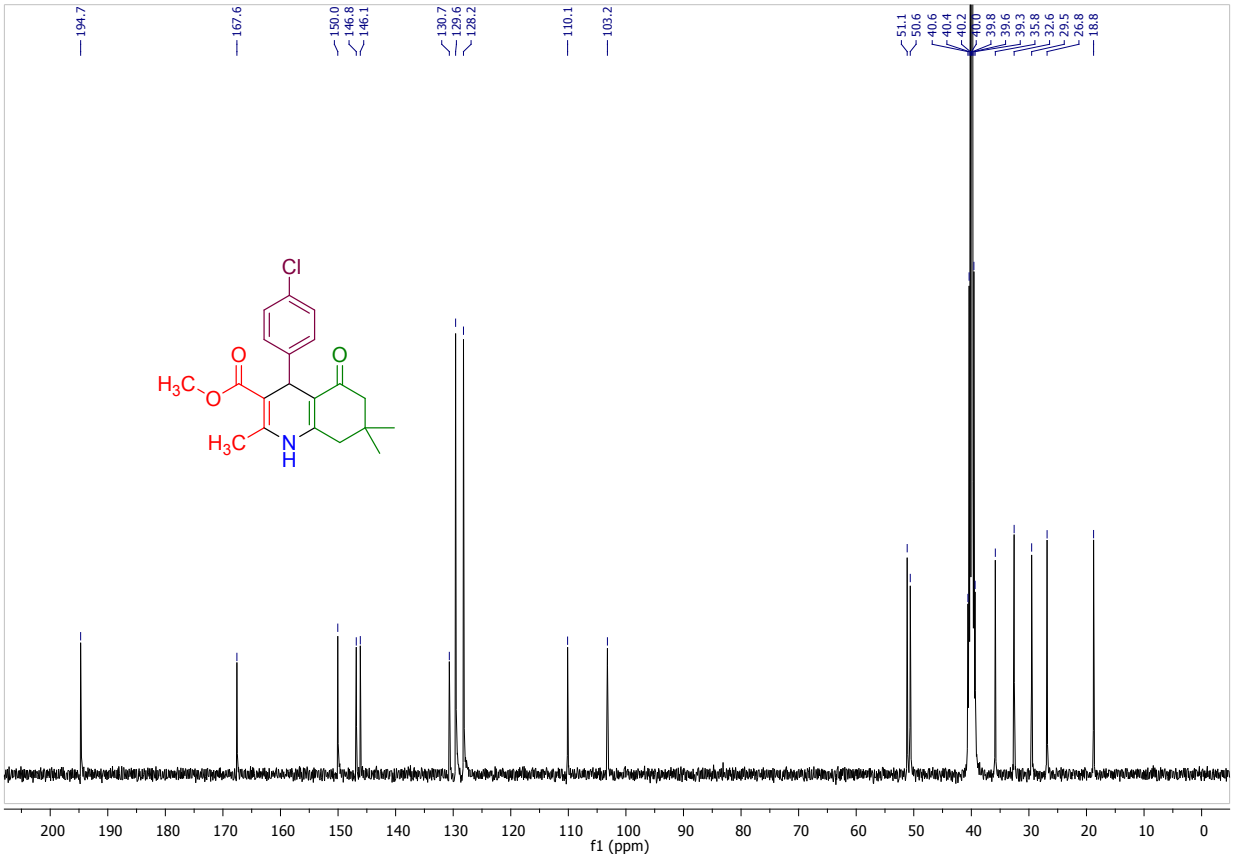
29. ^{13}C NMR spectrum of ethyl 4-(3-hydroxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1m**)



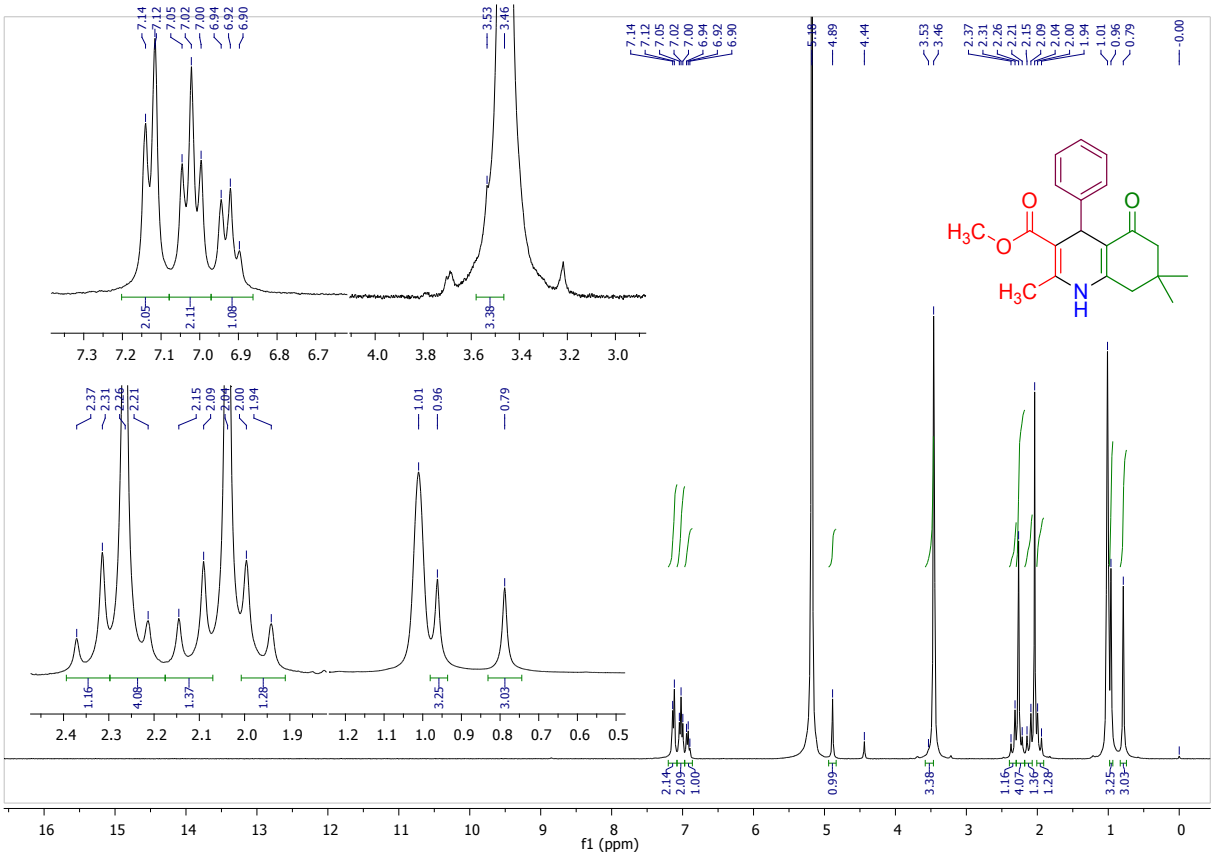
30. ^{1}H NMR spectrum of methyl 4-(4-chlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1n**)



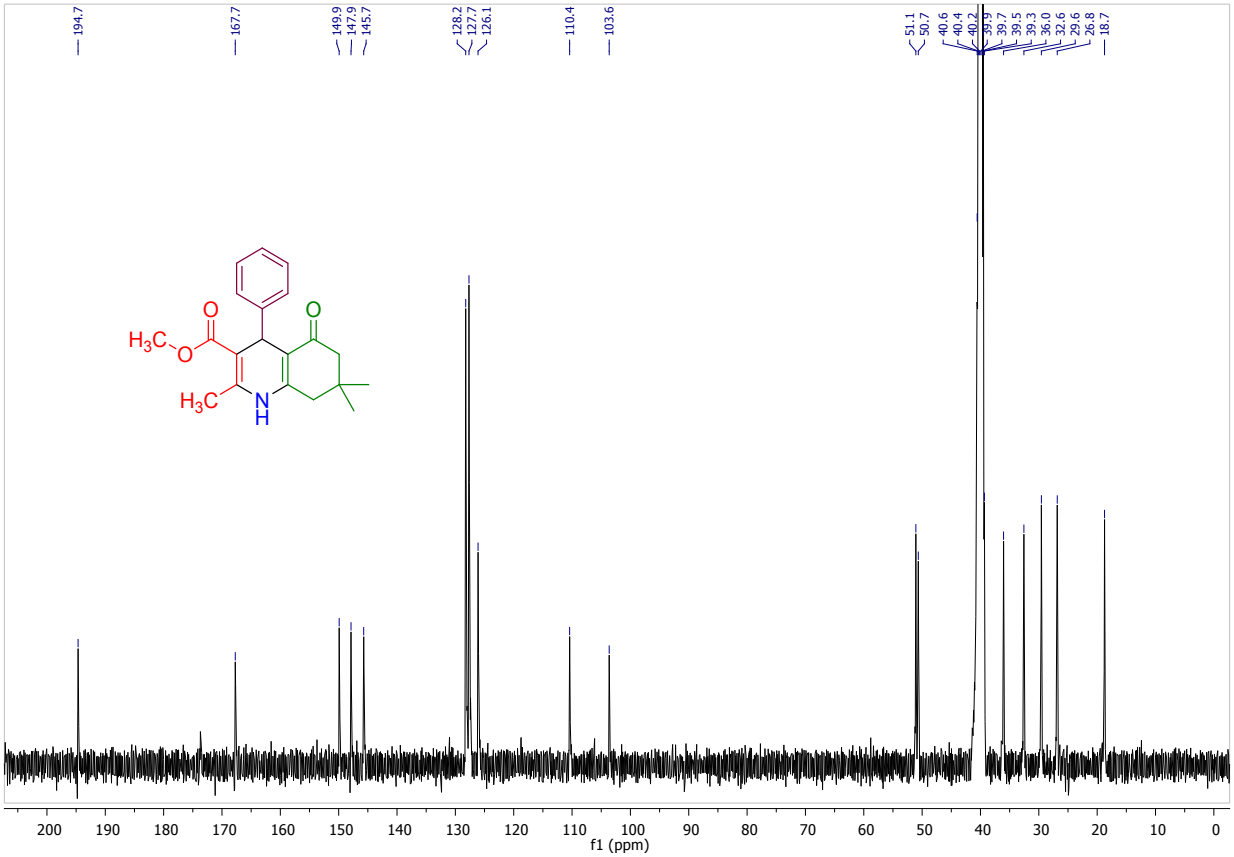
31. ^{13}C NMR spectrum of methyl 4-(4-chlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1n**)



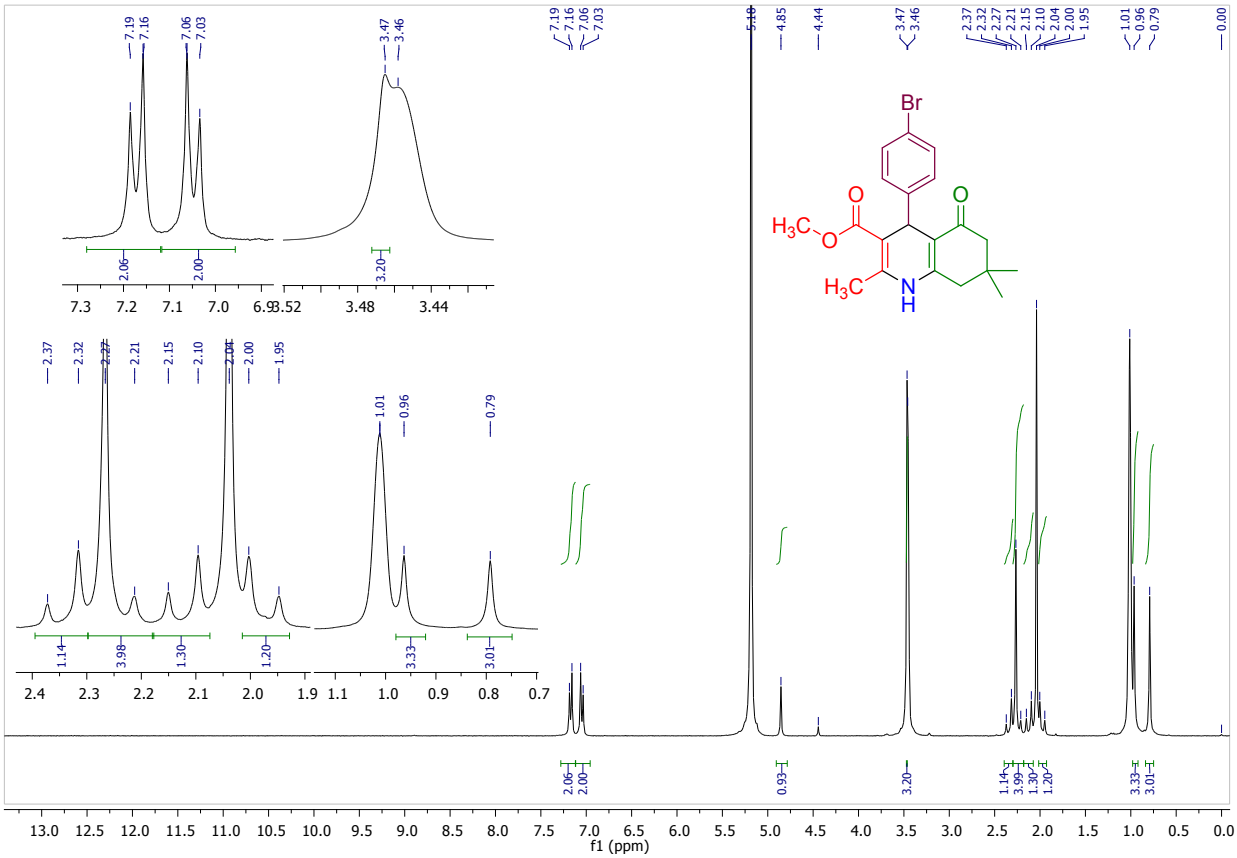
32. ^{1}H NMR spectrum of methyl 2,7,7-trimethyl-5-oxo-4-phenyl-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate in Ethanol-d_6: (**1o**)



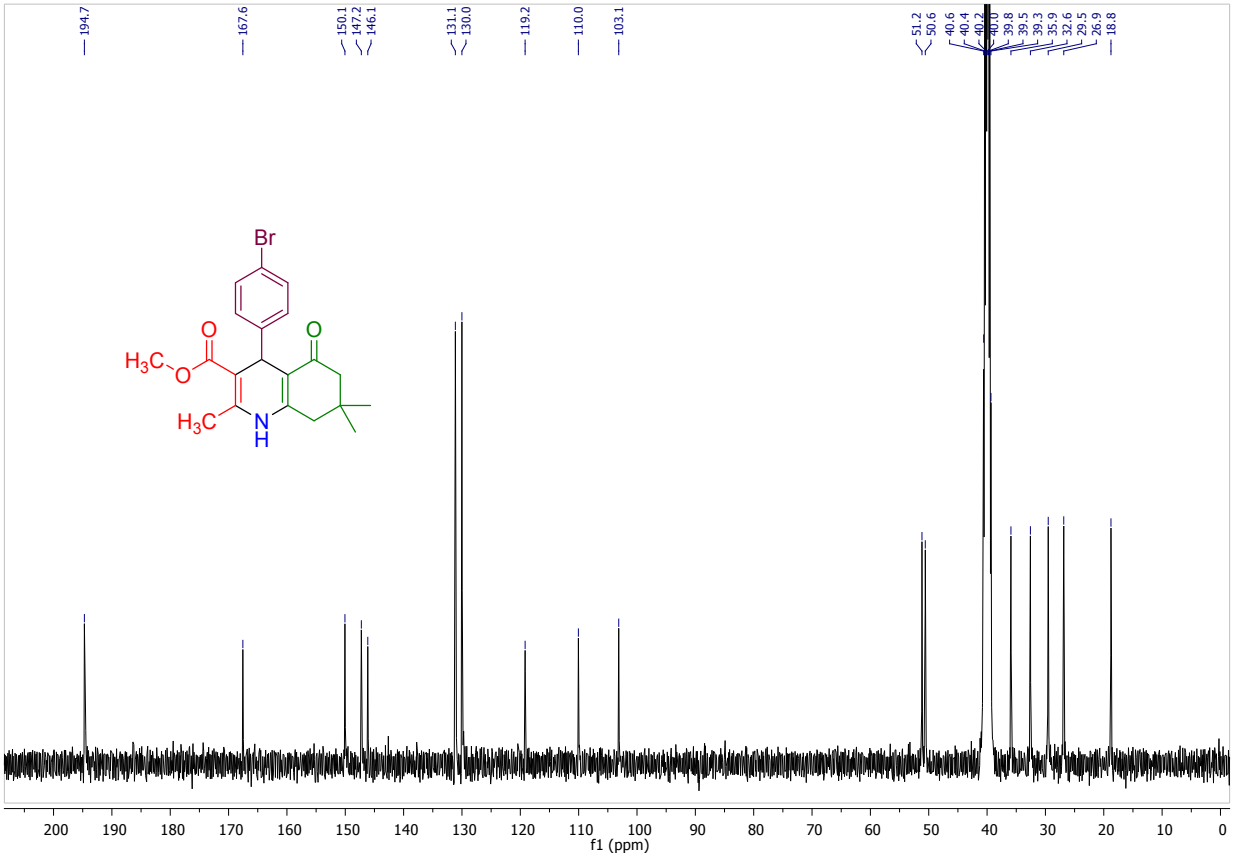
33. ^{13}C NMR spectrum of methyl 2,7,7-trimethyl-5-oxo-4-phenyl-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1o**)



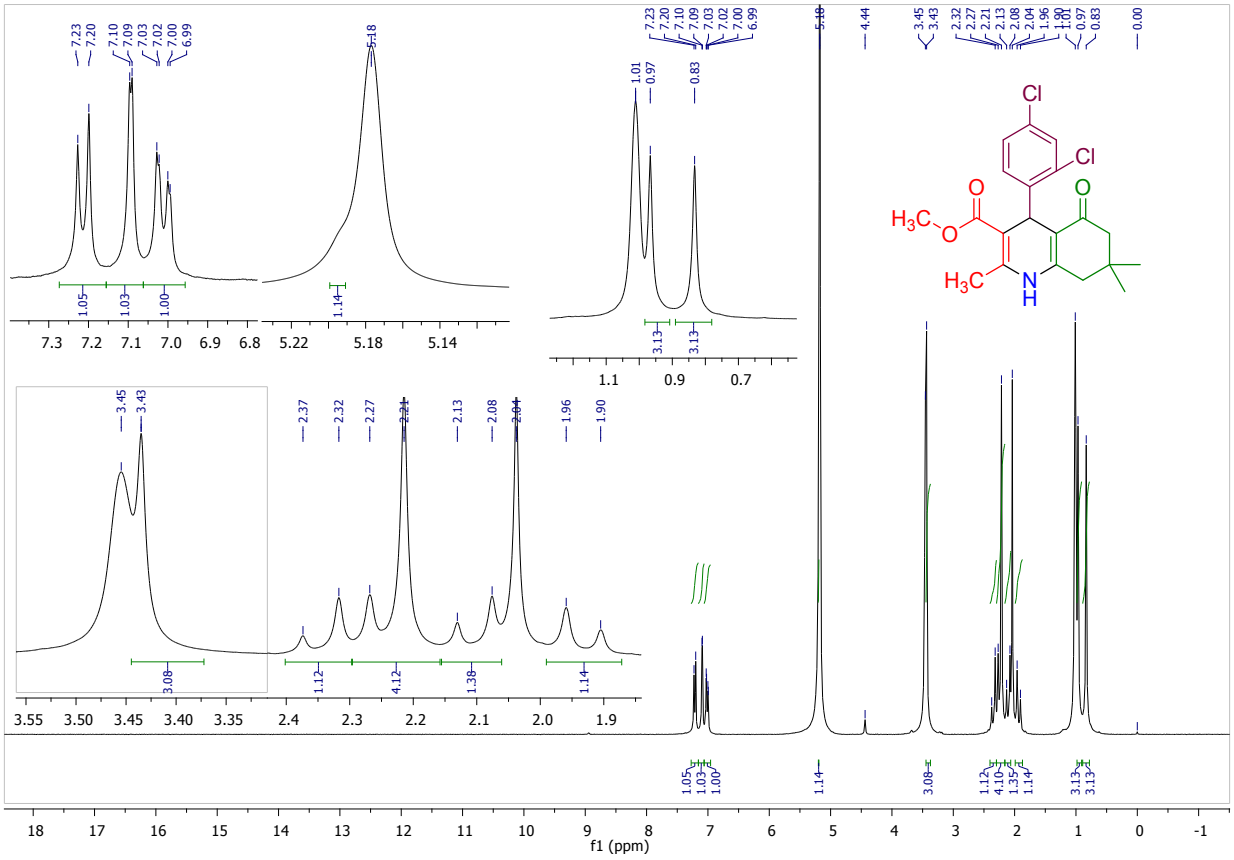
34. ^{1}H NMR spectrum of methyl 4-(4-bromophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate in Ethanol-d_6: (**1p**)



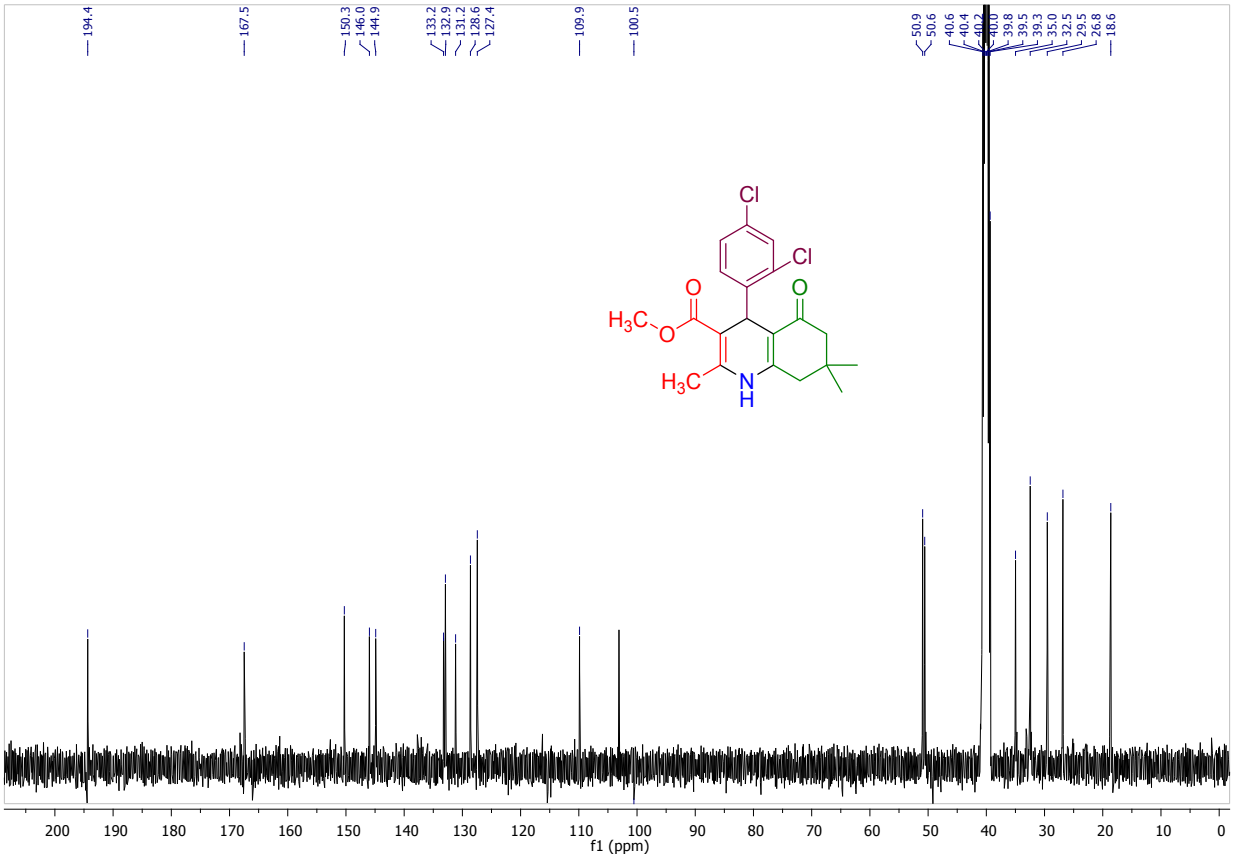
35. ^{13}C NMR spectrum of methyl 4-(4-bromophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1p**)



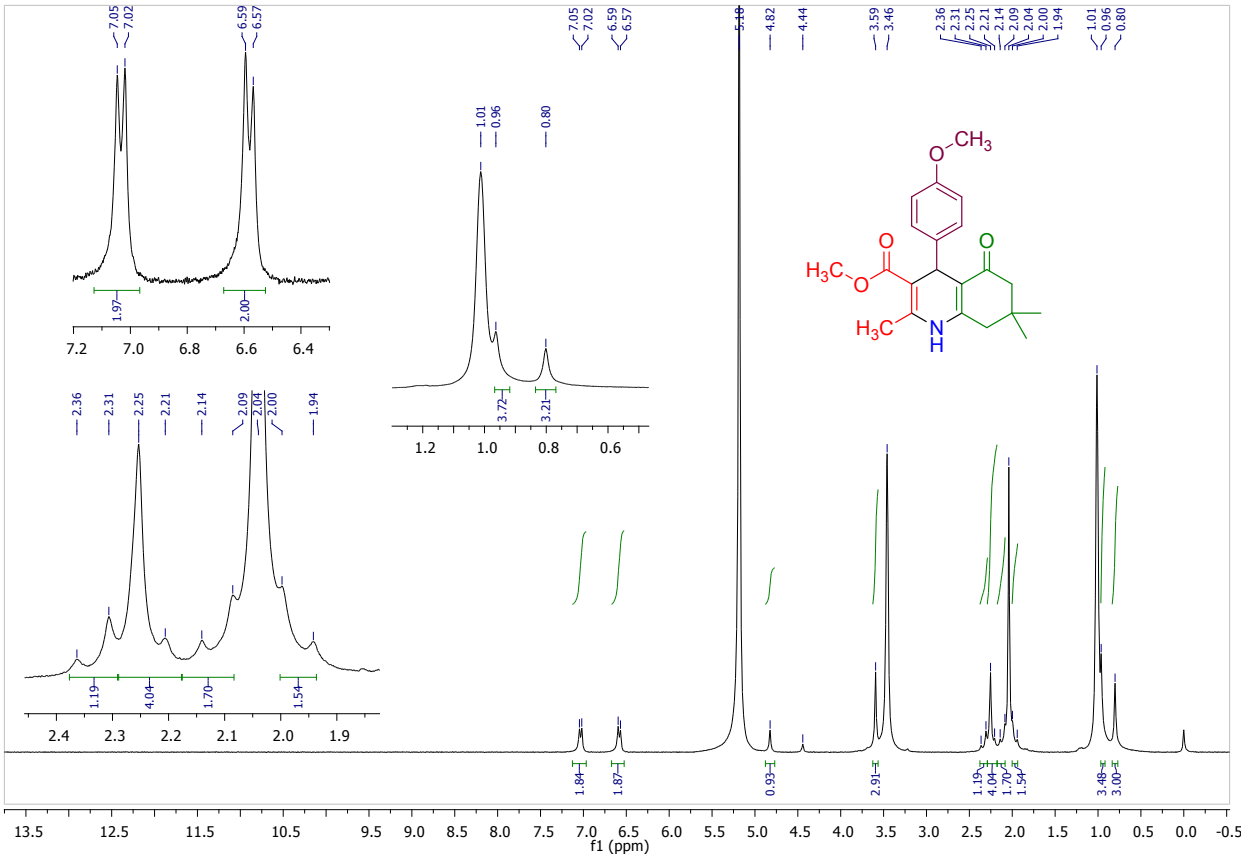
36. ^{1}H NMR spectrum of methyl 4-(2,4-dichlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate in Ethanol-d_6: (**1q**)



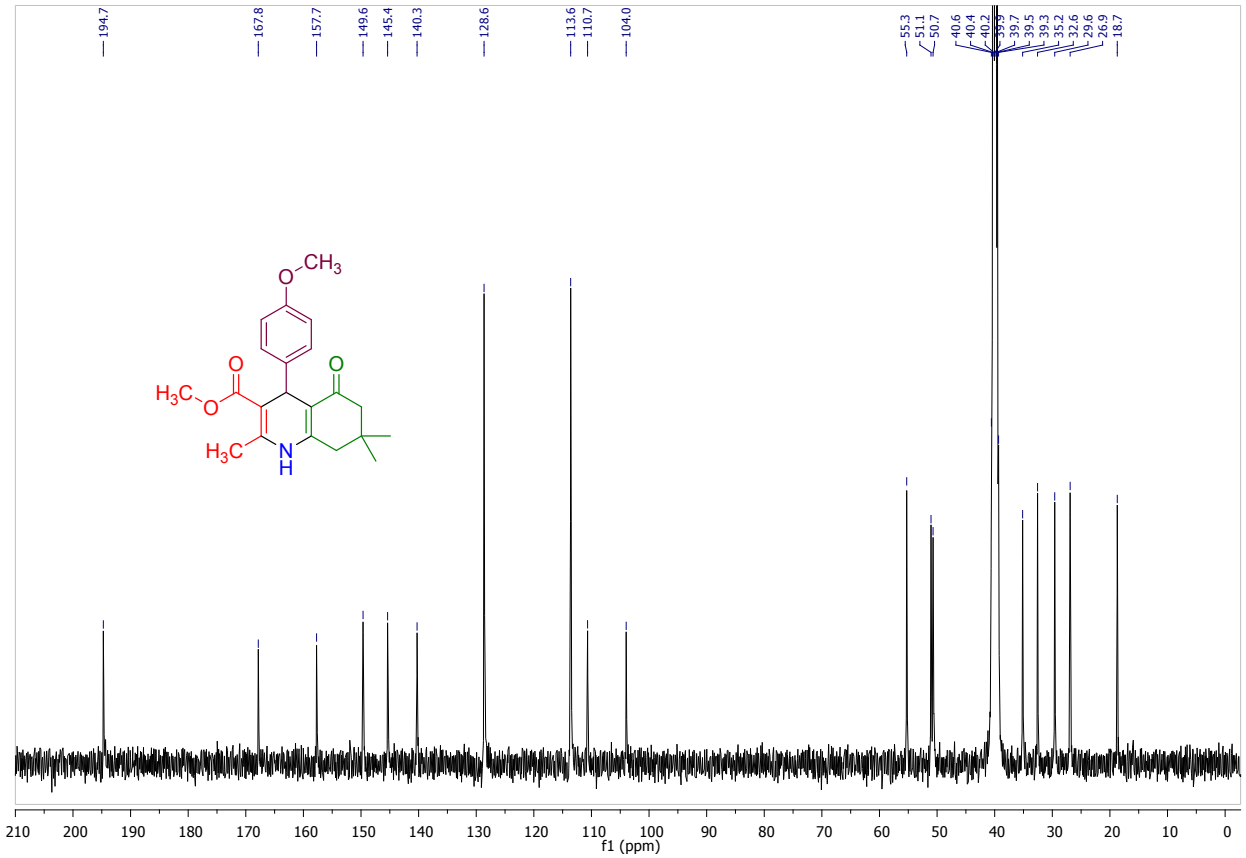
37. ^{13}C NMR spectrum of methyl 4-(2,4-dichlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1q**)



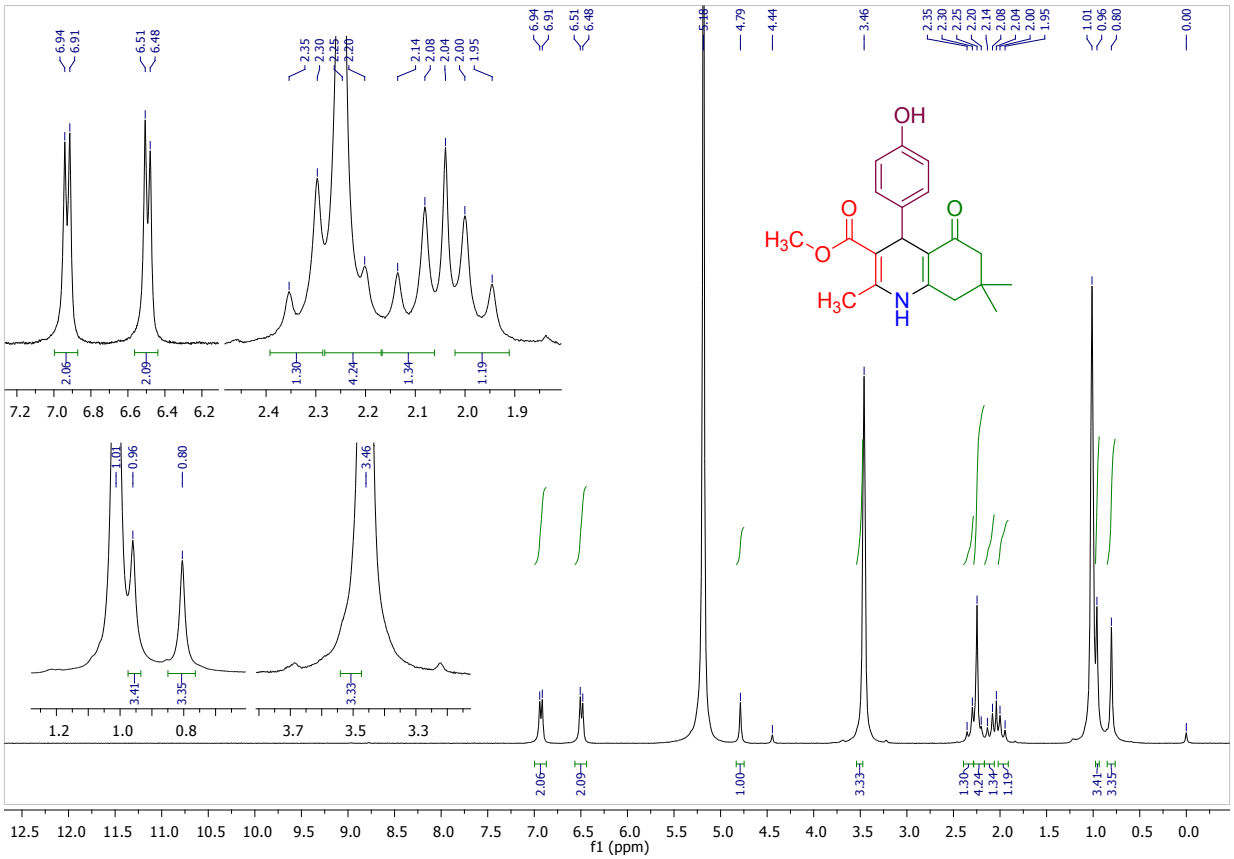
38. ^{1}H NMR spectrum of methyl 4-(4-methoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate in Ethanol-d_6: (**1r**)



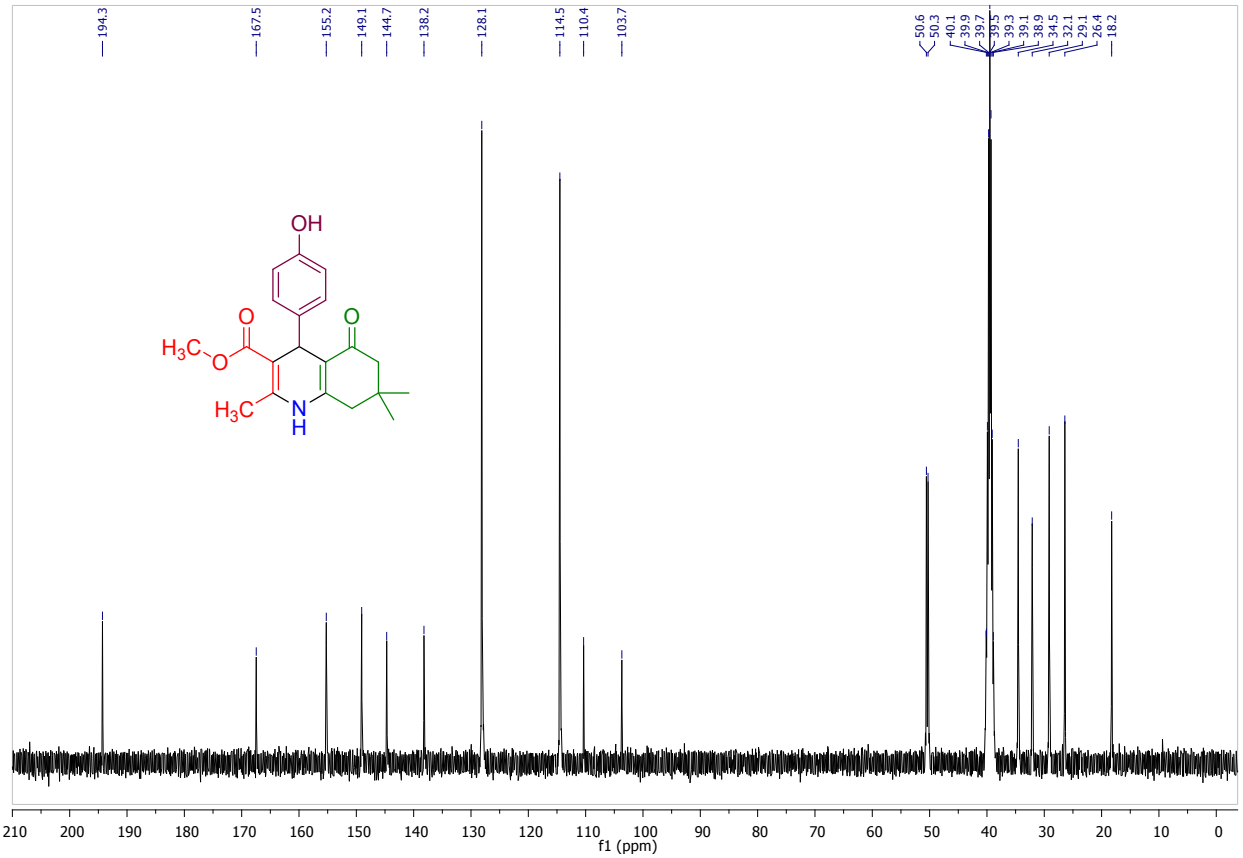
39. ^{13}C NMR spectrum of methyl 4-(4-methoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1r**)



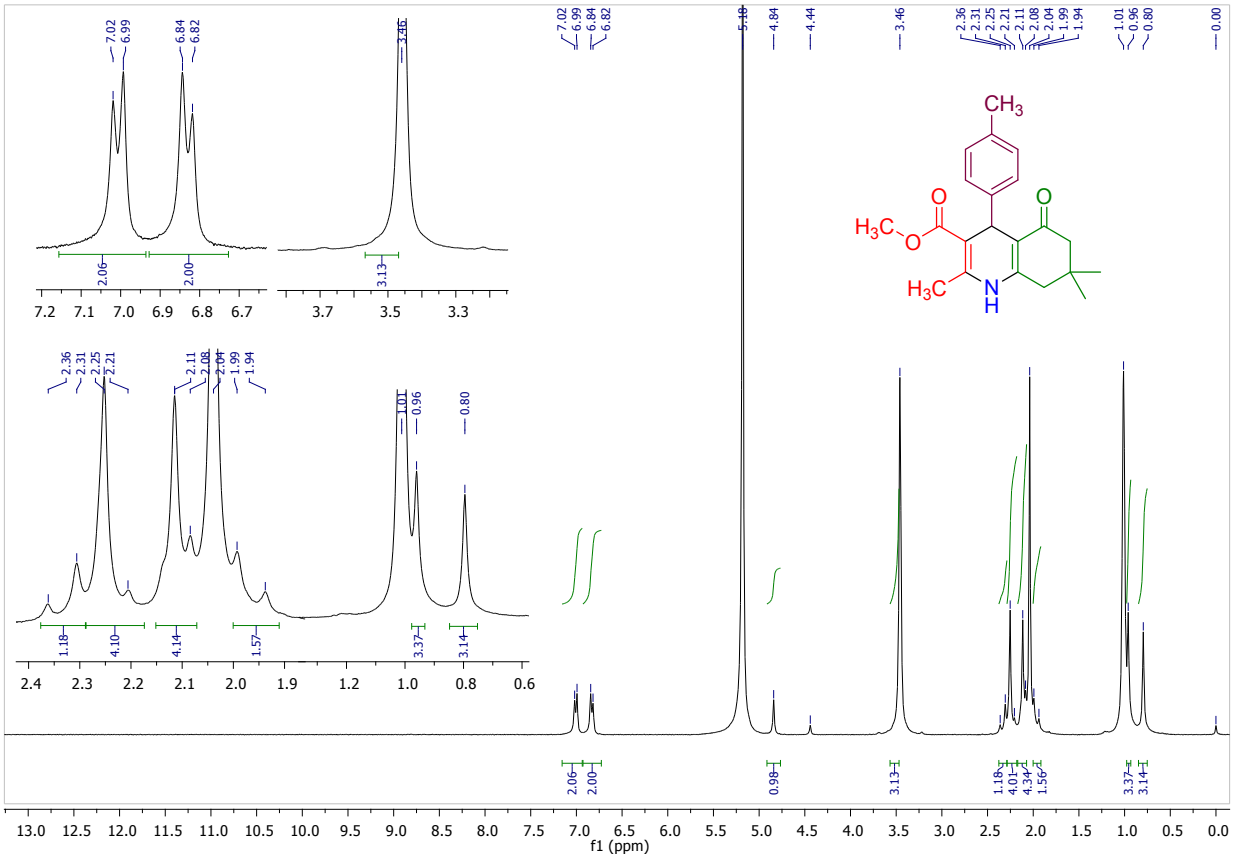
40. ^{1}H NMR spectrum of methyl 4-(4-hydroxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1s**)



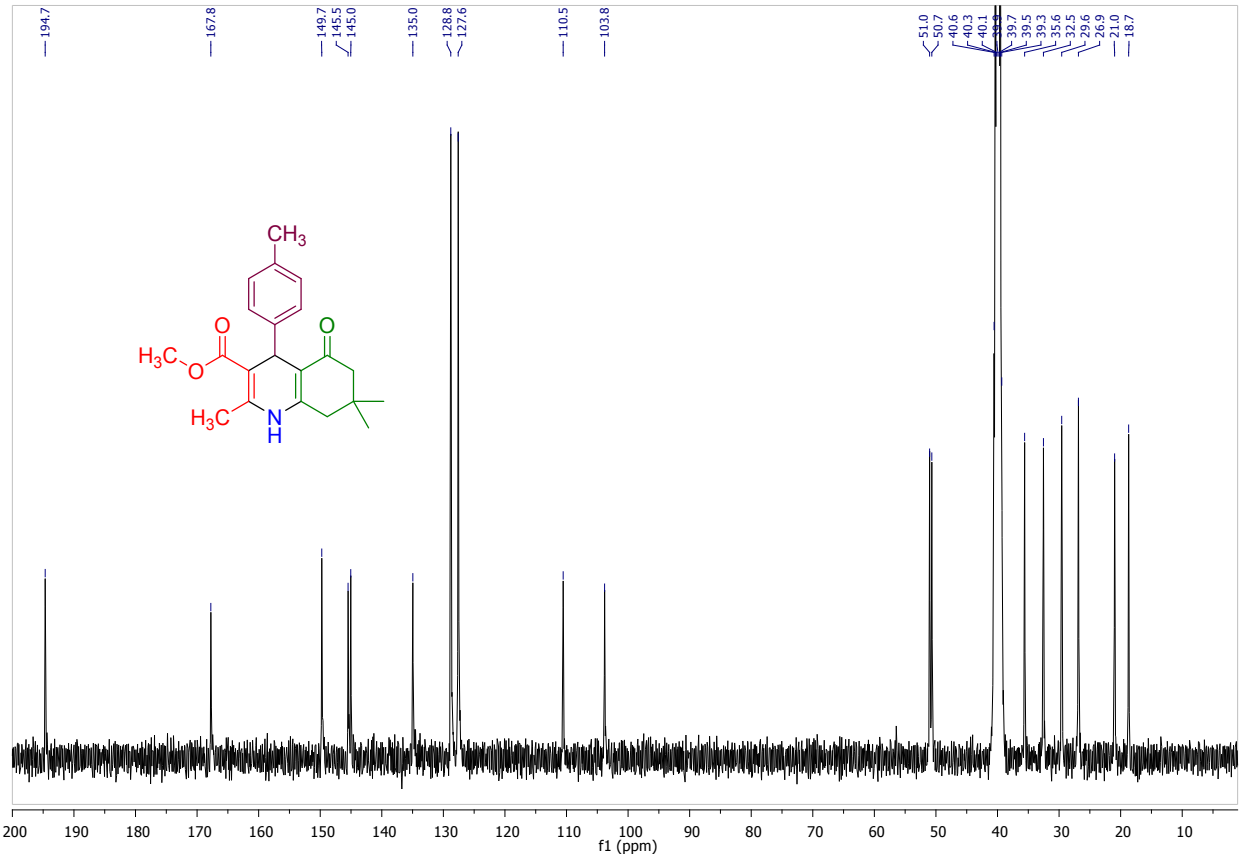
41. ^{13}C NMR spectrum of methyl 4-(4-hydroxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1s**)



42. ^{1}H NMR spectrum of methyl 2,7,7-trimethyl-5-oxo-4-(p-tolyl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate in Ethanol-d_6: (**1t**)



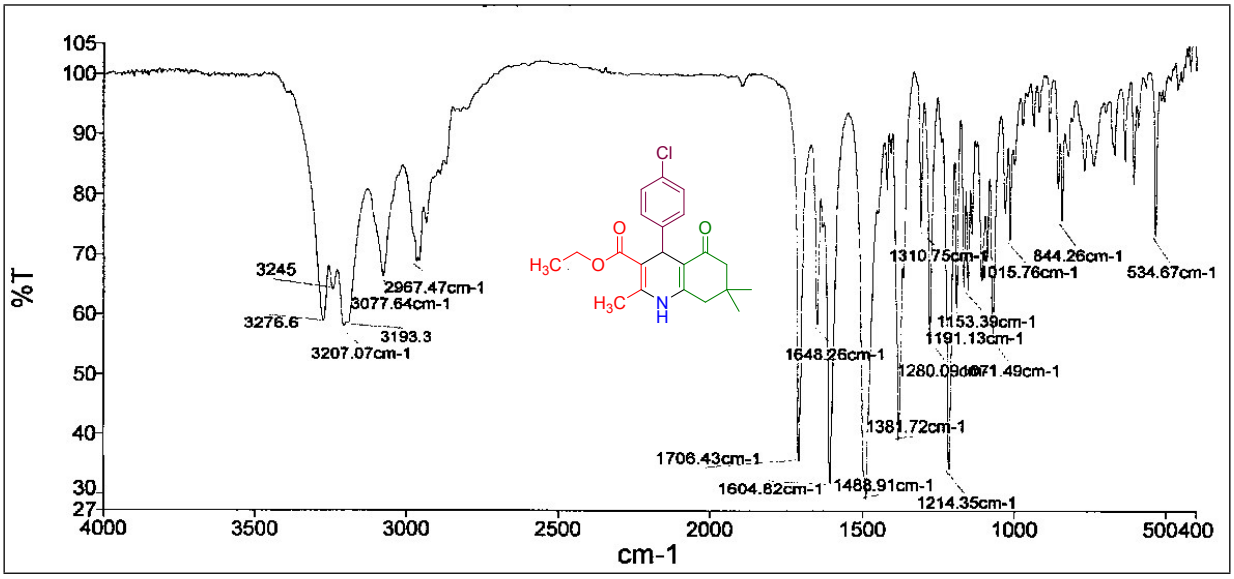
43. ^{13}C NMR spectrum of methyl 2,7,7-trimethyl-5-oxo-4-(p-tolyl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1t**)



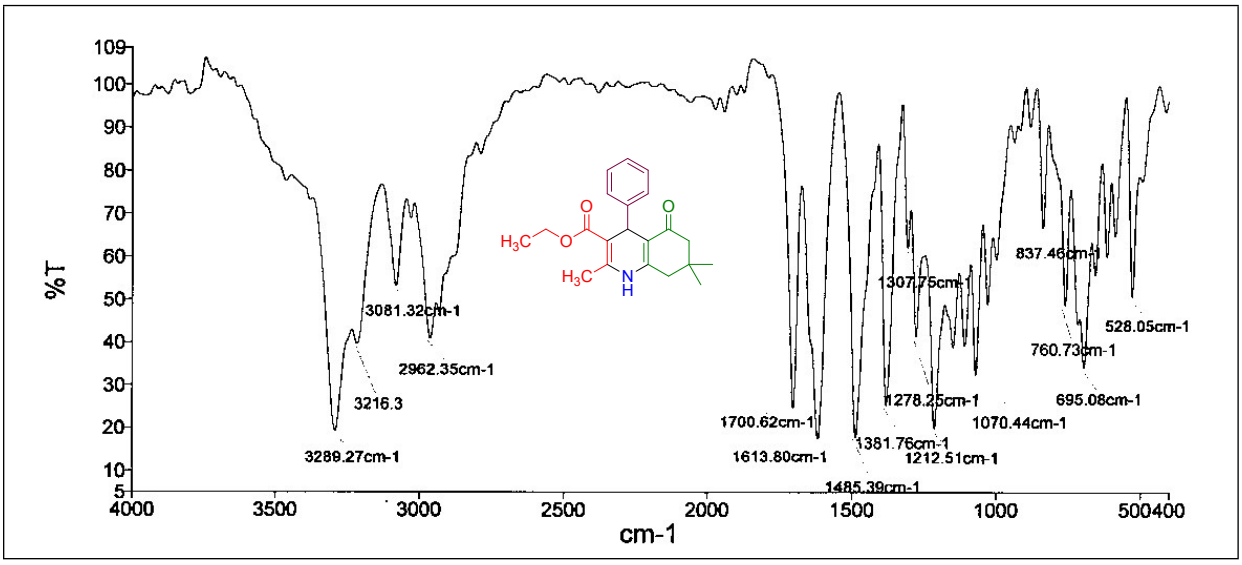
PART 2

FT-IR

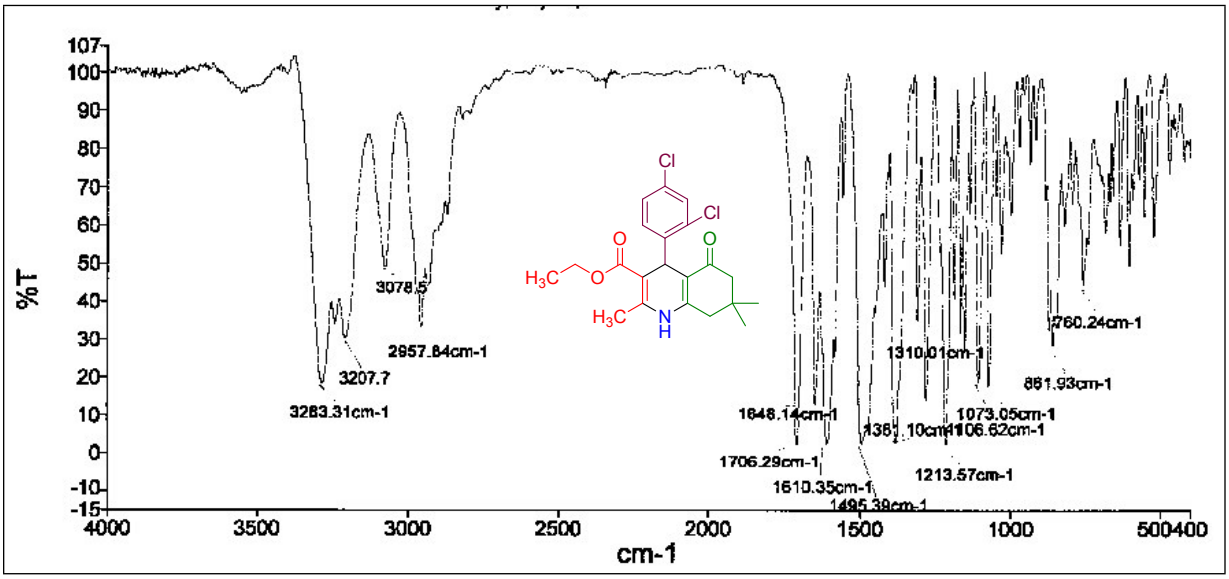
44. FT-IR spectra of ethyl 4-(4-chlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1a**)



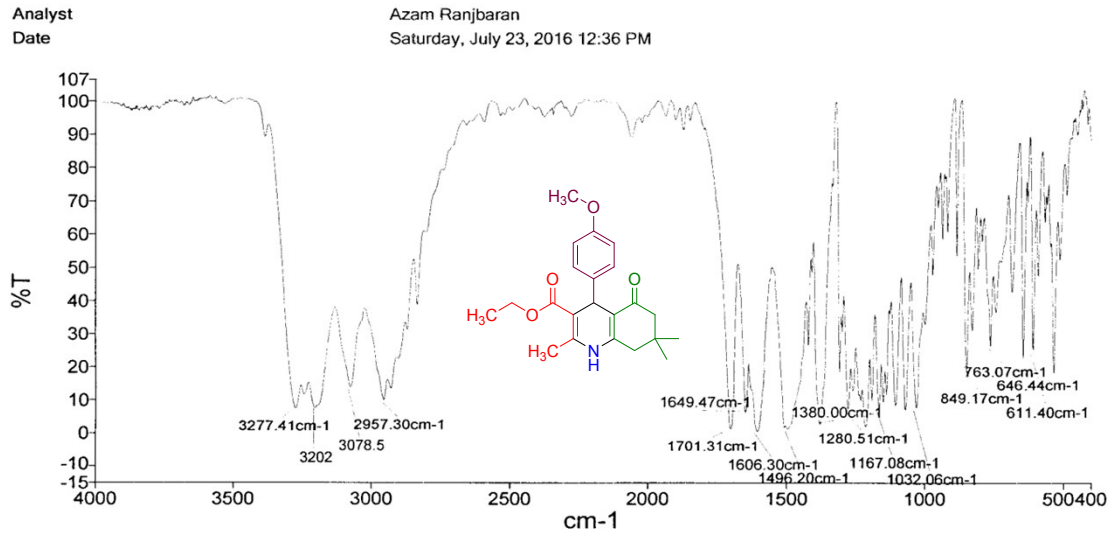
45. FT-IR spectra of ethyl 2,7,7-trimethyl-5-oxo-4-phenyl-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1b**)



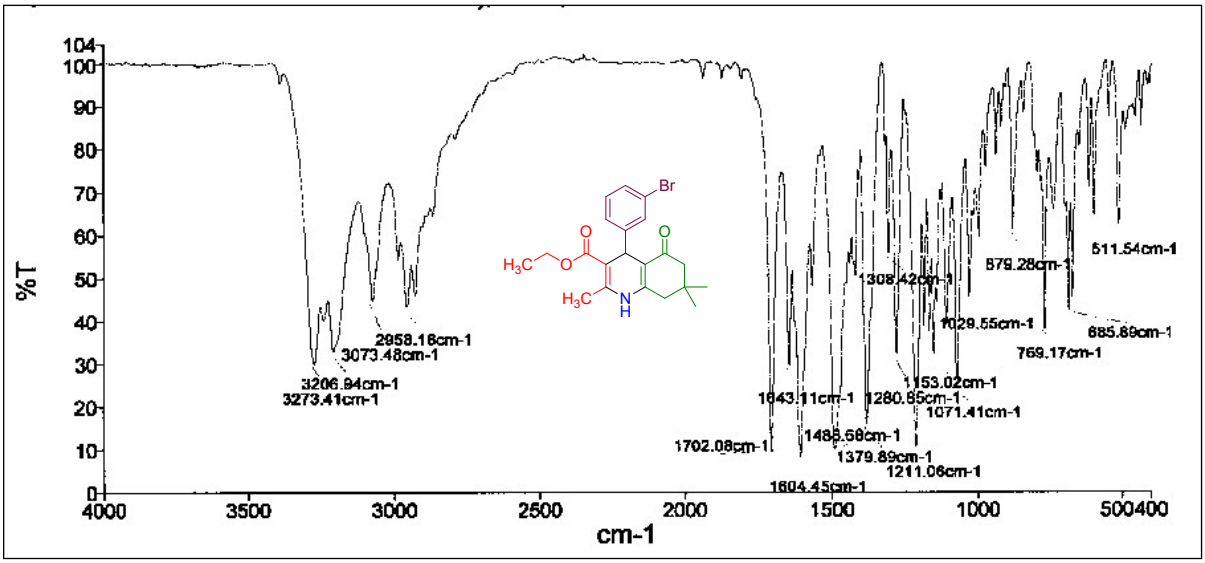
46. FT-IR spectra of ethyl 4-(2,4-dichlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1c**)



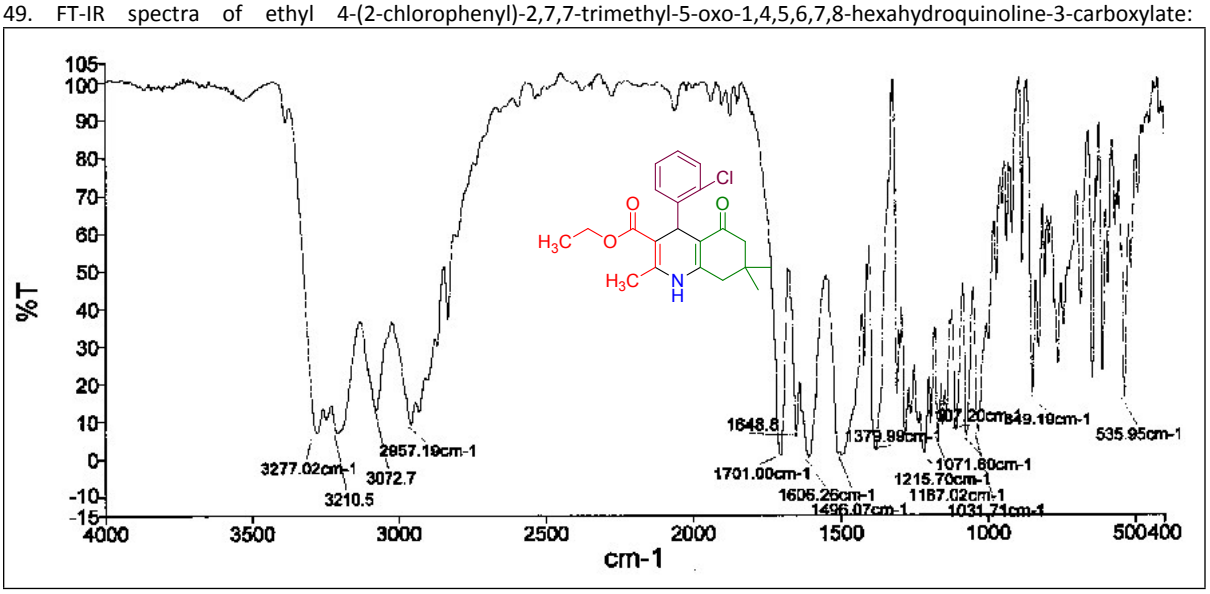
47. FT-IR spectra of ethyl 4-(4-methoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1d**)



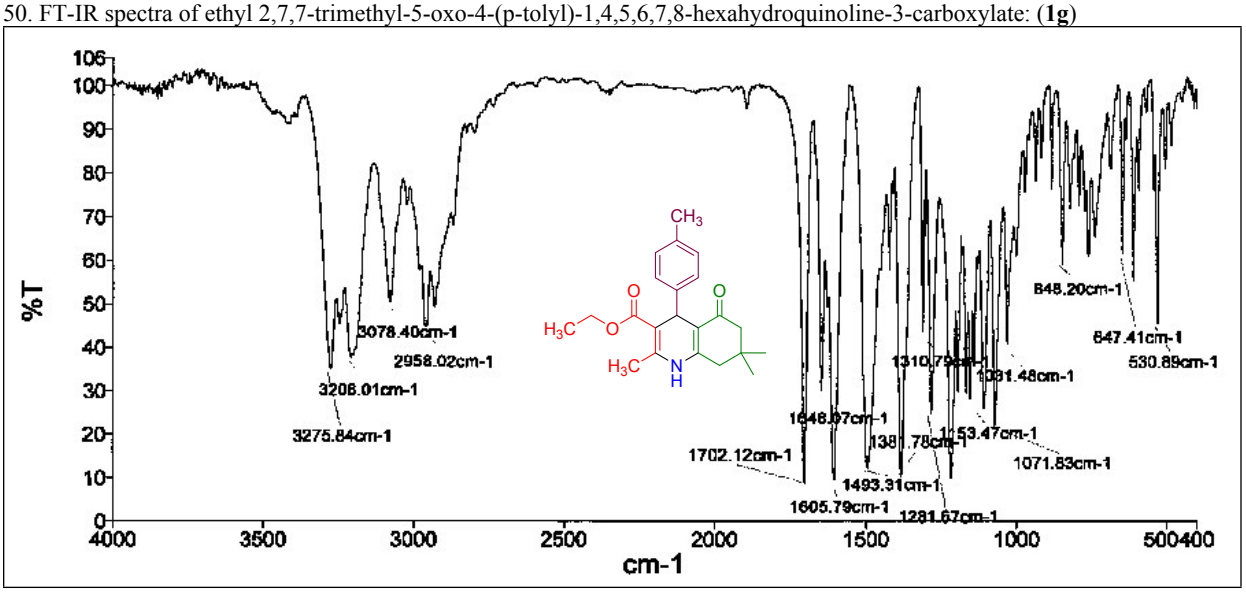
48. FT-IR spectra of ethyl 4-(3-bromophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1e**)



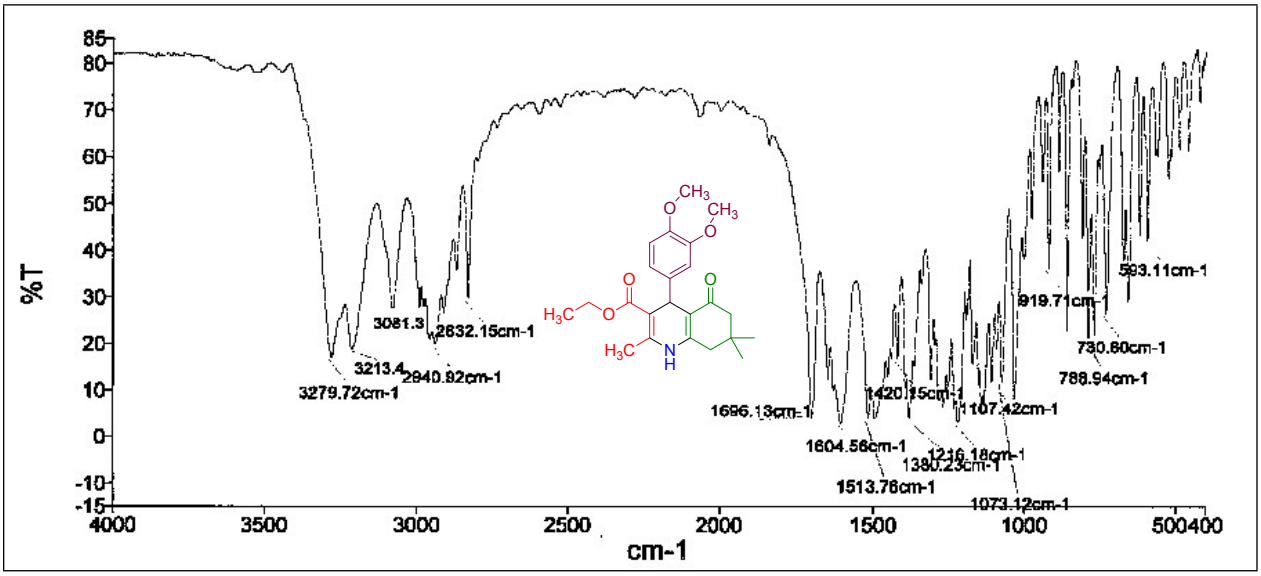
49. FT-IR spectra of ethyl 4-(2-chlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1f**)



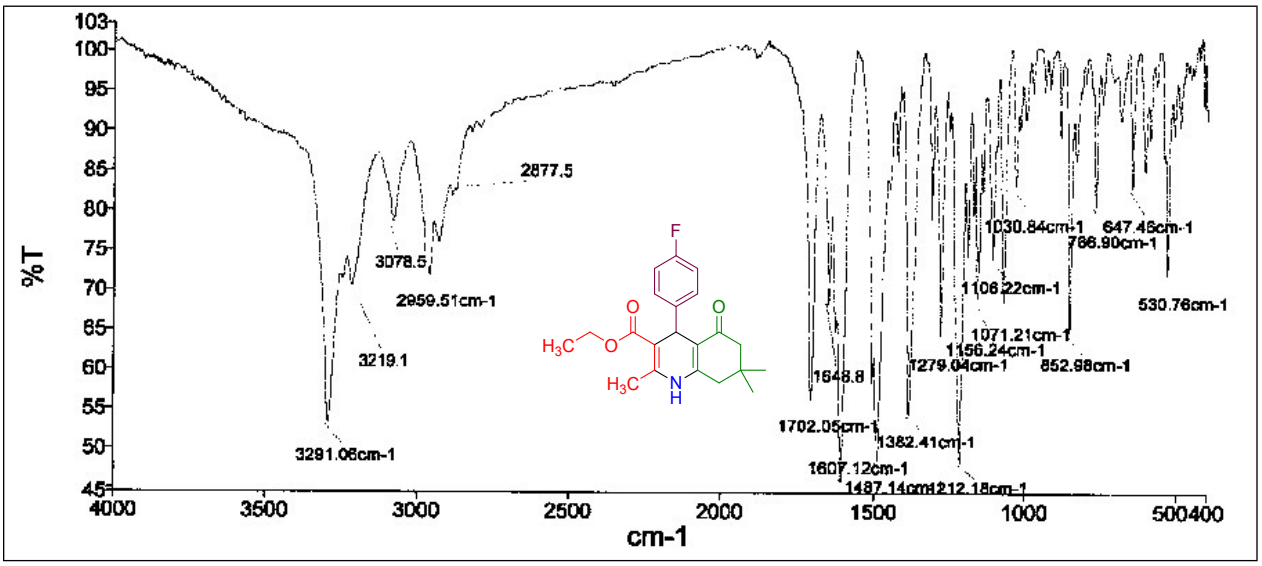
50. FT-IR spectra of ethyl 2,7,7-trimethyl-5-oxo-4-(p-tolyl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1g**)



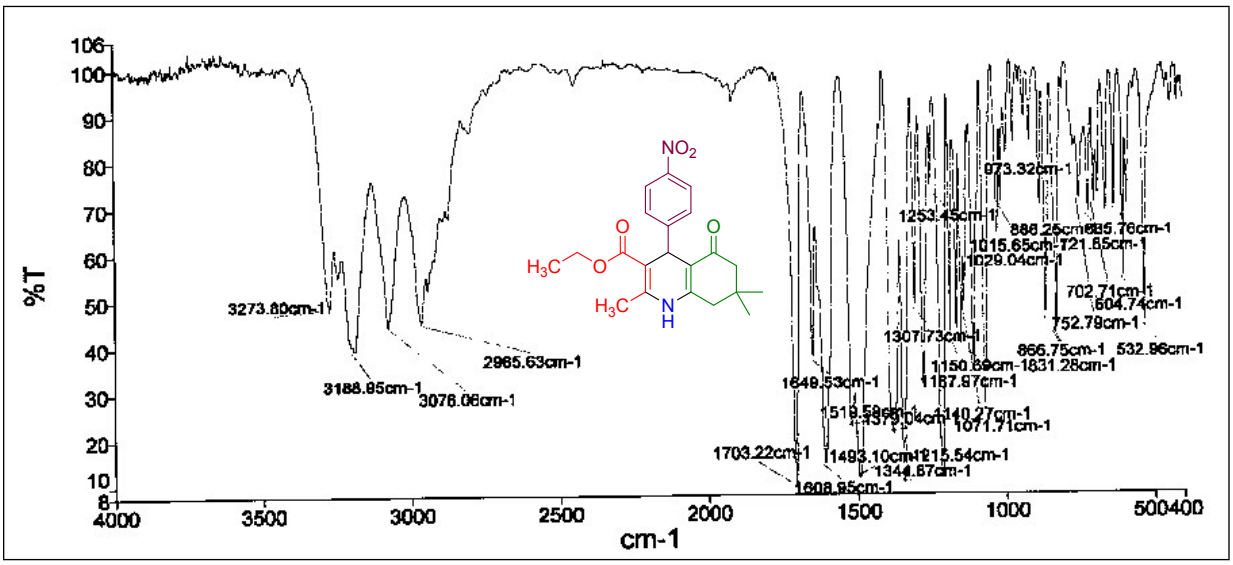
51. FT-IR spectra of ethyl 4-(3,4-dimethoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1h**)



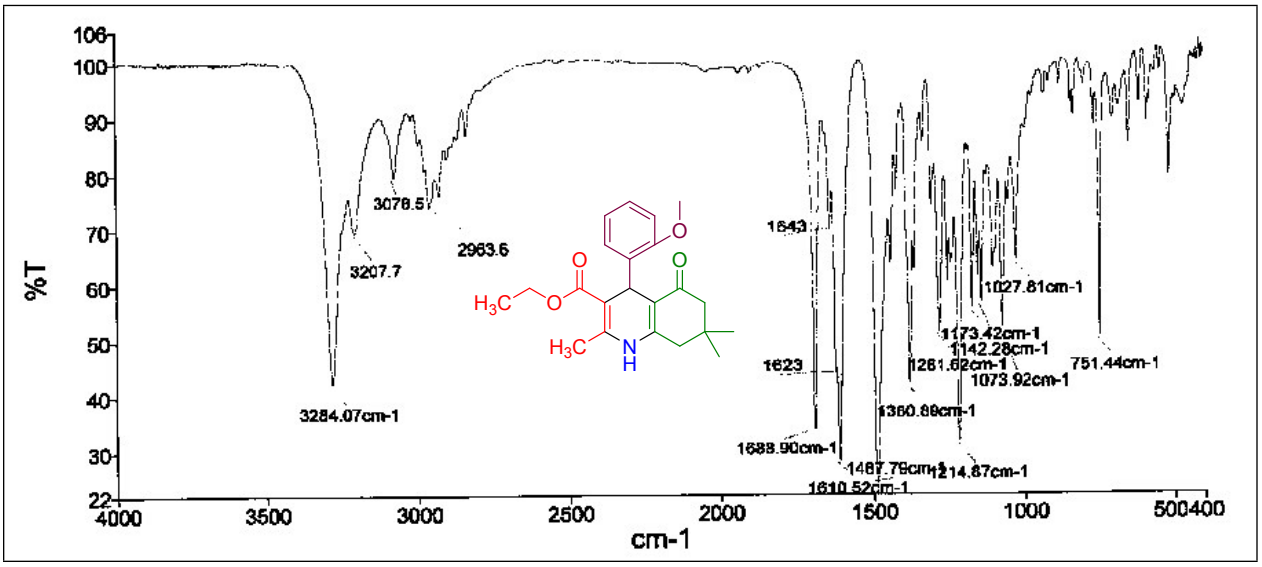
52. FT-IR spectra of ethyl 4-(4-fluorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1i**)



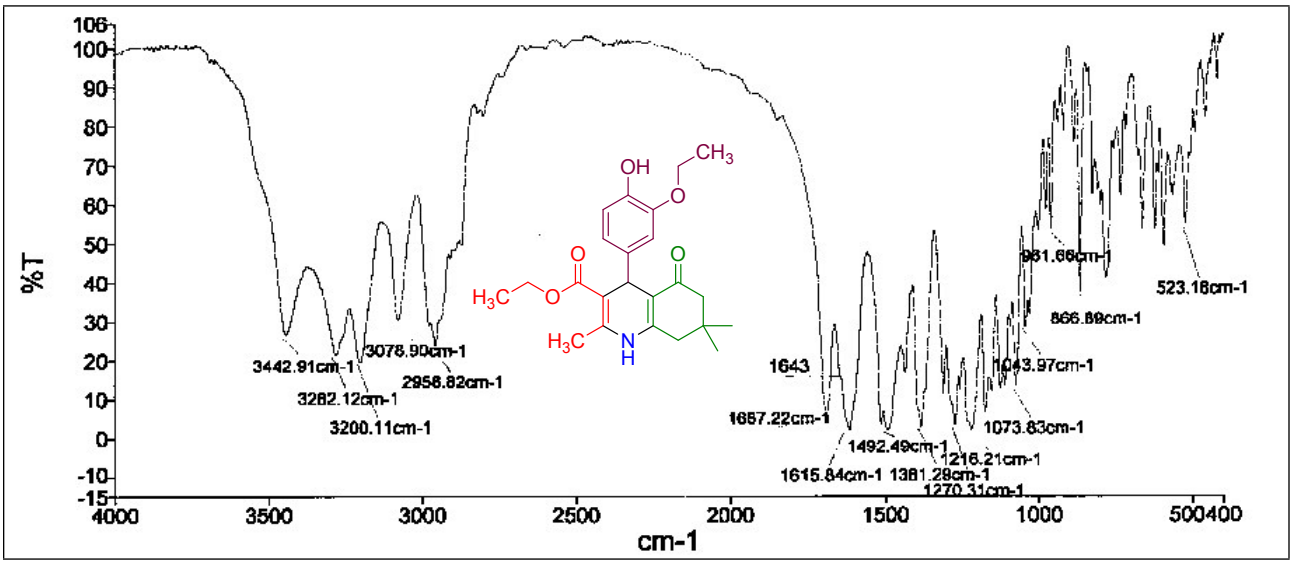
53. FT-IR spectra of ethyl 2,7,7-trimethyl-4-(4-nitrophenyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1j**)



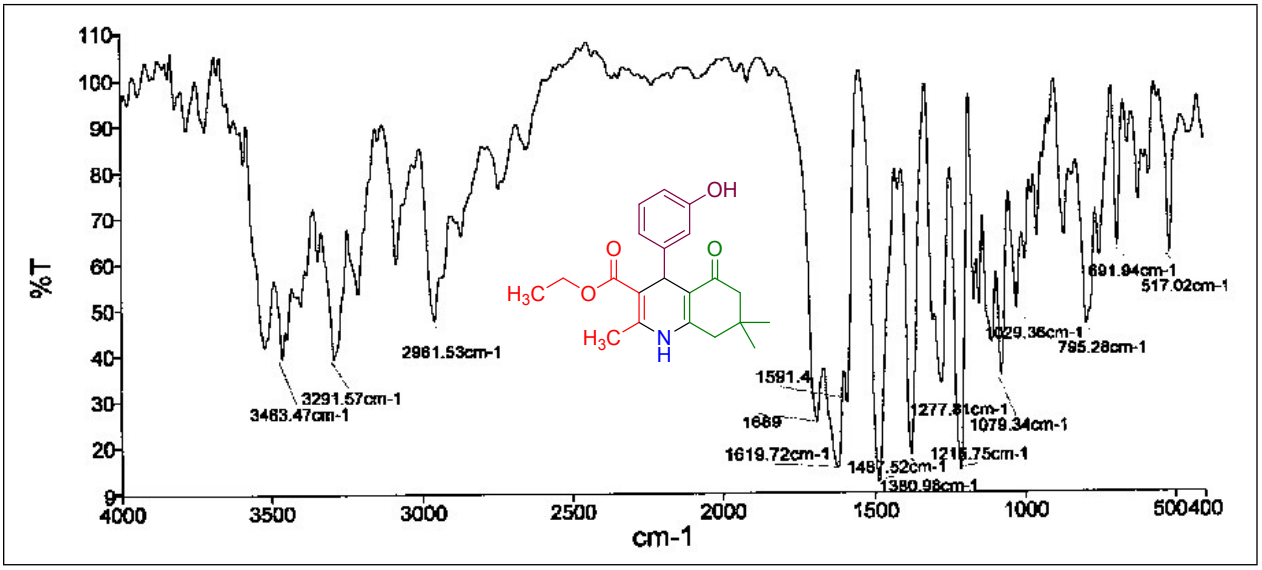
54. FT-IR spectra of ethyl 4-(2-methoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1k**)



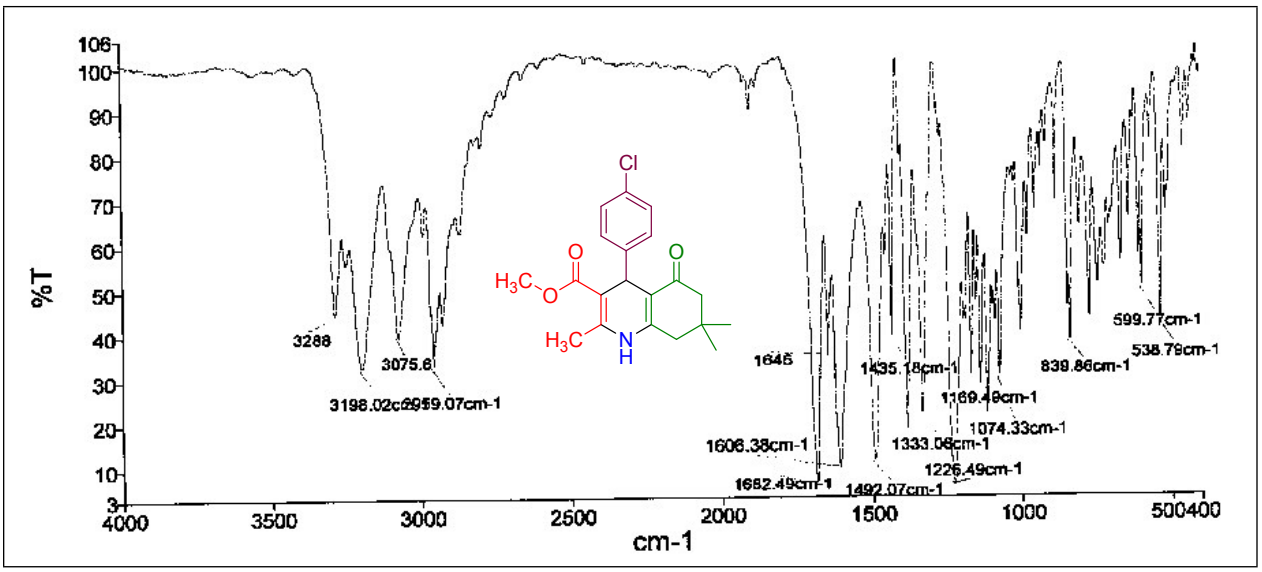
55. FT-IR spectra of ethyl 4-(3-ethoxy-4-hydroxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1l**)



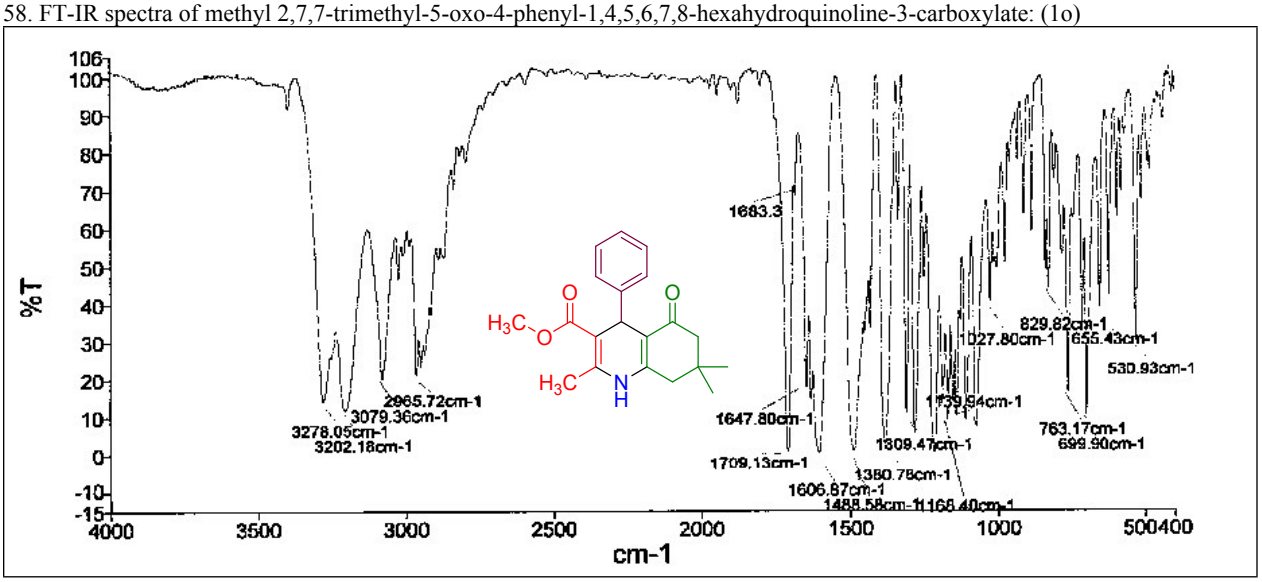
56. FT-IR spectra of ethyl 4-(3-hydroxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1m**)



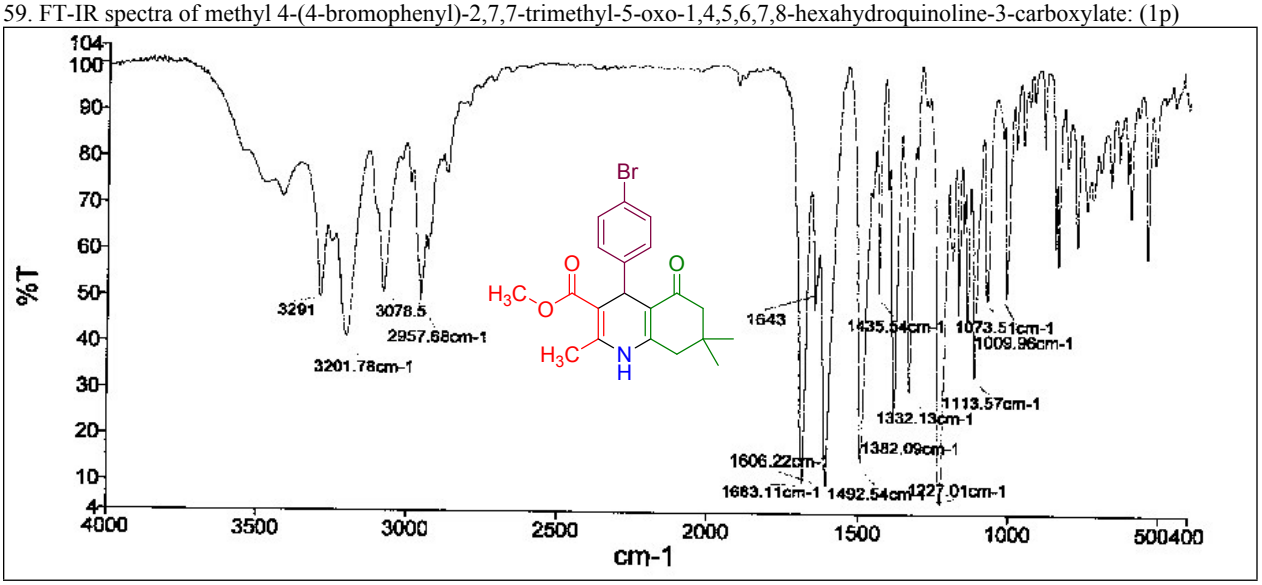
57. FT-IR spectra of methyl 4-(4-chlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (**1n**)



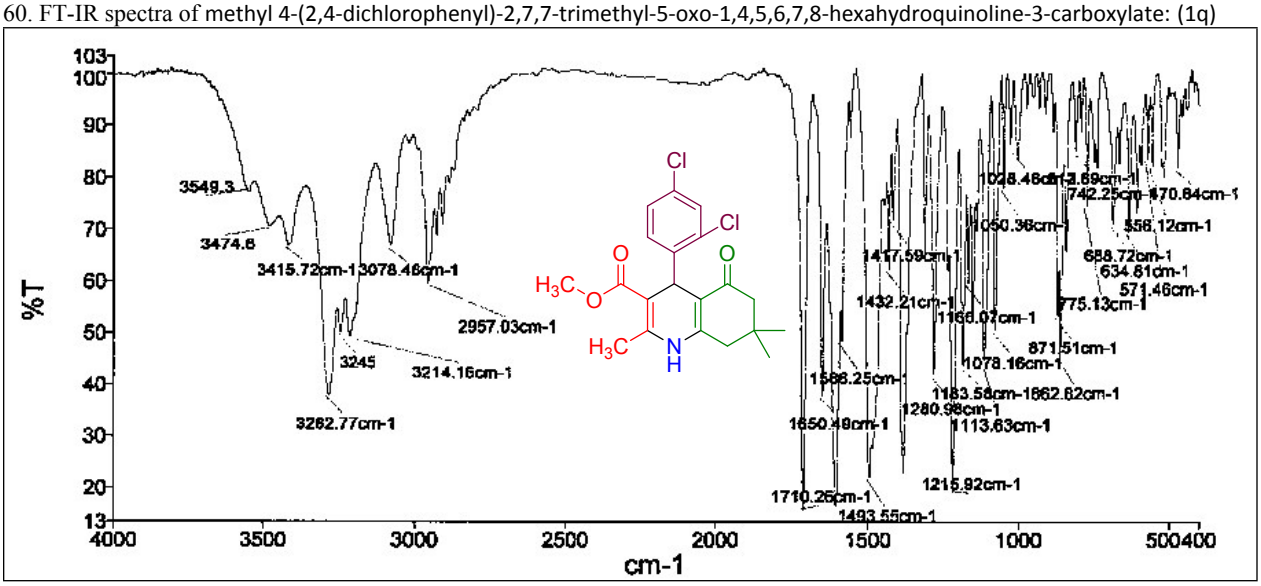
58. FT-IR spectra of methyl 2,7,7-trimethyl-5-oxo-4-phenyl-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (1o)



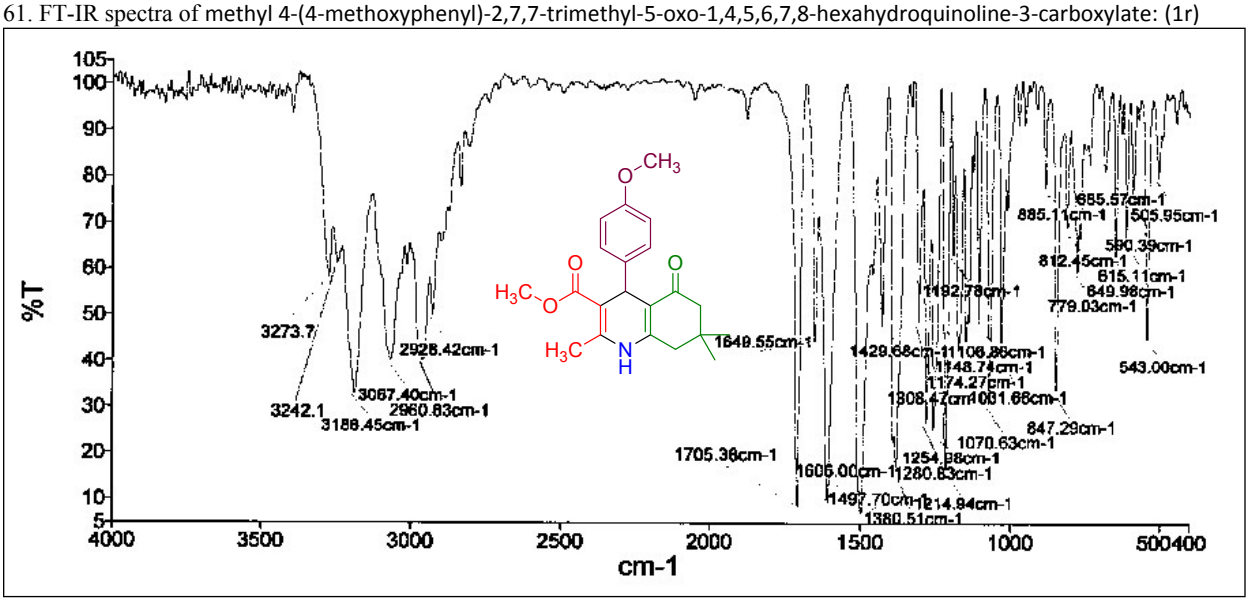
59. FT-IR spectra of methyl 4-(4-bromophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (1p)



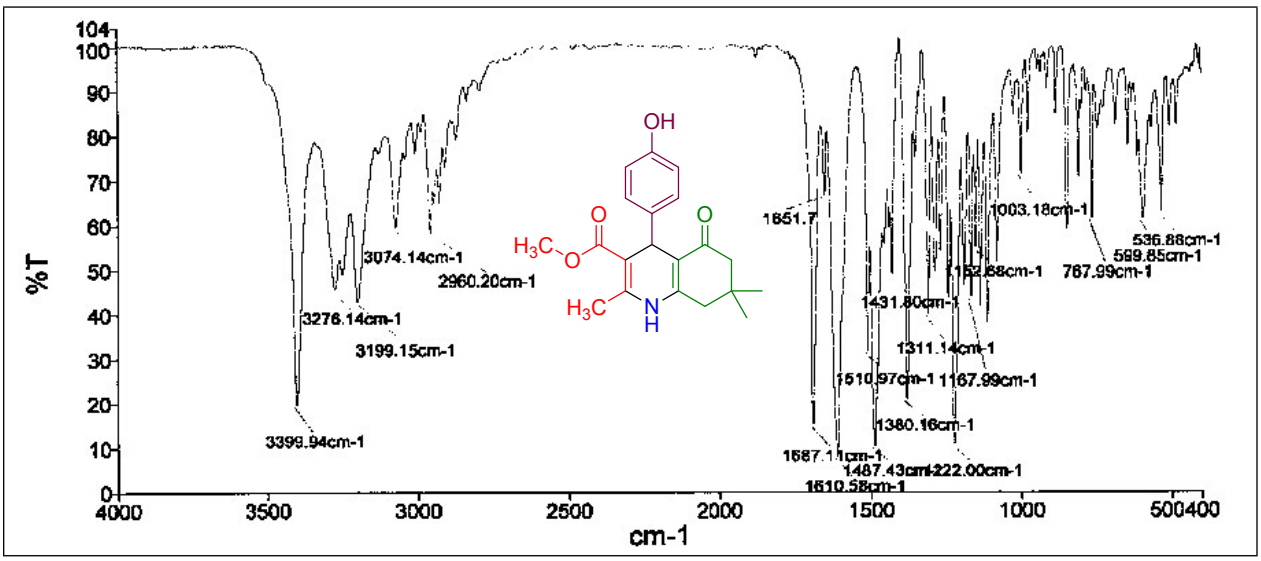
60. FT-IR spectra of methyl 4-(2,4-dichlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (1q)



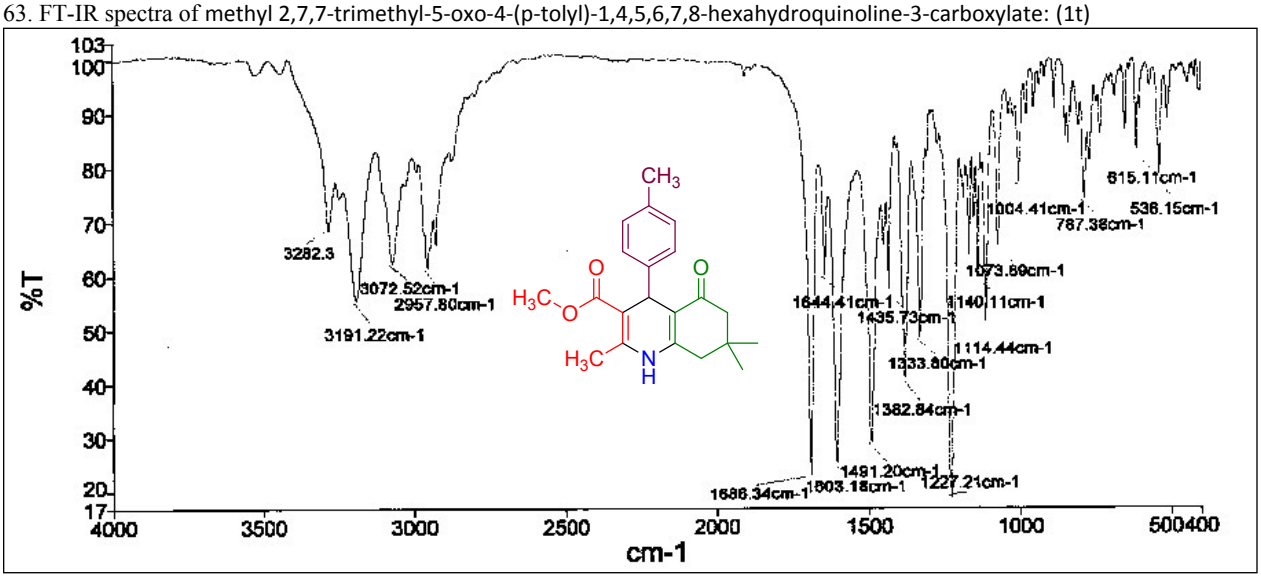
61. FT-IR spectra of methyl 4-(4-methoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (1r)



62. FT-IR spectra of methyl 4-(4-hydroxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (1s)

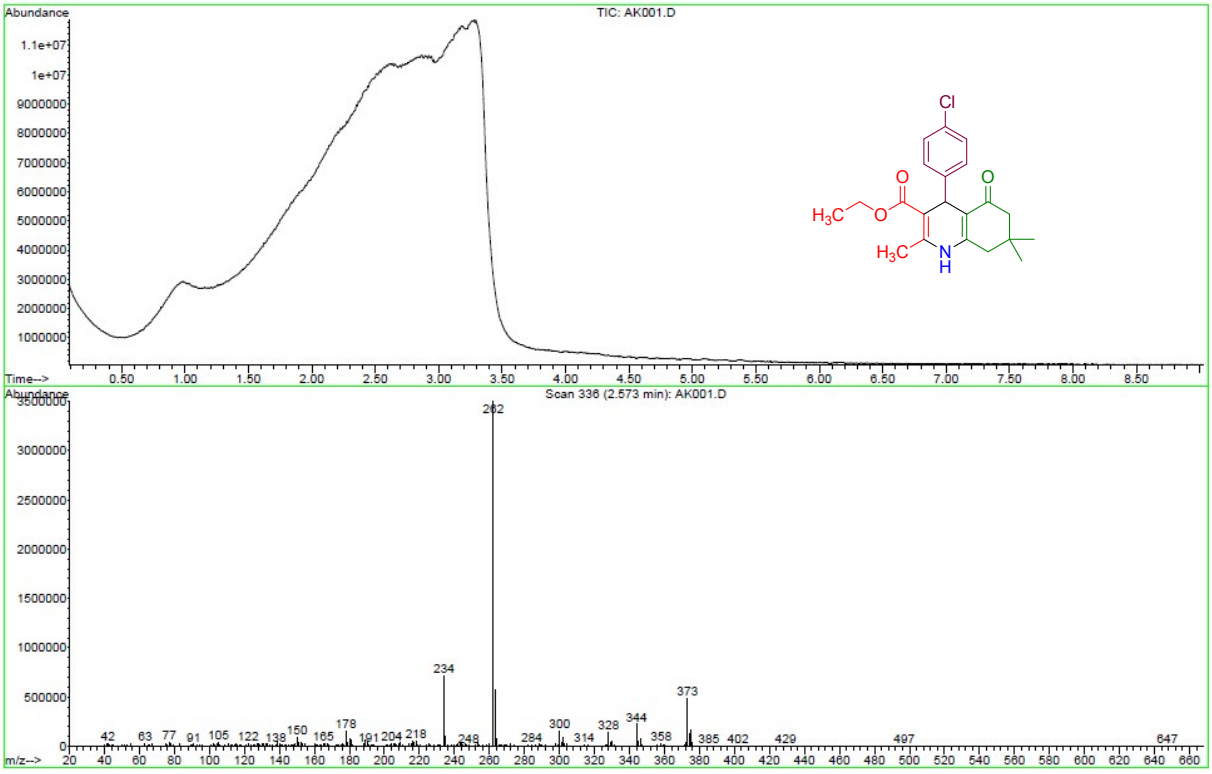


63. FT-IR spectra of methyl 2,7,7-trimethyl-5-oxo-4-(p-tolyl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate: (1t)

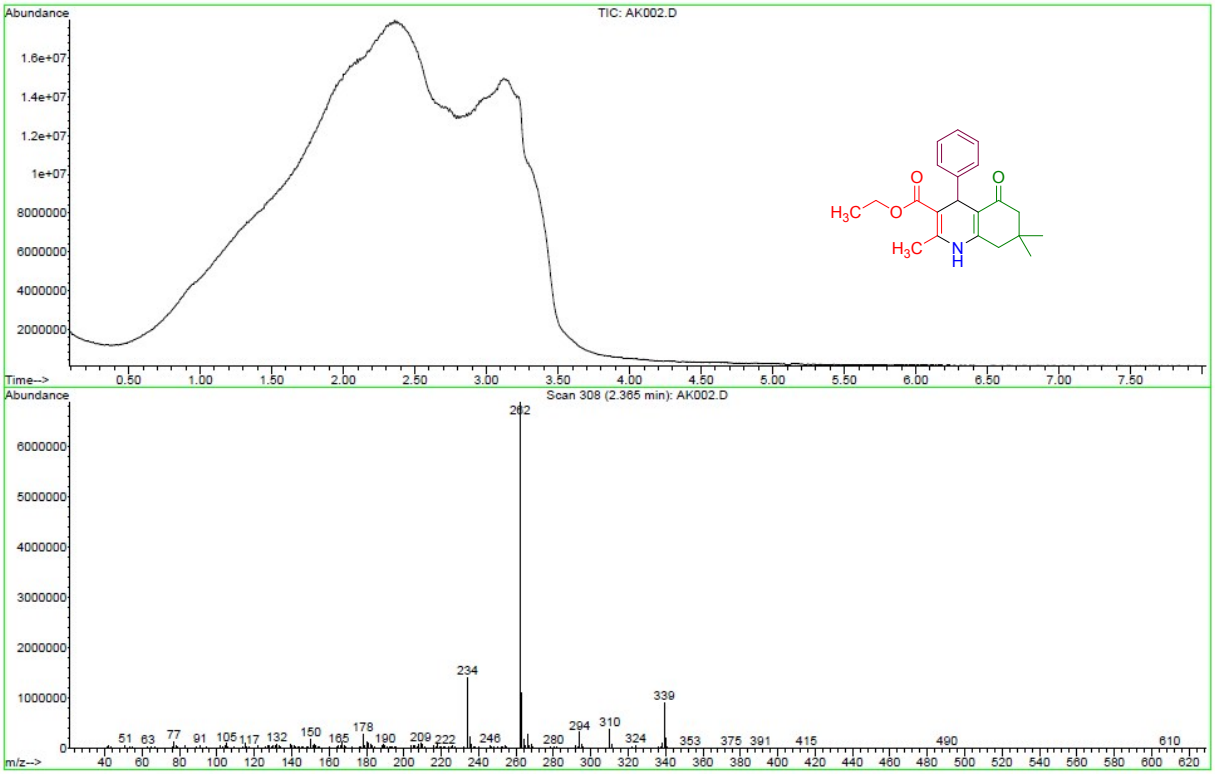


PART 3
Low Resolution Mass

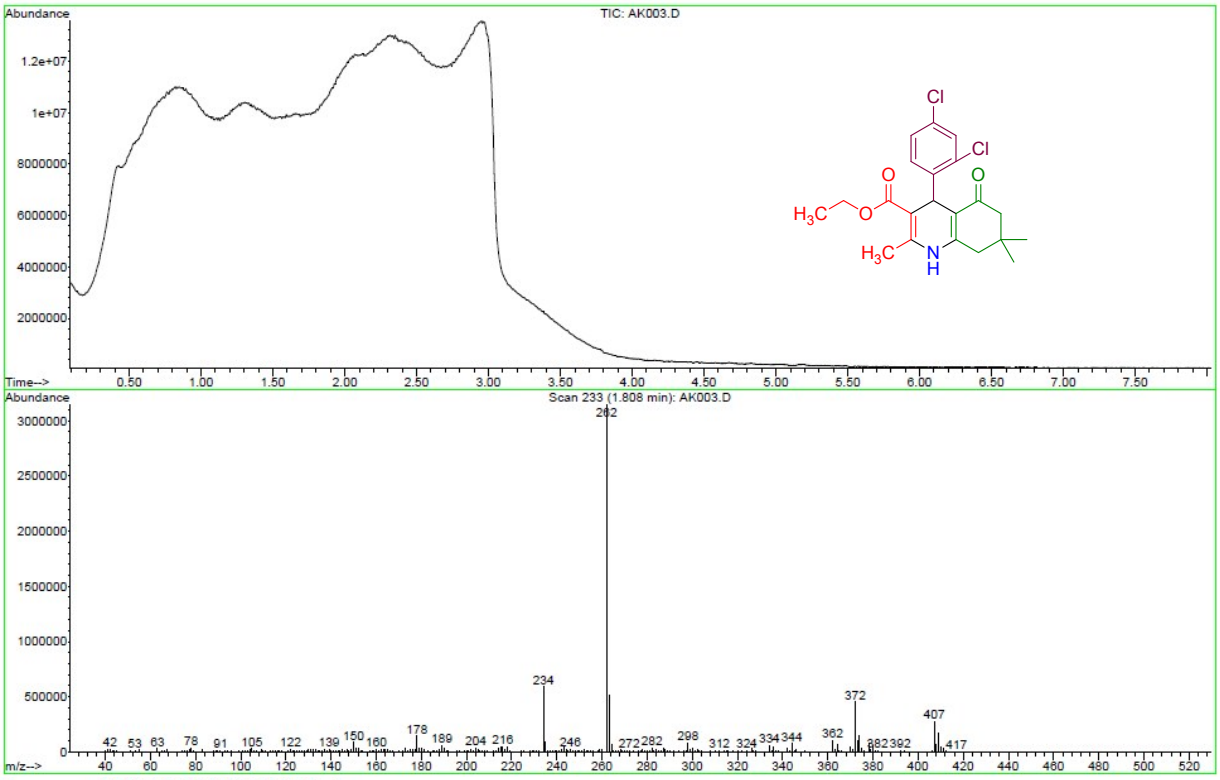
```
File       : C:\MSDCHEM\1\DATA\AK001.D
Operator   : Pablo
Acquired   : 26 Jul 2016  10:40     using AcqMethod MSALTA
Instrument :    Instrumen
Sample Name: Muestra 1a,  C21H24ClNO3 , MW=373.14
Misc Info  : msalta, dip
Vial Number: 1
```



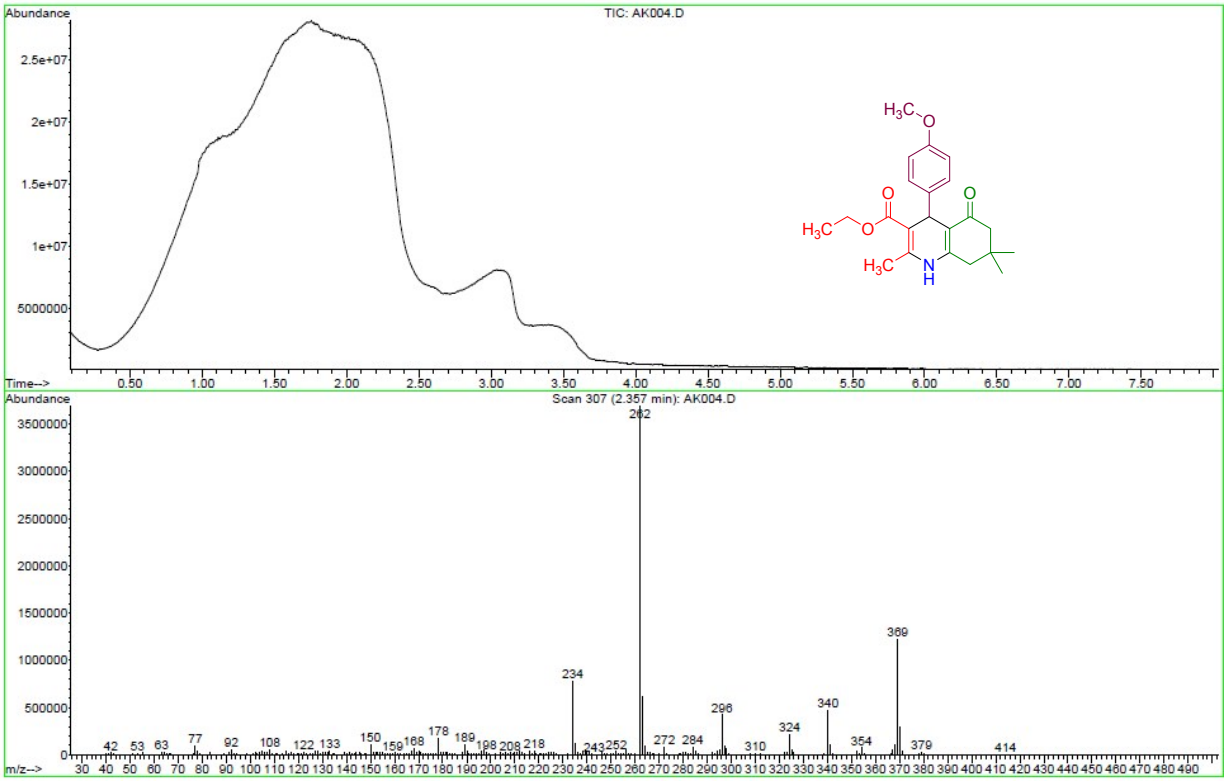

```
File       : C:\MSDCHEM\1\DATA\AK002.D
Operator   : Pablo
Acquired   : 26 Jul 2016  10:52     using AcqMethod MSALTA
Instrument :    Instrumen
Sample Name: Muestra 1b,  C21H25NO3 , MW=339.18
Misc Info  : msalta, dip
Vial Number: 1
```



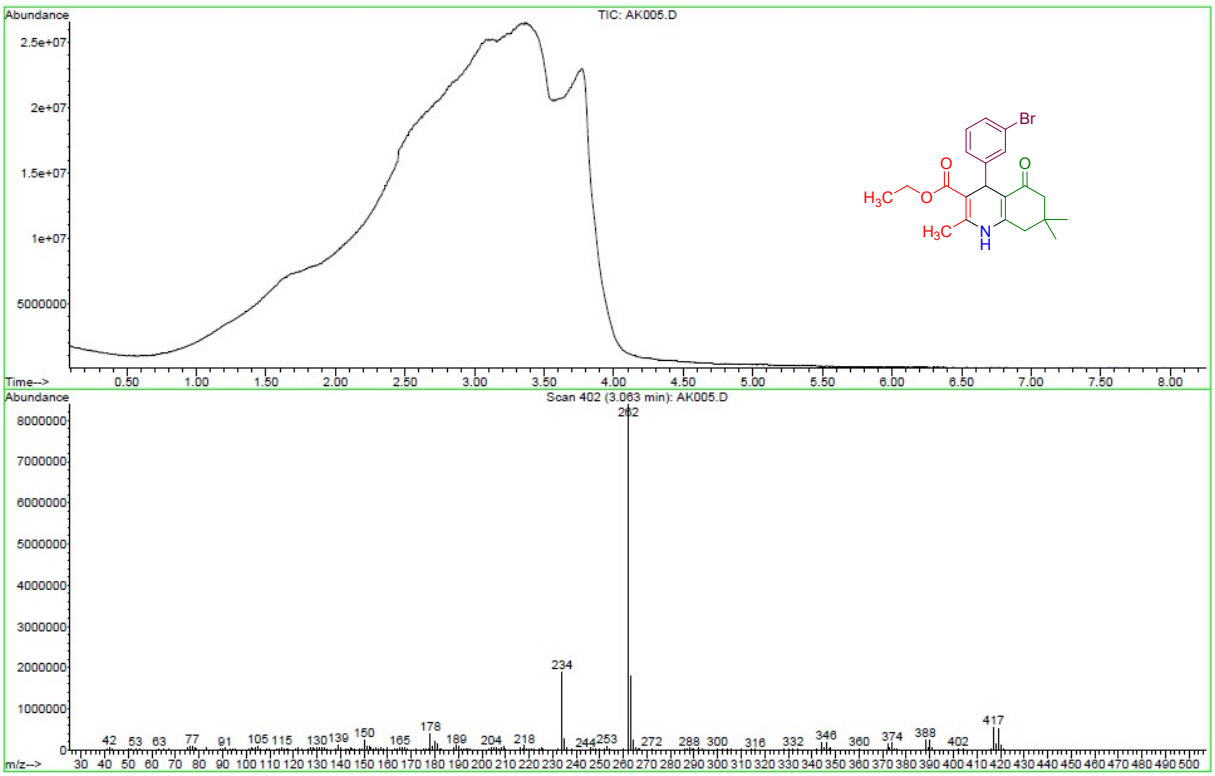
File : C:\MSDCHEM\1\DATA\AK003.D
Operator : Pablo
Acquired : 26 Jul 2016 11:03 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 1c, C21H23Cl2NO3 , MW=407.11
Misc Info : msalta, dip
Vial Number: 1



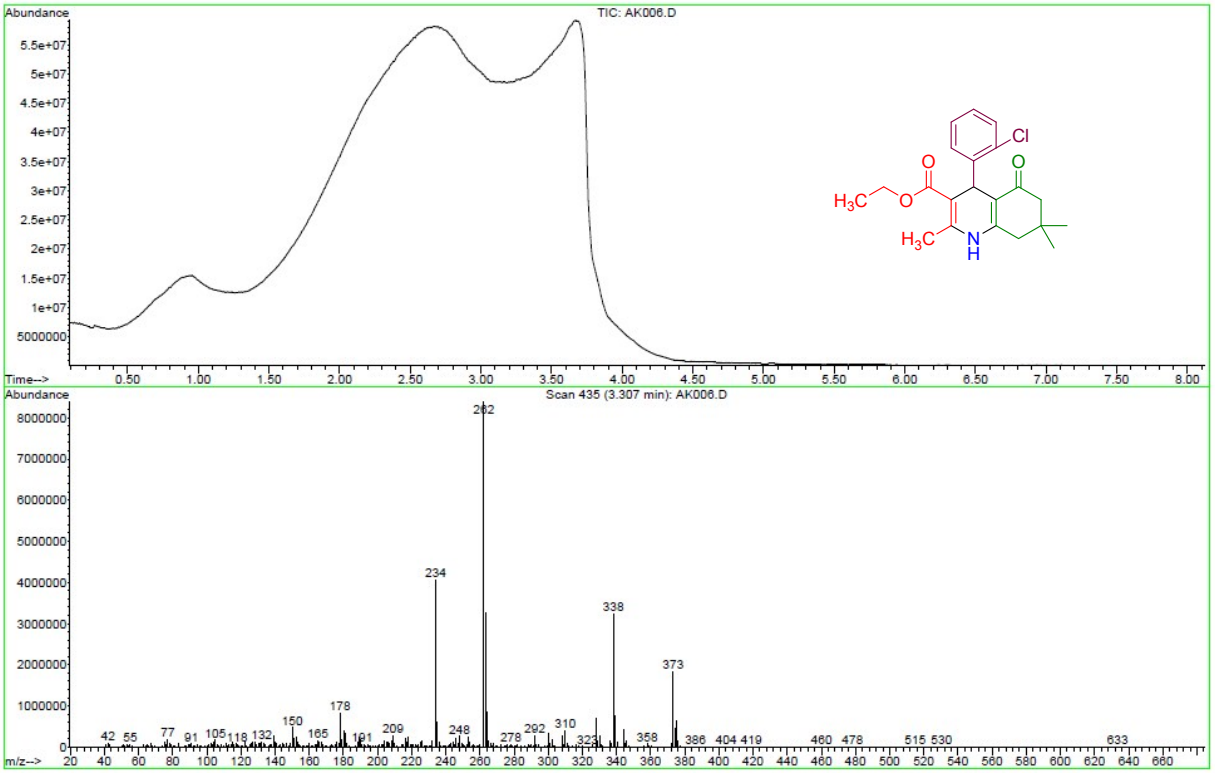
File : C:\MSDCHEM\1\DATA\AK004.D
Operator : Pablo
Acquired : 26 Jul 2016 11:15 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 1d, C22H27NO4 , MW=369.19
Misc Info : msalta, dip
Vial Number: 1



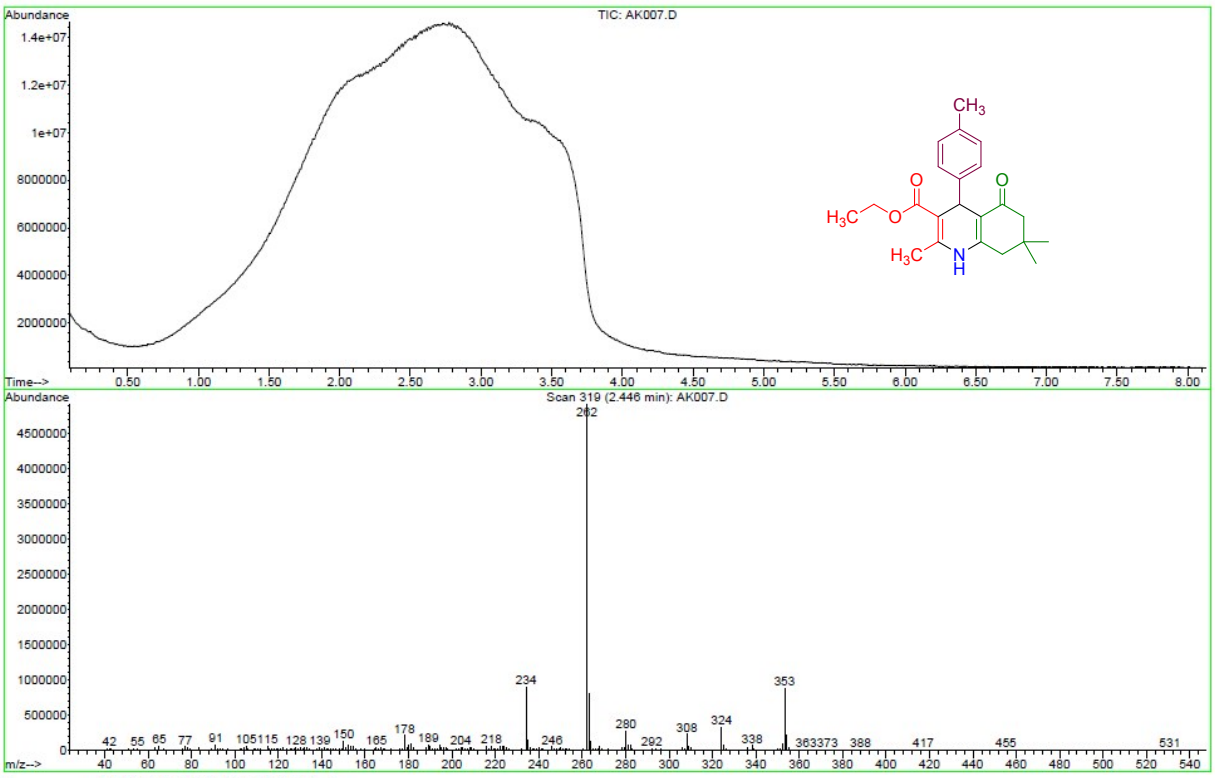
File : C:\MSDCHEM\1\DATA\AK005.D
Operator : Pablo
Acquired : 26 Jul 2016 11:26 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 1e, C21H24BrNO3 , MW=417.09
Misc Info : msalta, dip
Vial Number: 1



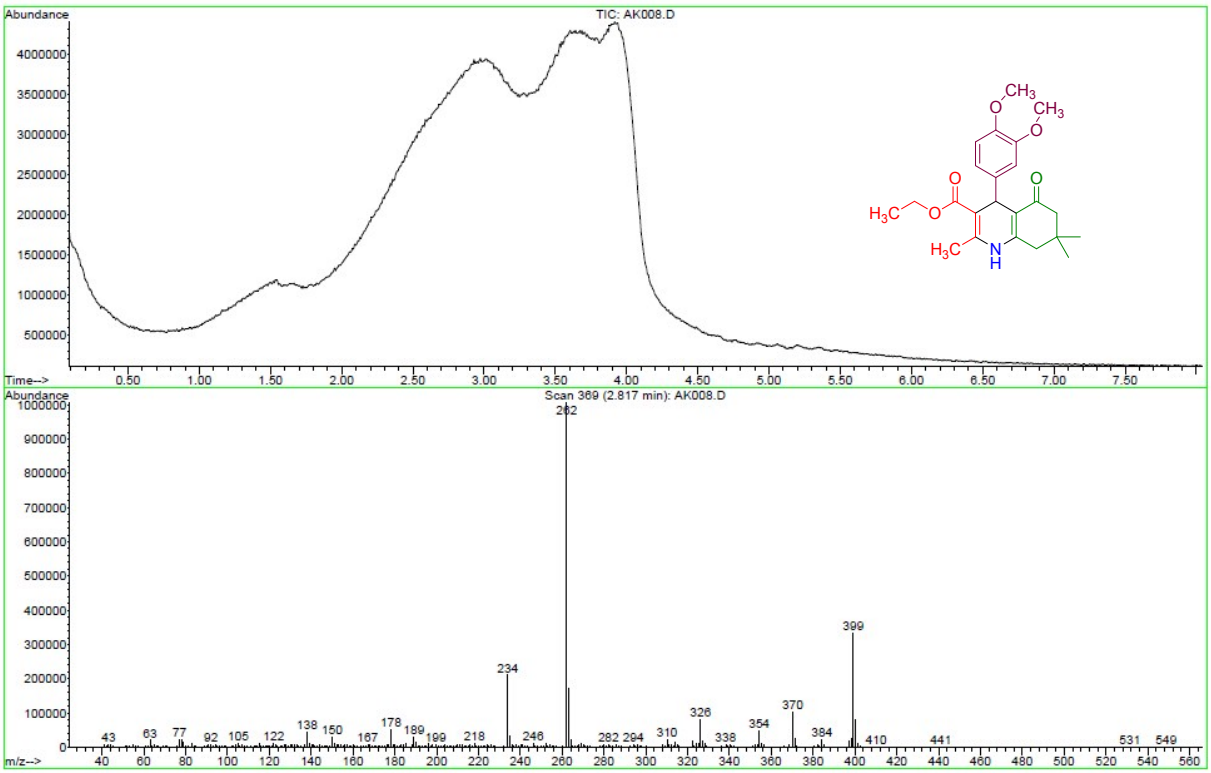
File : C:\MSDCHEM\1\DATA\AK006.D
Operator : Pablo
Acquired : 26 Jul 2016 11:38 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 1f, C21H24ClNO3 , MW=373.14
Misc Info : msalta, dip
Vial Number: 1



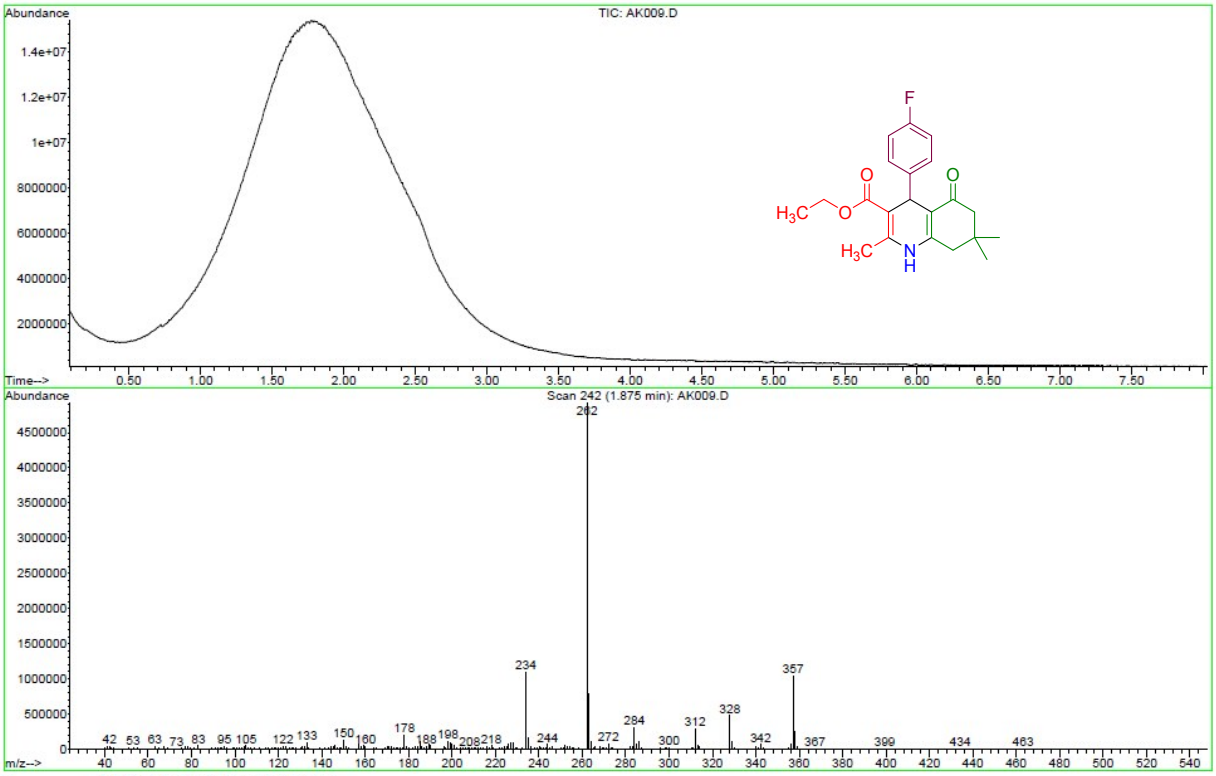
File : C:\MSDCHEM\1\DATA\AK007.D
Operator : Pablo
Acquired : 26 Jul 2016 11:52 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 1g, C22H27NO3 , MW=353.20
Misc Info : msalta, dip
Vial Number: 1



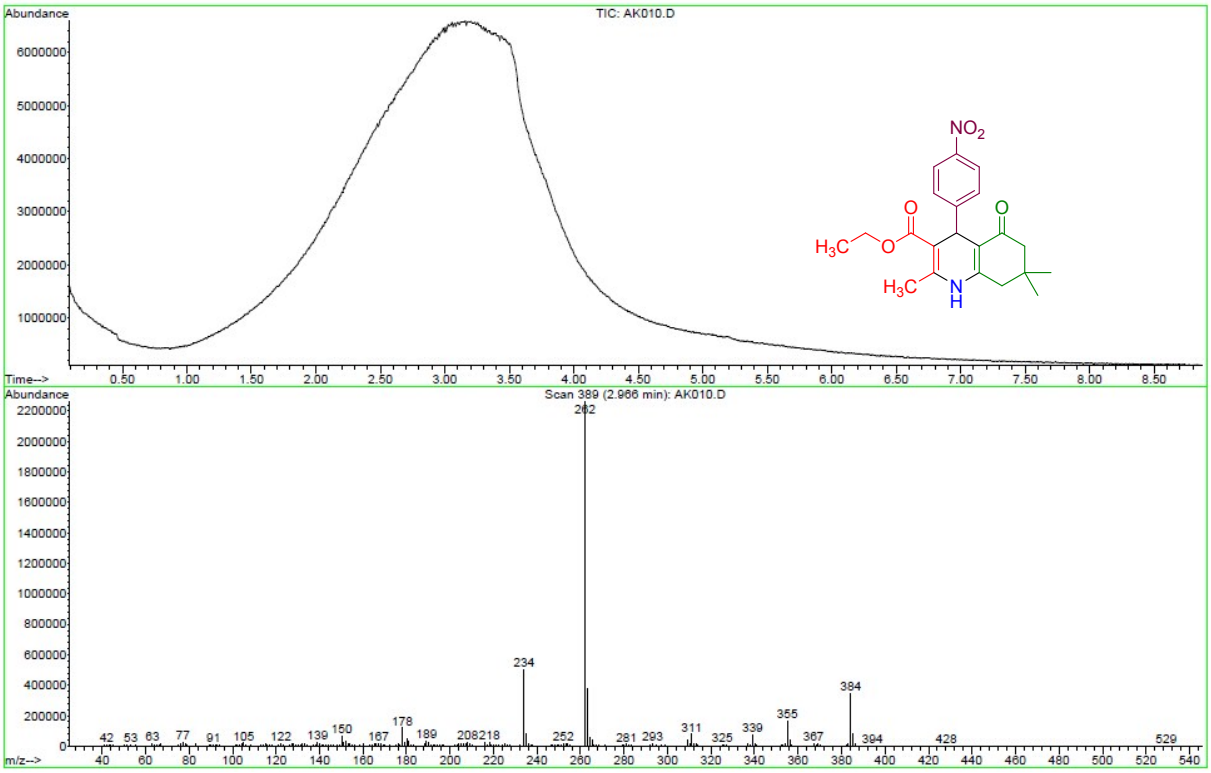
File : C:\MSDCHEM\1\DATA\AK008.D
Operator : Pablo
Acquired : 26 Jul 2016 12:08 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 1h, C23H29NO5 , MW=399.20
Misc Info : msalta, dip
Vial Number: 1



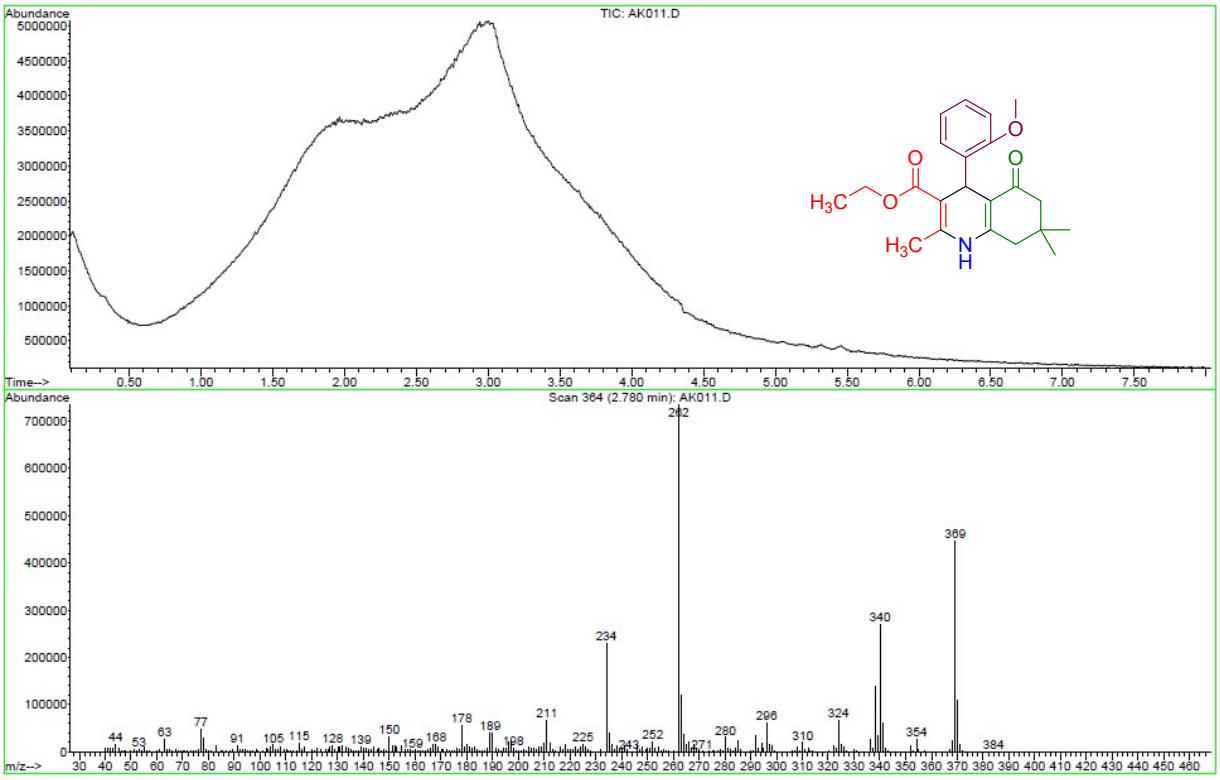
File : C:\MSDCHEM\1\DATA\AK009.D
Operator : Pablo
Acquired : 26 Jul 2016 13:54 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 1i, C21H24FNO3 , MW=357.17
Misc Info : msalta, dip
Vial Number: 1



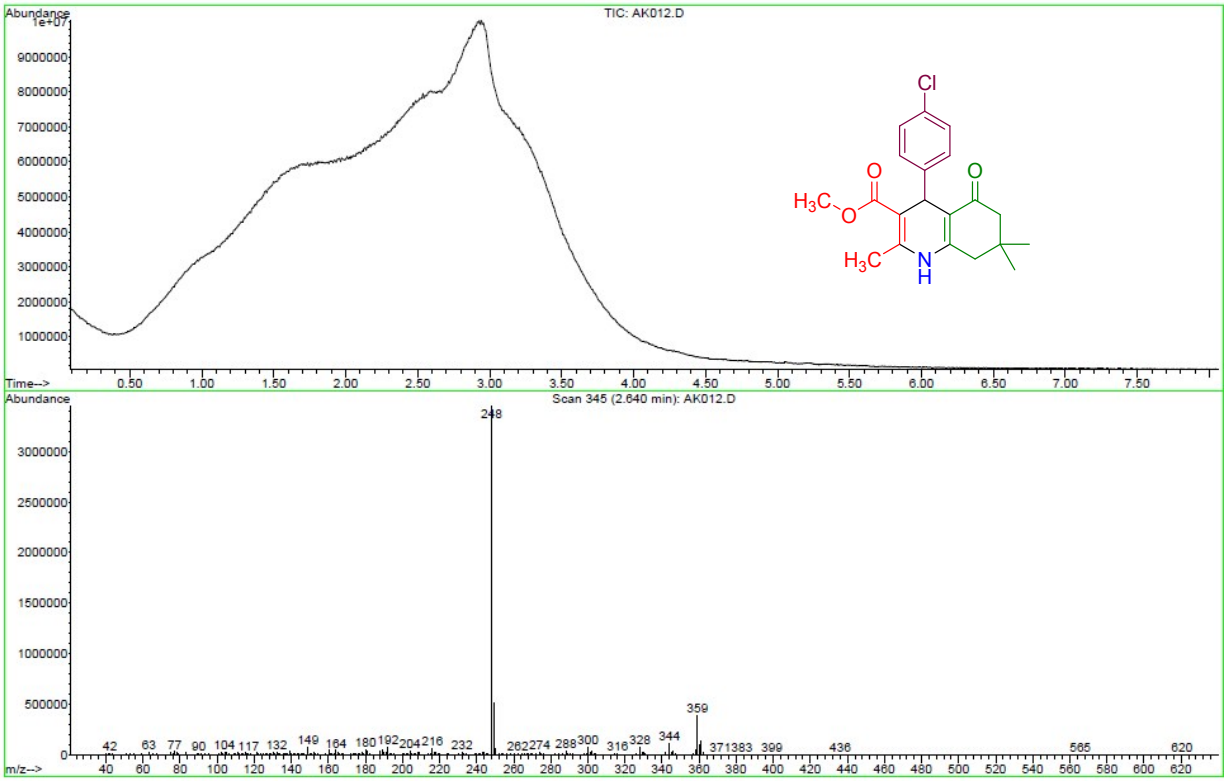
File : C:\MSDCHEM\1\DATA\AK010.D
Operator : Pablo
Acquired : 26 Jul 2016 14:05 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 1j, C21H24N2O5 , MW=384.17
Misc Info : msalta, dip
Vial Number: 1



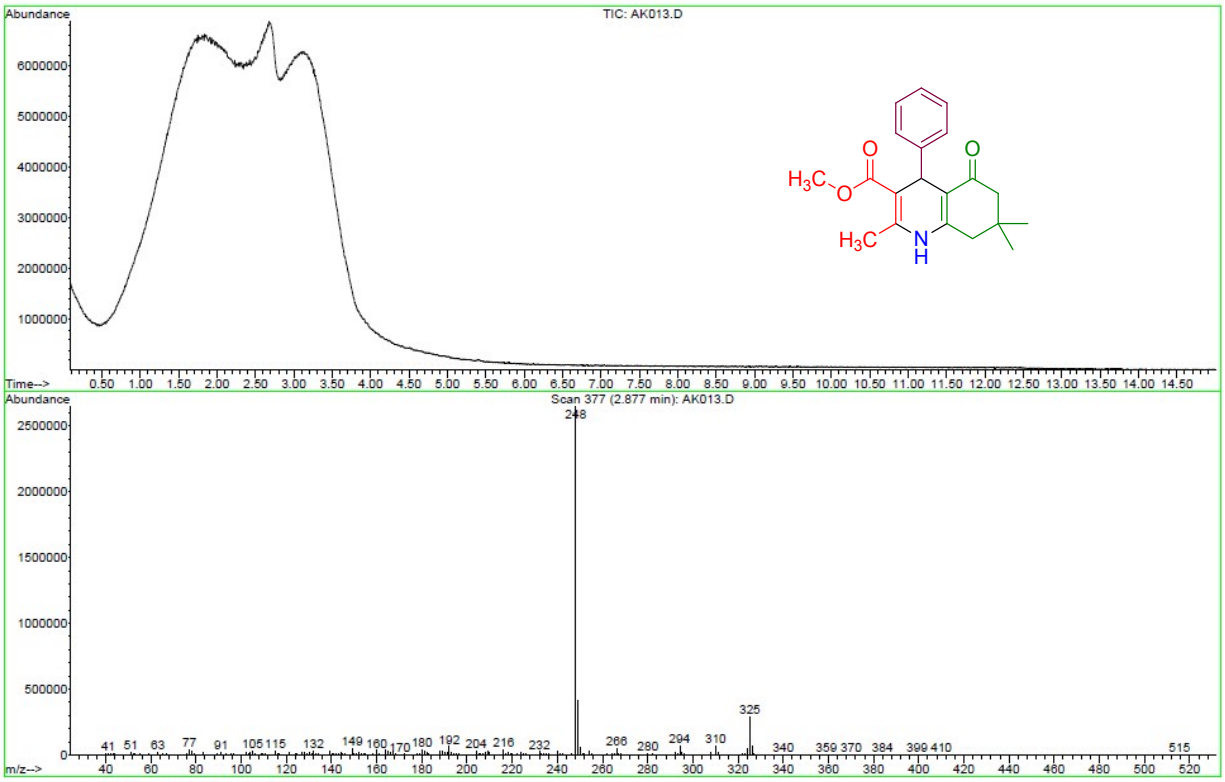
File : C:\MSDCHEM\1\DATA\AK011.D
Operator : Pablo
Acquired : 27 Jul 2016 8:38 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 11, C22H27NO4 , MW=369.19
Misc Info : msalta, dip
Vial Number: 1



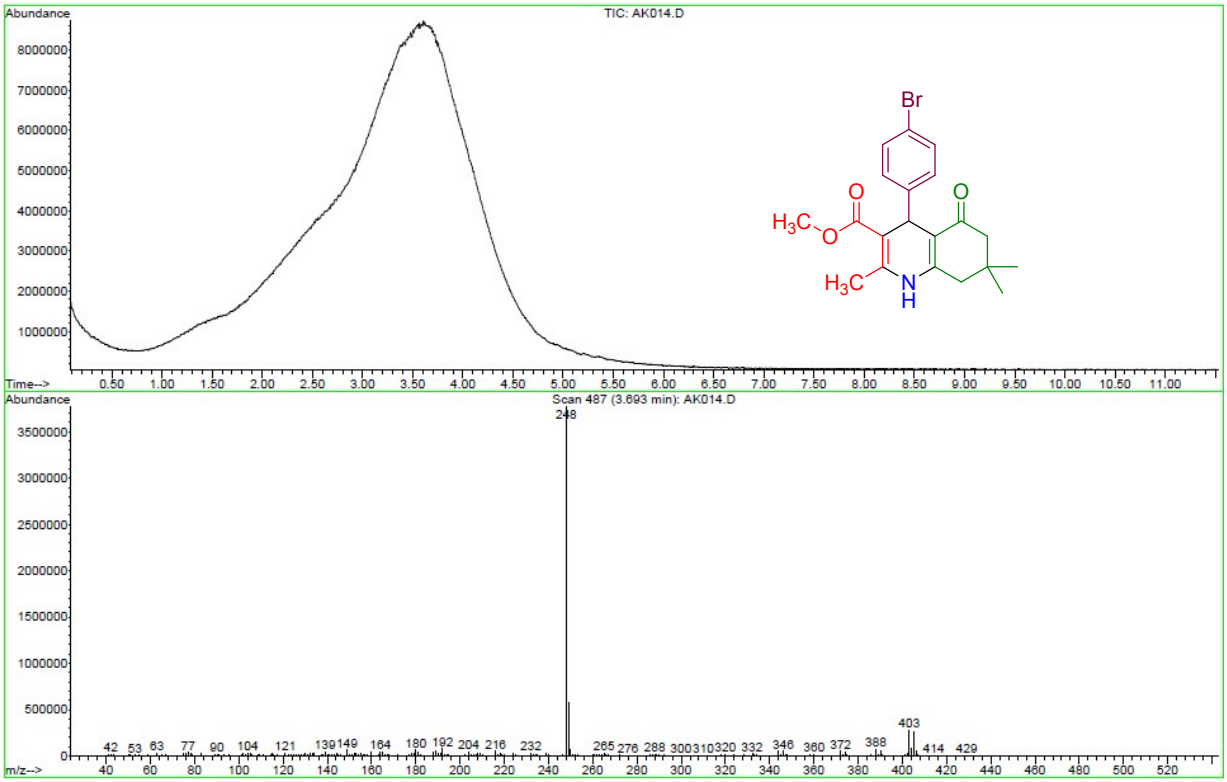
File : C:\MSDCHEM\1\DATA\AK012.D
Operator : Pablo
Acquired : 27 Jul 2016 8:49 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 12, C20H22ClNO3 , MW=359.13
Misc Info : msalta, dip
Vial Number: 1



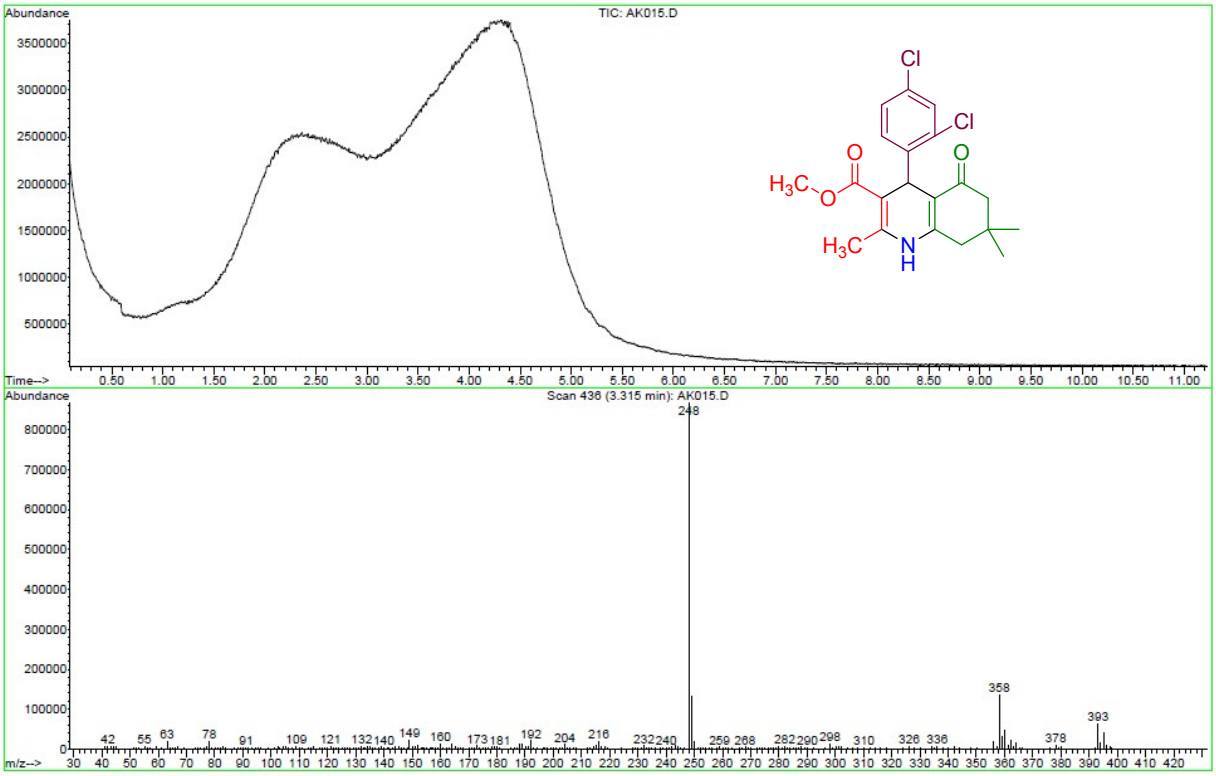
File : C:\MSDCHEM\1\DATA\AK013.D
Operator : Pablo
Acquired : 27 Jul 2016 9:01 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 13, C20H23NO3 , MW=325.17
Misc Info : msalta, dip
Vial Number: 1



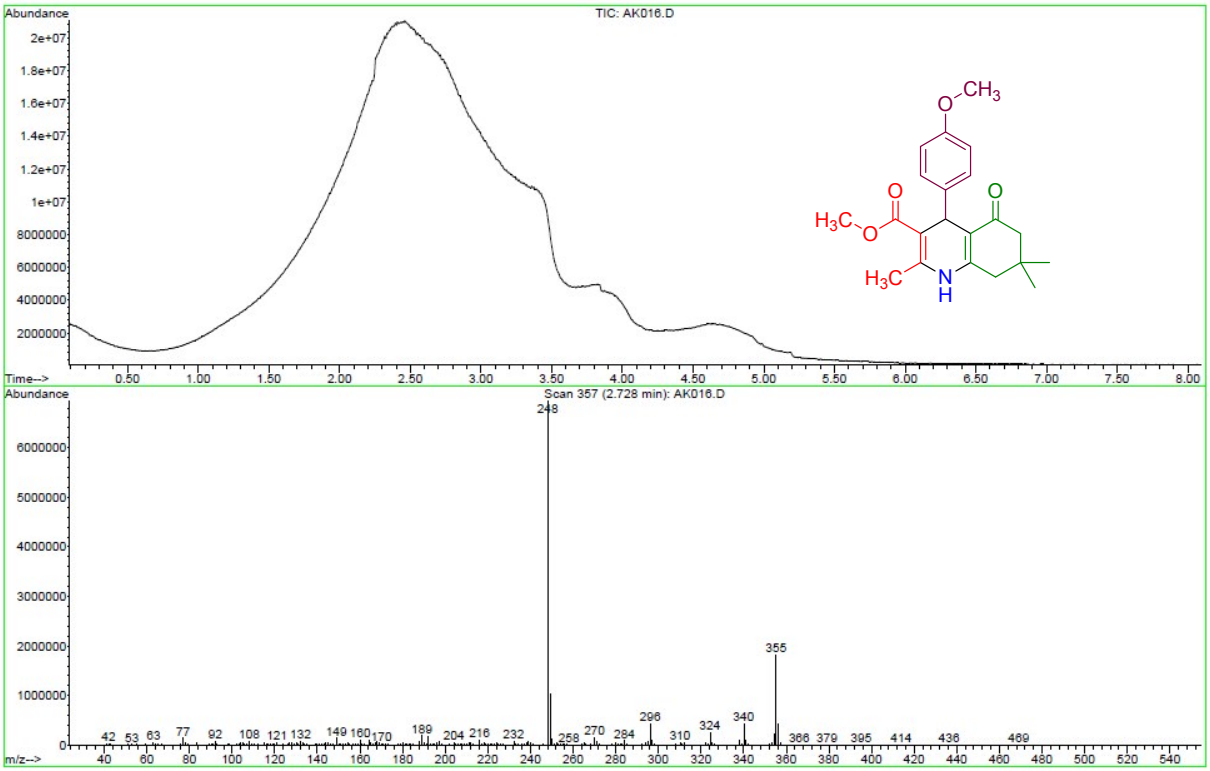
File : C:\MSDCHEM\1\DATA\AK014.D
Operator : Pablo
Acquired : 27 Jul 2016 9:19 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 14, C20H22BrNO3 , MW=403.08
Misc Info : msalta, dip
Vial Number: 1



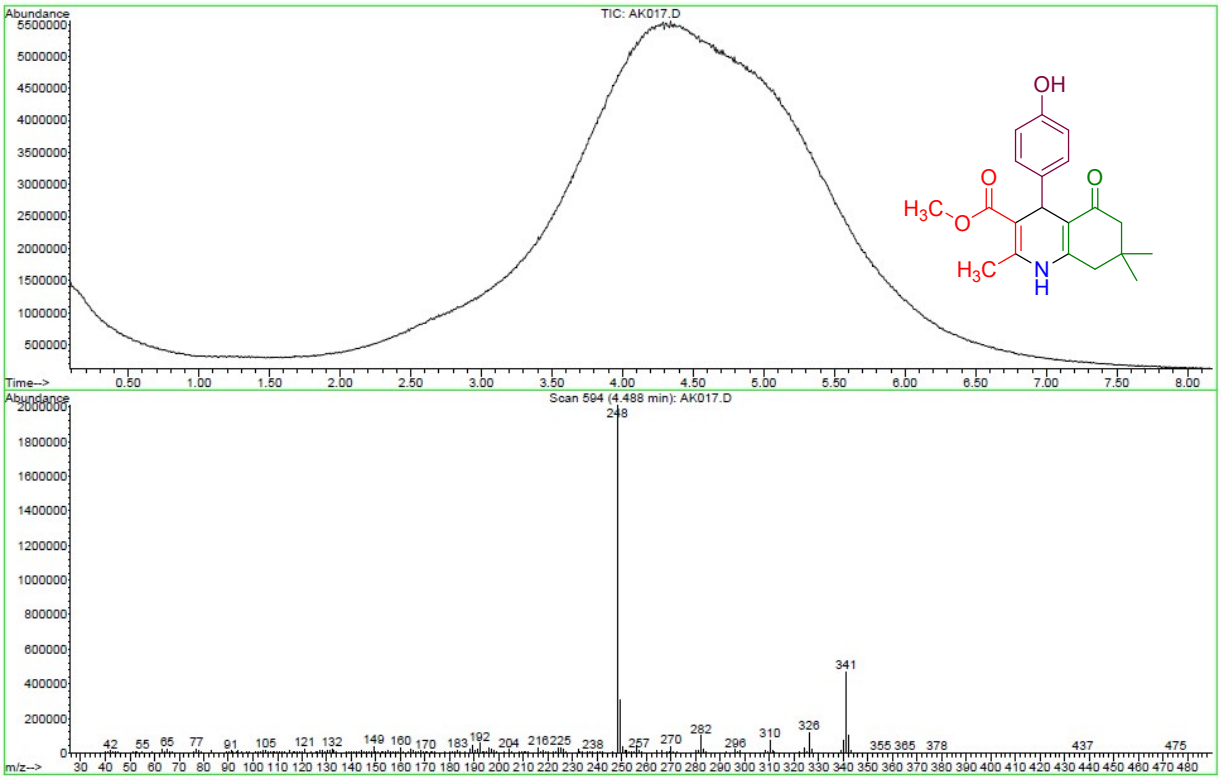
File : C:\MSDCHEM\1\DATA\AK015.D
Operator : Pablo
Acquired : 27 Jul 2016 10:32 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 15, C20H21Cl2NO3 , MW=393.09
Misc Info : msalta, dip
Vial Number: 1



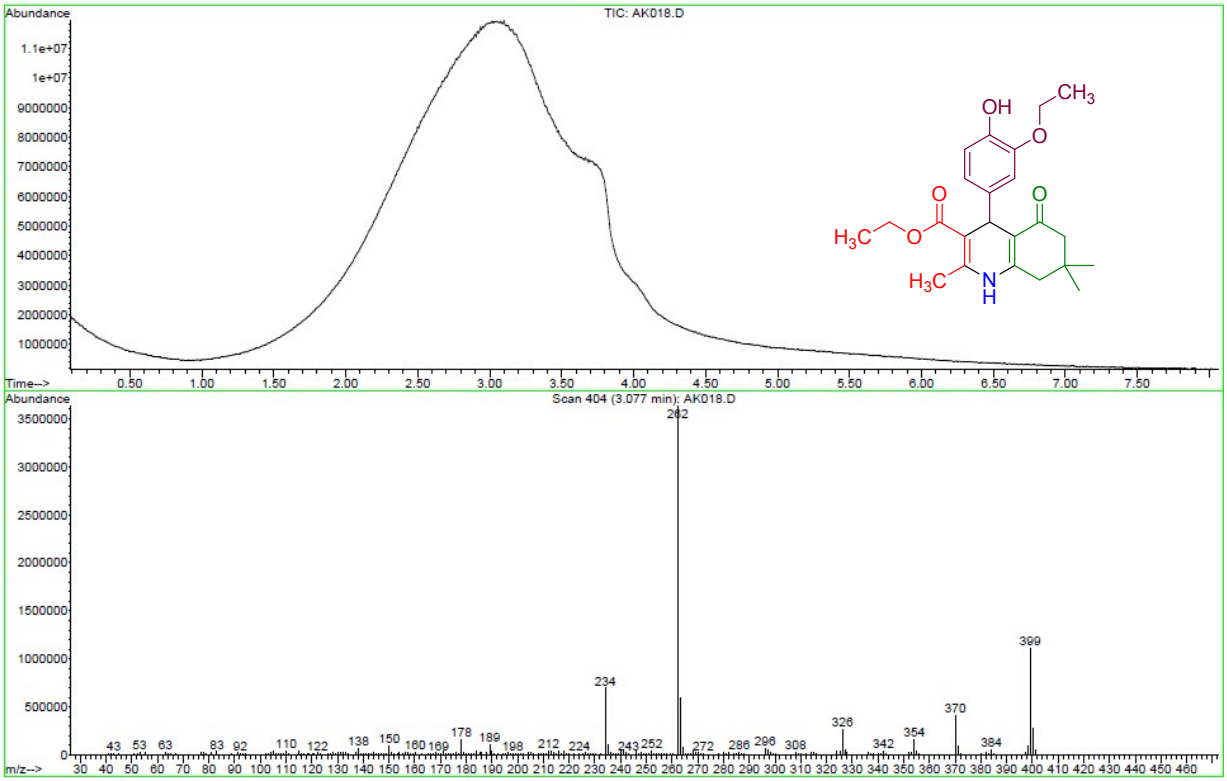
File : C:\MSDCHEM\1\DATA\AK016.D
Operator : Pablo
Acquired : 27 Jul 2016 10:49 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 16, C21H25NO4 , MW=355.18
Misc Info : msalta, dip
Vial Number: 1



File : C:\MSDCHEM\1\DATA\AK017.D
Operator : Pablo
Acquired : 27 Jul 2016 11:00 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 17, C20H23NO4 , MW=341.16
Misc Info : msalta, dip
Vial Number: 1



File : C:\MSDCHEM\1\DATA\AK018.D
Operator : Pablo
Acquired : 27 Jul 2016 11:11 using AcqMethod MSALTA
Instrument : Instrumen
Sample Name: Muestra 18, C23H29NO5 , MW=399.20
Misc Info : msalta, dip
Vial Number: 1



```
File       : C:\MSDCHEM\1\DATA\AK019.D
Operator   : Pablo
Acquired   : 27 Jul 2016  11:23     using AcqMethod MSALTA
Instrument :    Instrumen
Sample Name: Muestra 19,  C21H25NO4 , MW=355.18
Misc Info  : msalta, dip
Vial Number: 1
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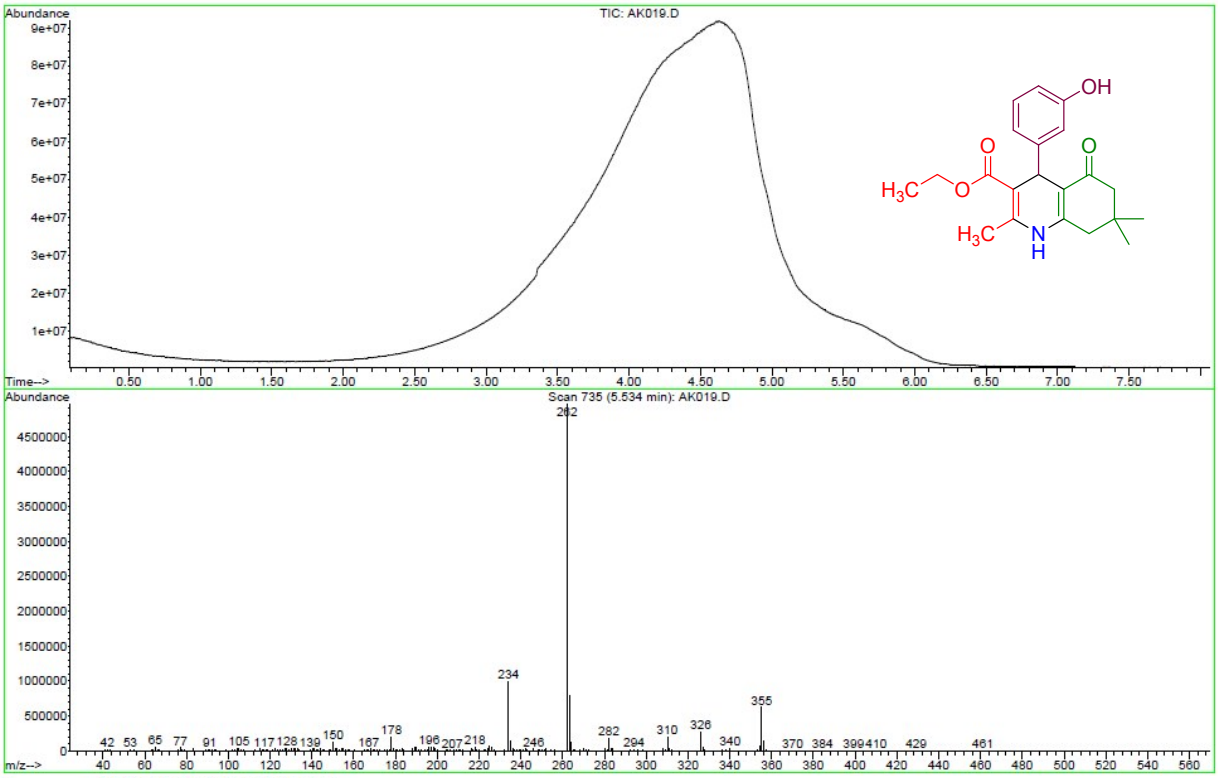
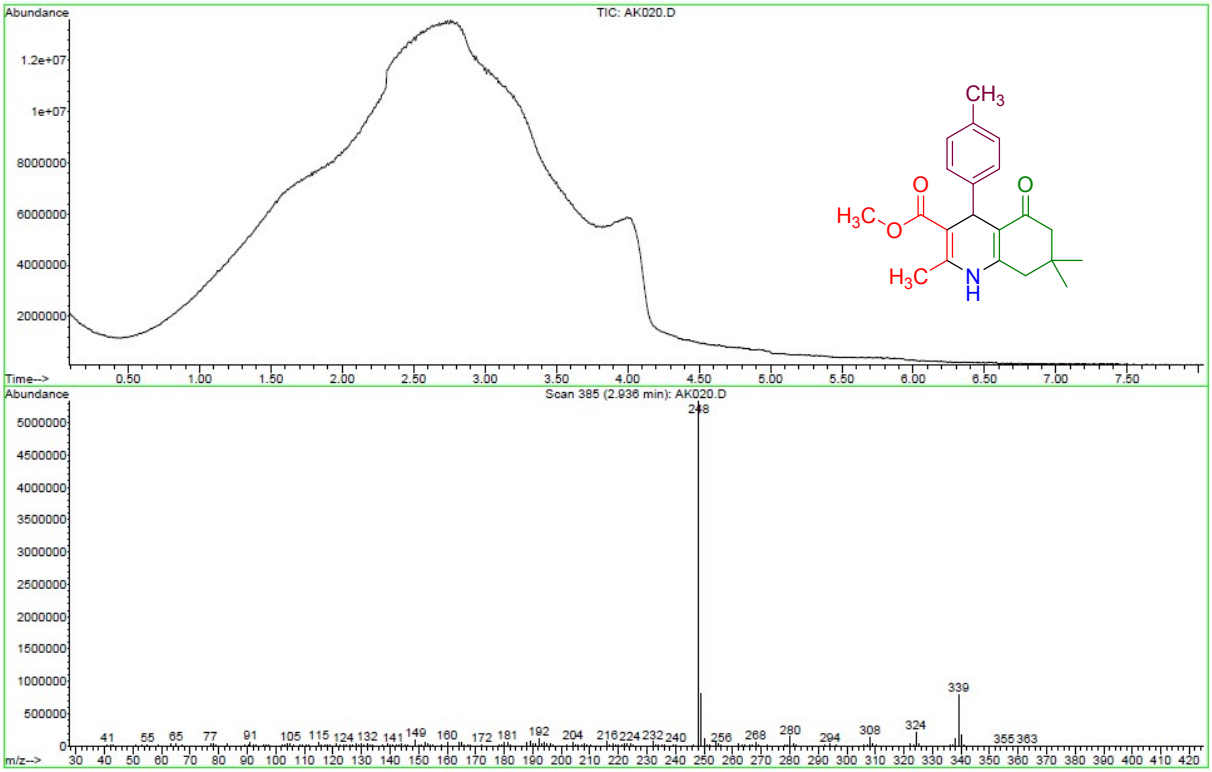



```
File       : C:\MSDCHEM\1\DATA\AK020.D
Operator   : Pablo
Acquired   : 27 Jul 2016  11:34     using AcqMethod MSALTA
Instrument :    Instrumen
Sample Name: Muestra 20,  C21H25NO3 , MW=339.18
Misc Info  : msalta, dip
Vial Number: 1
```



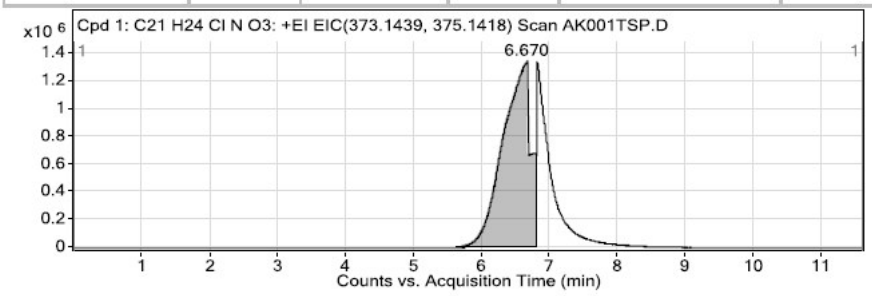
PART 4
High Resolution Mass

Data File	AK001TSP.D	**Sample Name**	
Position	1	**Instrument Name**	GCQTOF
Operator Name		**Acq Method**	ORGANICA_EI_4G_TSP.M
Acquired Time	7/26/2016 11:29:42 AM	**IRM Calibration Status**	Success
DA Method	UA.m	**Comment**	

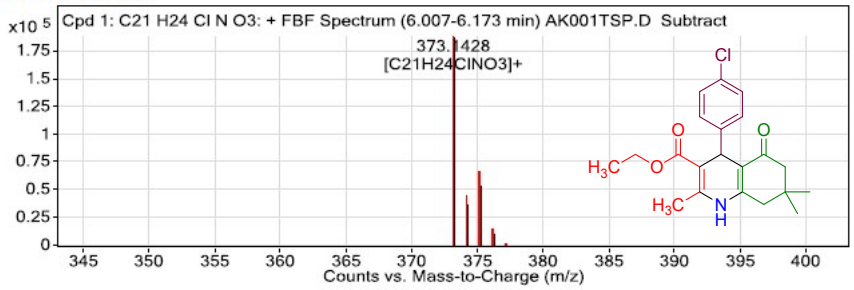
Compound Table

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass Error (ppm)	Obs. m/z	Ret.T	Find Comp. Algorith
C21 H24 Cl N O3	373.1445	373.1437	91.43	-2.03	373.1428	6.67	Find By Formula

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass error (ppm)	*Obs. m/z*	Find Cpds Algorith
C21 H24 Cl N O3	373.1445	373.1437	91.43	-2.03	373.1428	Find By Formula



MS Zoomed Spectrum

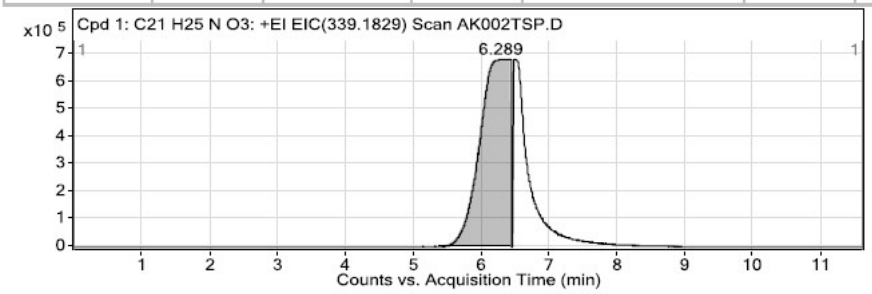


Data File	AK002TSP.D	**Sample Name**	
Position	1	**Instrument Name**	GCQTOF
Operator Name		**Acq Method**	ORGANICA_EI_4G_TSP.M
Acquired Time	7/26/2016 12:05:22 PM	**IRM Calibration Status**	Success
DA Method	UA.m	**Comment**	

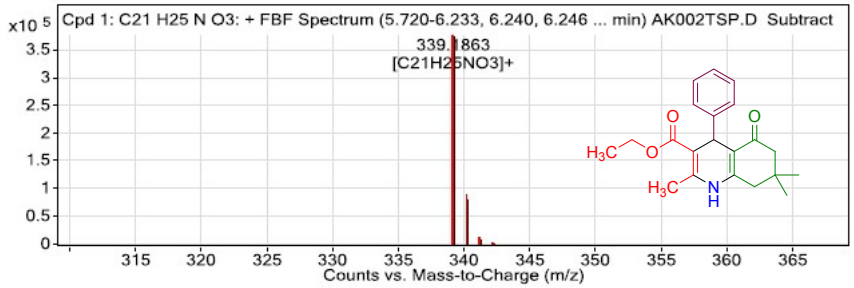
Compound Table

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass Error (ppm)	Obs. m/z	Ret.T	Find Comp. Algorith
C21 H25 N O3	339.1834	339.1863	74.09	8.52	339.1863	6.289	Find By Formula

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass error (ppm)	*Obs. m/z*	Find Cpds Algorith
C21 H25 N O3	339.1834	339.1863	74.09	8.52	339.1863	Find By Formula



MS Zoomed Spectrum

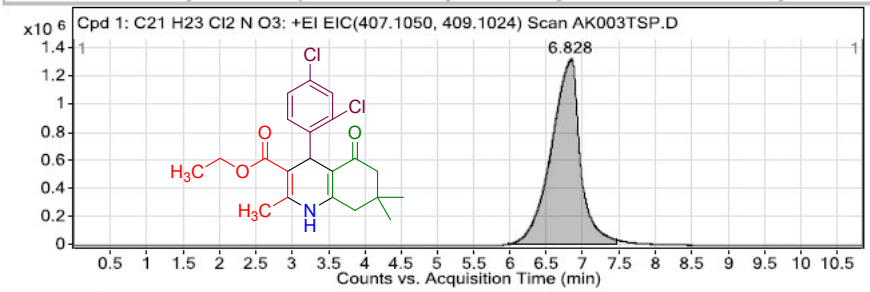


Data File	AK003TSP.D	**Sample Name**	Unavailable
Position	Unavailable	**Instrument Name**	Unavailable
Operator Name	Unavailable	**Acq Method**	
Acquired Time	Unavailable	**IRM Calibration Status**	Success
DA Method	UA.m	**Comment**	Sample information is unavailable

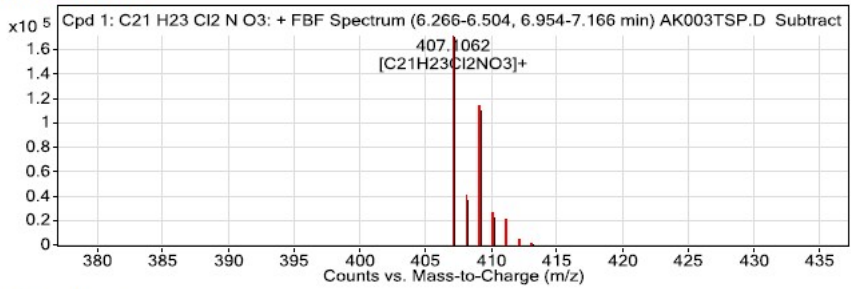
Compound Table

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass Error (ppm)	Obs. m/z	Ret.T	Find Comp. Algorith
C21 H23 Cl2 N O3	407.1055	407.1065	95.66	2.49	407.1062	6.828	Find By Formula

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass error (ppm)	*Obs. m/z*	Find Cpds Algorith
C21 H23 Cl2 N O3	407.1055	407.1065	95.66	2.49	407.1062	Find By Formula



MS Zoomed Spectrum

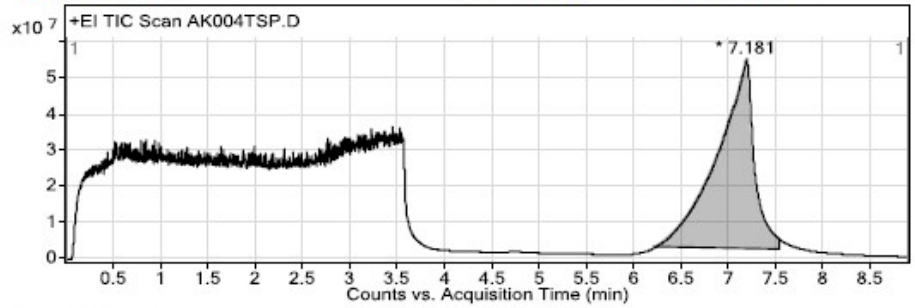


Data Filename	AK004TSP.D	**Sample Name**	
Sample Type		**Position**	1
Instrument Name	GCQTOF	**User Name**	
Acq Method	ORGANICA_EI_4G_TSP.M	**Acquired Time**	7/26/2016 12:48:37 PM
IRM Calibration Status	Success	**DA Method**	UA.m
Comment			

Expected Barcode		**Sample Amount**	
Dual Inj Vol		**TuneName**	atunes.ei.tune.xml
TunePath	D:\MassHunter\GCMS\1\7200\	**TuneDateStamp**	7/26/2016 10:46:36 AM
MSFirmwareVersion	G.7200.01.13	**OperatorName**	
RunCompletedFlag	True	**Acquisition SW Version**	MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013

User Chromatograms

Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** EI

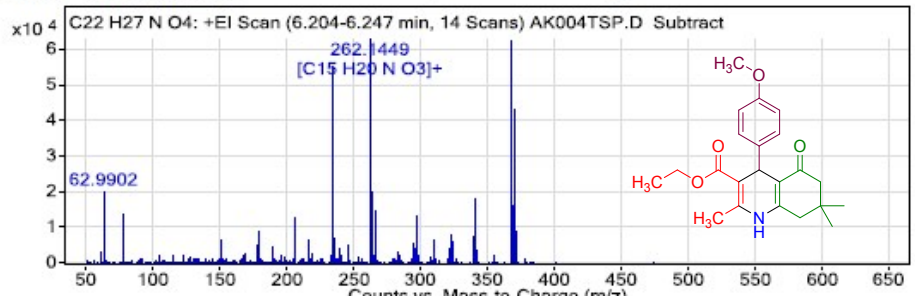


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	6.204	7.181	7.541	52799138.41	1441864093	100

User Spectra

Spectrum Source Peak (1) in "+ TIC Scan - AK004TSP.D" **Collision Energy** 0 **Ionization Mode** EI

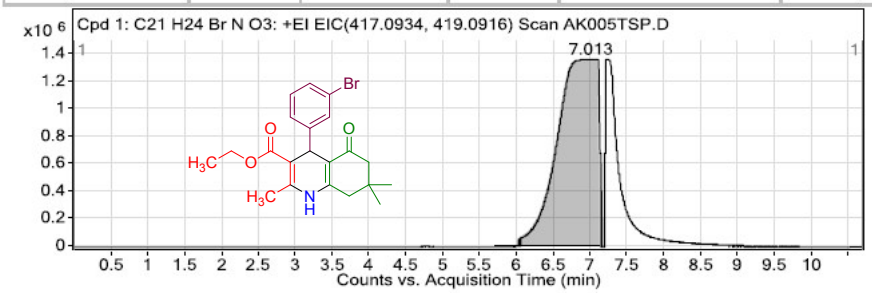


Data File	AK005TSP.D	**Sample Name**	
Position	1	**Instrument Name**	GCQTOF
Operator Name		**Acq Method**	ORGANICA_EI_4G_TSP.M
Acquired Time	7/26/2016 1:08:51 PM	**IRM Calibration Status**	Success
DA Method	UA.m	**Comment**	

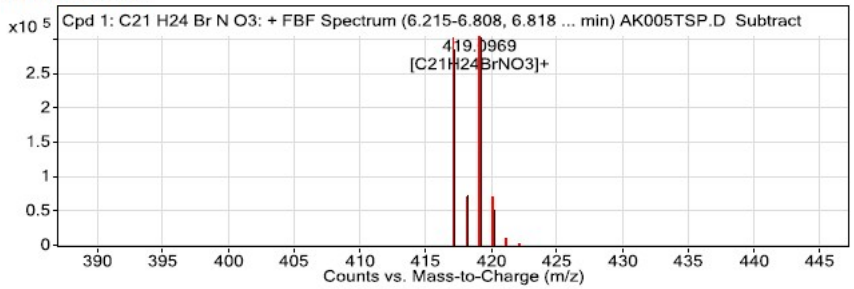
Compound Table

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass Error (ppm)	Obs. m/z	Ret.T	Find Comp. Algorith
C21 H24 Br N O3	417.094	417.096	76.61	4.94	419.0969	7.013	Find By Formula

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass error (ppm)	*Obs. m/z*	Find Cpds Algorith
C21 H24 Br N O3	417.094	417.096	76.61	4.94	419.0969	Find By Formula



MS Zoomed Spectrum

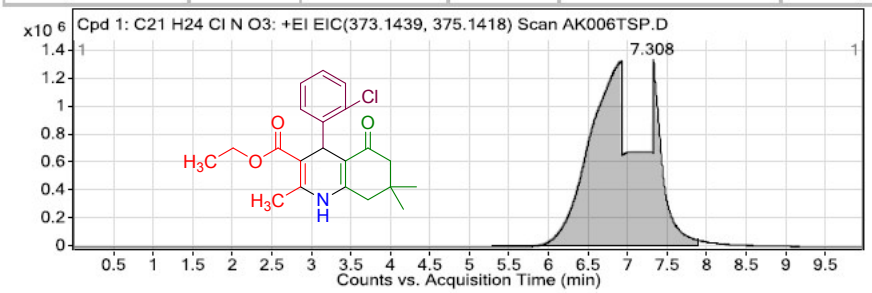


Data File	AK006TSP.D	**Sample Name**	
Position	1	**Instrument Name**	GCQTOF
Operator Name		**Acq Method**	ORGANICA_EI_4G_TSP.M
Acquired Time	7/26/2016 1:40:33 PM	**IRM Calibration Status**	Success
DA Method	UA.m	**Comment**	

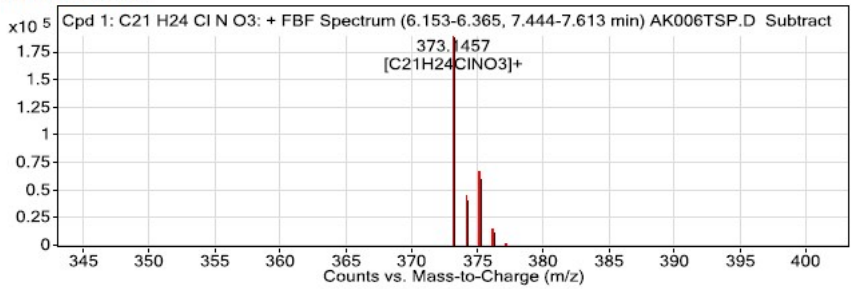
Compound Table

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass Error (ppm)	Obs. m/z	Ret.T	Find Comp. Algorith
C21 H24 Cl N O3	373.1445	373.1461	91.04	4.39	373.1457	7.308	Find By Formula

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass error (ppm)	*Obs. m/z*	Find Cpds Algorith
C21 H24 Cl N O3	373.1445	373.1461	91.04	4.39	373.1457	Find By Formula



MS Zoomed Spectrum

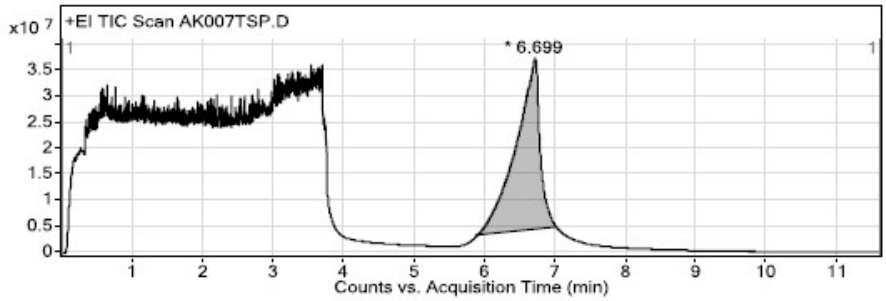


Data Filename	AK007TSP.D	**Sample Name**	
Sample Type		**Position**	1
Instrument Name	GCQTOF	**User Name**	
Acq Method	ORGANICA_EI_4G_TSP.M	**Acquired Time**	7/26/2016 1:58:45 PM
IRM Calibration Status	Success	**DA Method**	UA.m
Comment			

Expected Barcode		**Sample Amount**	
Dual Inj Vol		**TuneName**	atunes.ei.tune.xml
TunePath	D:\MassHunter\GCMS\1\7200\	**TuneDateStamp**	7/26/2016 11:55:23 AM
MSFirmwareVersion	G.7200.01.13	**OperatorName**	
RunCompletedFlag	True	**Acquisition SW Version**	MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013

User Chromatograms

Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** EI

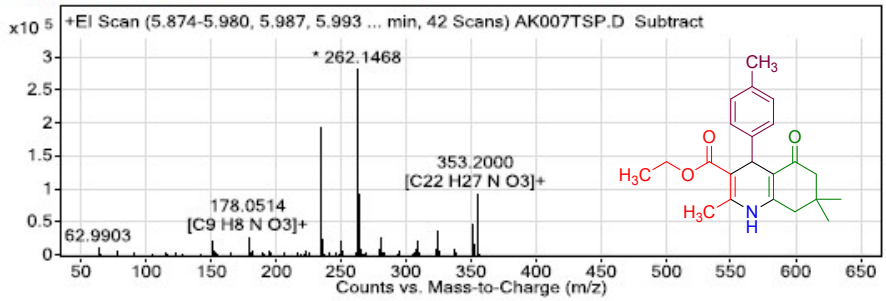


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	5.874	6.699	7.016	32984452.52	788602954.9	100

User Spectra

Spectrum Source	**Collision Energy**	**Ionization Mode**
Peak (1) in "+ TIC Scan - AK007TSP.D"	0	EI

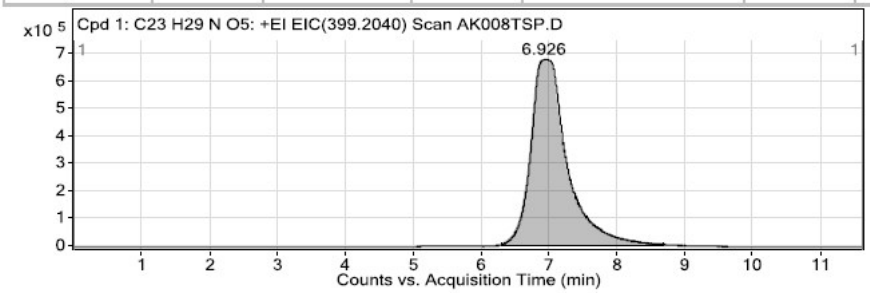


Data File	AK008TSP.D	**Sample Name**	
Position	1	**Instrument Name**	GCQTOF
Operator Name		**Acq Method**	ORGANICA_EI_4G_TSP.M
Acquired Time	7/27/2016 8:55:10 AM	**IRM Calibration Status**	Success
DA Method	UA.m	**Comment**	

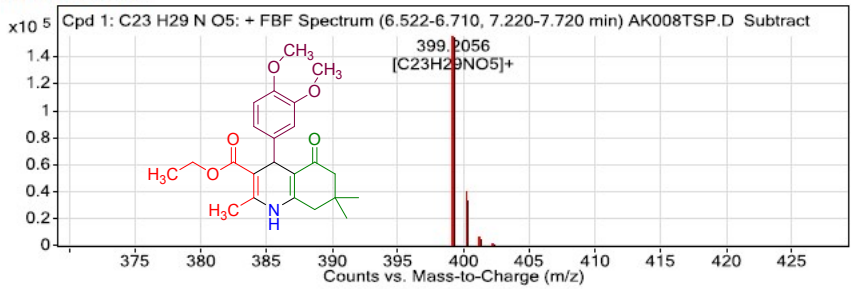
Compound Table

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass Error (ppm)	Obs. m/z	Ret.T	Find Comp. Algorith
C23 H29 N O5	399.2046	399.2062	91.12	4.07	399.2056	6.926	Find By Formula

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass error (ppm)	*Obs. m/z*	Find Cpds Algorith
C23 H29 N O5	399.2046	399.2062	91.12	4.07	399.2056	Find By Formula



MS Zoomed Spectrum

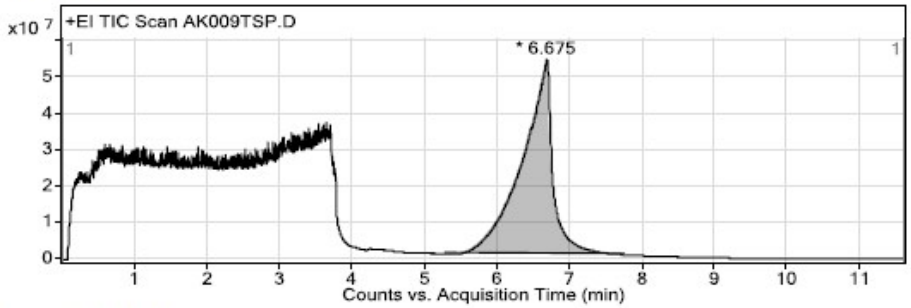


Data Filename	AK009TSP.D	**Sample Name**	
Sample Type		**Position**	1
Instrument Name	GCQTOF	**User Name**	
Acq Method	ORGANICA_EI_4G_TSP.M	**Acquired Time**	7/27/2016 9:15:29 AM
IRM Calibration Status	Success	**DA Method**	UA.m
Comment			

Expected Barcode		**Sample Amount**	
Dual Inj Vol		**TuneName**	atunes.ei.tune.xml
TunePath	D:\MassHunter\GCMS\1\7200\	**TuneDateStamp**	7/27/2016 7:13:13 AM
MSFirmwareVersion	G.7200.01.13	**OperatorName**	
RunCompletedFlag	True	**Acquisition SW Version**	MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013

User Chromatograms

Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** EI

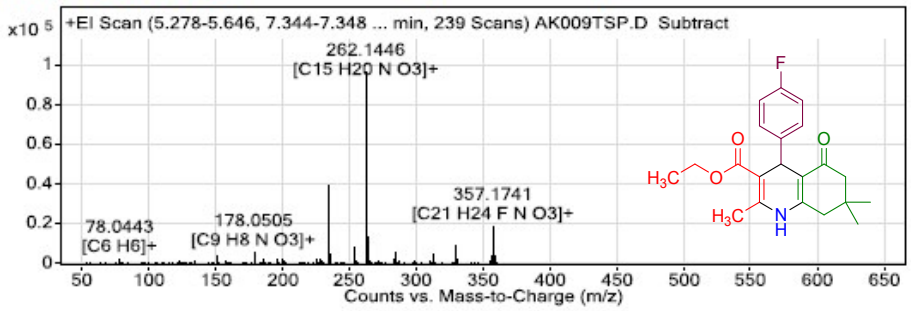


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	5.278	6.675	7.765	53445390.85	1570038458	100

User Spectra

Spectrum Source Peak (1) in "+ TIC Scan - AK009TSP.D" **Collision Energy** 0 **Ionization Mode** EI

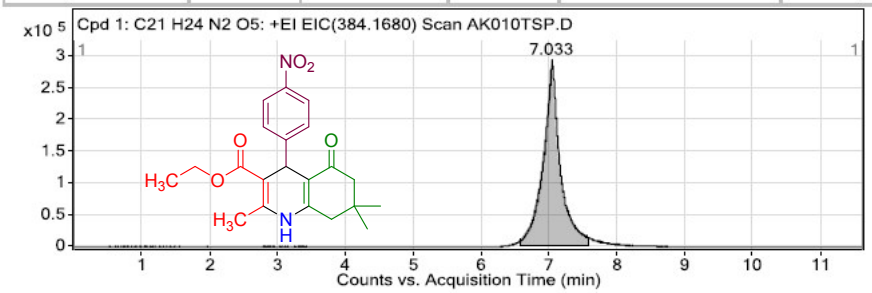


Data File	AK010TSP.D	**Sample Name**	
Position	1	**Instrument Name**	GCQTOF
Operator Name		**Acq Method**	ORGANICA_EI_4G_TSP.M
Acquired Time	7/27/2016 9:47:51 AM	**IRM Calibration Status**	Success
DA Method	UA.m	**Comment**	

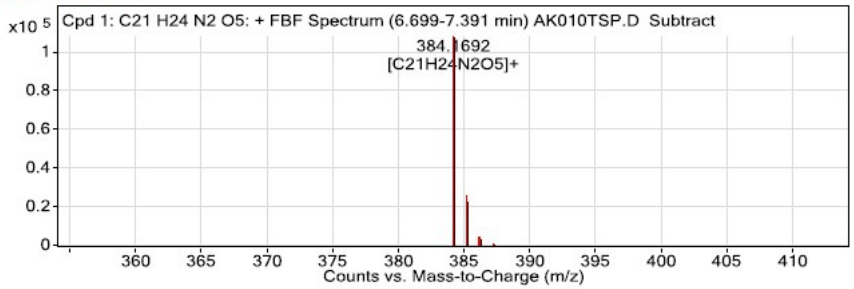
Compound Table

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass Error (ppm)	Obs. m/z	Ret.T	Find Comp. Algorith
C21 H24 N2 O5	384.1685	384.1697	94.68	3.02	384.1692	7.033	Find By Formula

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass error (ppm)	*Obs. m/z*	Find Cpds Algorith
C21 H24 N2 O5	384.1685	384.1697	94.68	3.02	384.1692	Find By Formula



MS Zoomed Spectrum

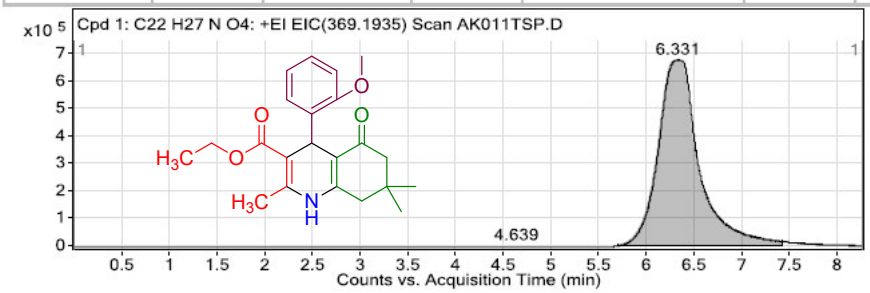


Data File	AK011TSP.D	**Sample Name**	
Position	1	**Instrument Name**	GCQTOF
Operator Name		**Acq Method**	ORGANICA_EI_4G_TSP.M
Acquired Time	7/27/2016 10:10:06 AM	**IRM Calibration Status**	Success
DA Method	UA.m	**Comment**	

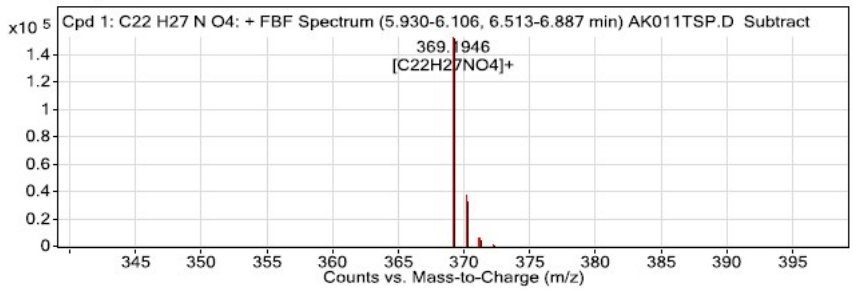
Compound Table

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass Error (ppm)	Obs. m/z	Ret.T	Find Comp. Algorith
C22 H27 N O4	369.194	369.1951	94.59	3.03	369.1946	6.331	Find By Formula

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass error (ppm)	*Obs. m/z*	Find Cpds Algorith
C22 H27 N O4	369.194	369.1951	94.59	3.03	369.1946	Find By Formula



MS Zoomed Spectrum

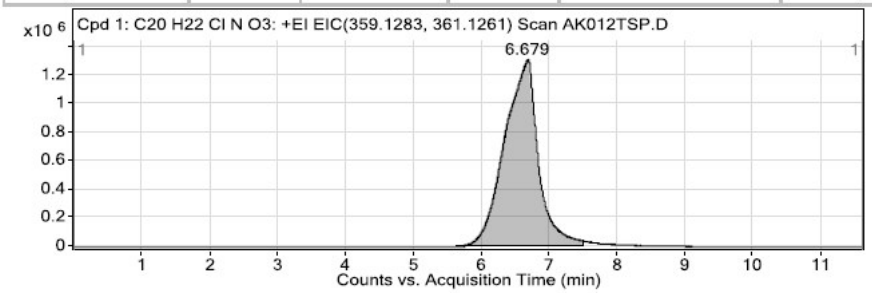


Data File	AK012TSP.D	**Sample Name**	
Position	1	**Instrument Name**	GCQTOF
Operator Name		**Acq Method**	ORGANICA_EI_4G_TSP.M
Acquired Time	7/27/2016 10:25:41 AM	**IRM Calibration Status**	Success
DA Method	UA.m	**Comment**	

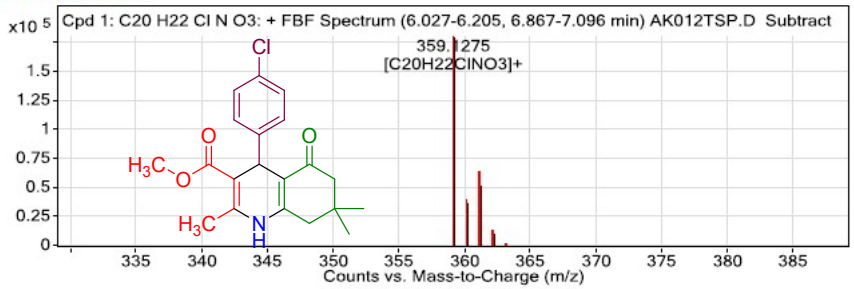
Compound Table

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass Error (ppm)	Obs. m/z	Ret.T	Find Comp. Algorith
C20 H22 Cl N O3	359.1288	359.1282	92.28	-1.62	359.1275	6.679	Find By Formula

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass error (ppm)	*Obs. m/z*	Find Cpds Algorith
C20 H22 Cl N O3	359.1288	359.1282	92.28	-1.62	359.1275	Find By Formula



MS Zoomed Spectrum

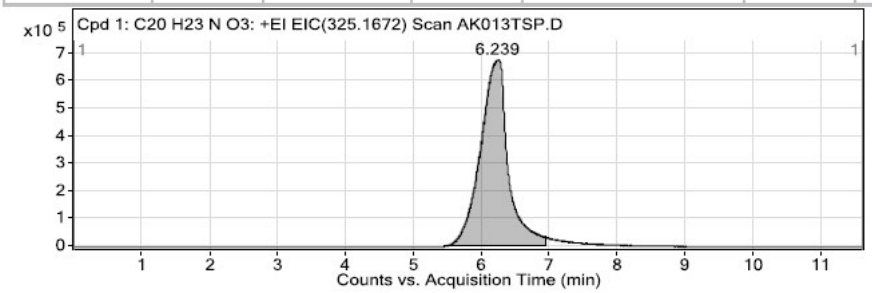


Data File	AK013TSP.D	**Sample Name**	
Position	1	**Instrument Name**	GCQTOF
Operator Name		**Acq Method**	ORGANICA_EI_4G_TSP.M
Acquired Time	7/27/2016 10:45:32 AM	**IRM Calibration Status**	Success
DA Method	UA.m	**Comment**	

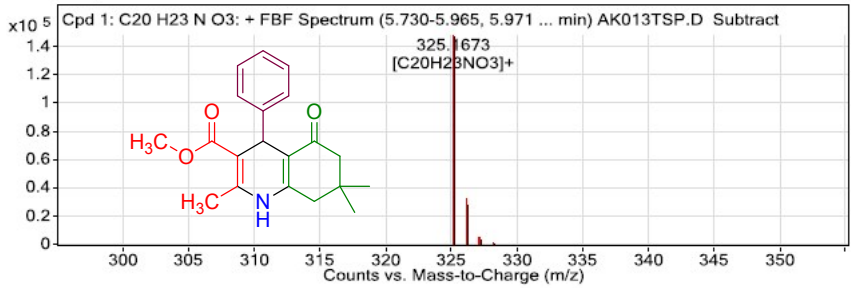
Compound Table

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass Error (ppm)	Obs. m/z	Ret.T	Find Comp. Algorith
C20 H23 N O3	325.1678	325.1678	97.57	0.11	325.1673	6.239	Find By Formula

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass error (ppm)	*Obs. m/z*	Find Cpds Algorith
C20 H23 N O3	325.1678	325.1678	97.57	0.11	325.1673	Find By Formula



MS Zoomed Spectrum

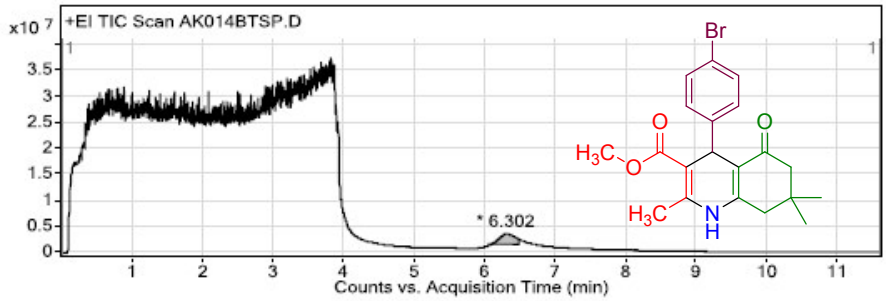


Data Filename	AK014BTSP.D	**Sample Name**	
Sample Type		**Position**	1
Instrument Name	GCQTOF	**User Name**	
Acq Method	ORGANICA_EI_4G_TSP.M	**Acquired Time**	7/28/2016 12:45:36 PM
IRM Calibration Status	Success	**DA Method**	UA.m
Comment			

Expected Barcode		**Sample Amount**	
Dual Inj Vol		**TuneName**	atunes.ei.tune.xml
TunePath	D:\MassHunter\GCMS\1\7200\	**TuneDateStamp**	7/28/2016 10:43:43 AM
MSFirmwareVersion	G.7200.01.13	**OperatorName**	
RunCompletedFlag	True	**Acquisition SW Version**	MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013 Copyright © 1989-2013 Agilent Technologies, Inc.

User Chromatograms

Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** EI

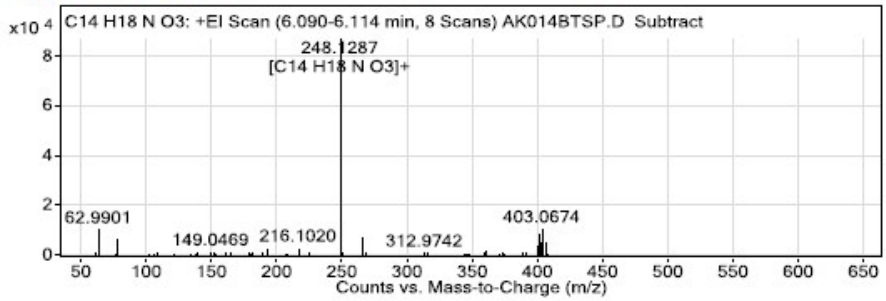


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	6.054	6.302	6.491	2284811.21	36745645.33	100

User Spectra

Spectrum Source	**Collision Energy**	**Ionization Mode**
Peak (1) in "+ TIC Scan - AK014BTSP.D"	0	EI

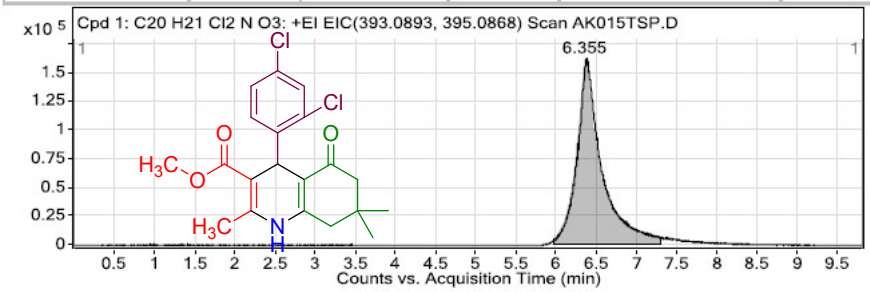


Data File	AK015TSP.D	**Sample Name**	Unavailable
Position	Unavailable	**Instrument Name**	Unavailable
Operator Name	Unavailable	**Acq Method**	
Acquired Time	Unavailable	**IRM Calibration Status**	Success
DA Method	UA.m	**Comment**	Sample information is unavailable

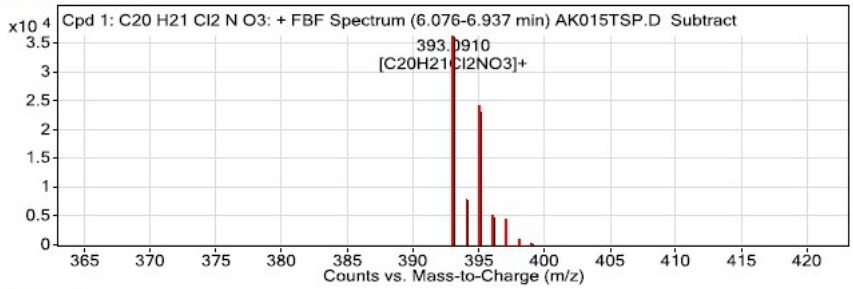
Compound Table

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass Error (ppm)	Obs. m/z	Ret.T	Find Comp. Algorith
C20 H21 Cl2 N O3	393.0898	393.0914	92.35	4	393.091	6.355	Find By Formula

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass error (ppm)	*Obs. m/z*	Find Cpds Algorith
C20 H21 Cl2 N O3	393.0898	393.0914	92.35	4	393.091	Find By Formula



MS Zoomed Spectrum

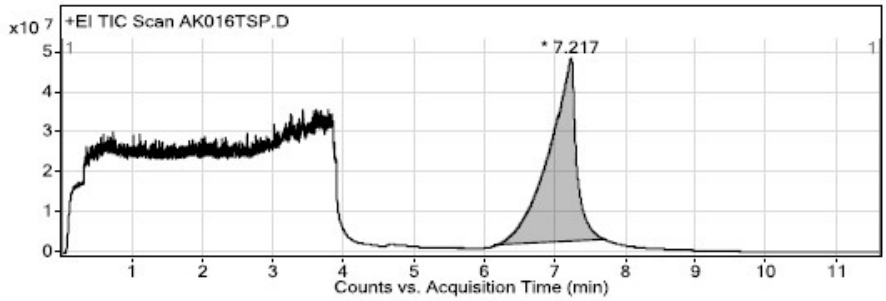


Data Filename	AK016TSP.D	**Sample Name**	
Sample Type		**Position**	1
Instrument Name	GCQTOF	**User Name**	
Acq Method	ORGANICA_EI_4G_TSP.M	**Acquired Time**	7/27/2016 12:22:19 PM
IRM Calibration Status	Success	**DA Method**	UA.m
Comment			

Expected Barcode		**Sample Amount**	
Dual Inj Vol		**TuneName**	atunes.ei.tune.xml
TunePath	D:\MassHunter\GCMS\1\7200\	**TuneDateStamp**	7/27/2016 10:20:48 AM
MSFirmwareVersion	G.7200.01.13	**OperatorName**	
RunCompletedFlag	True	**Acquisition SW Version**	MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013

User Chromatograms

Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** EI

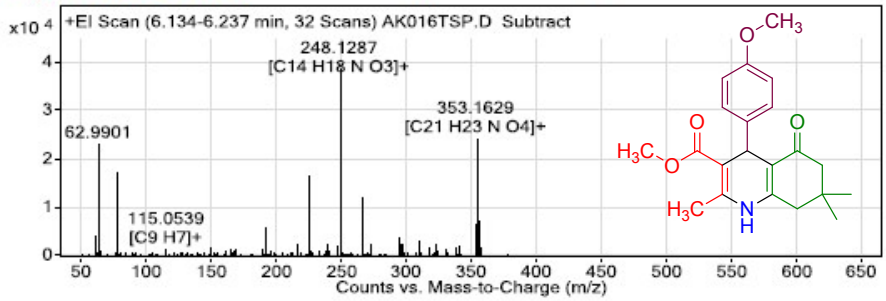


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	6.134	7.217	7.727	45734764.47	1256108048	100

User Spectra

Spectrum Source Peak (1) in "+ TIC Scan - AK016TSP.D" **Collision Energy** 0 **Ionization Mode** EI

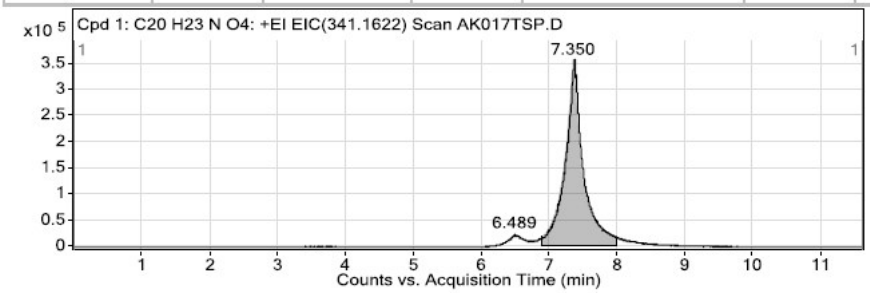


Data File	AK017TSP.D	**Sample Name**			
Position	1	**Instrument Name**	GCQTOF		
Operator Name		**Acq Method**	ORGANICA_EI_4G_TSP.M		
Acquired Time	7/27/2016 12:41:43 PM	**IRM Calibration Status**	Success		
DA Method	UA.m	**Comment**			

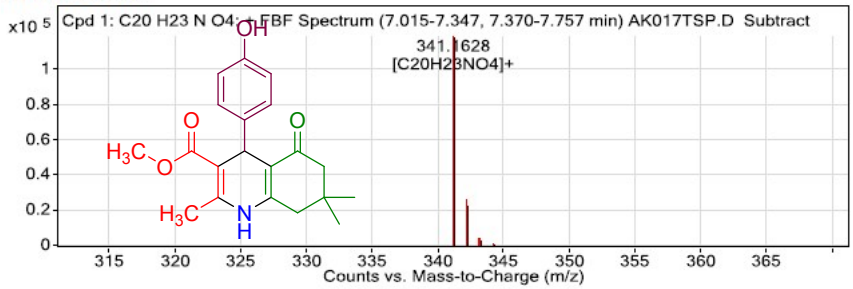
Compound Table

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass Error (ppm)	Obs. m/z	Ret.T	Find Comp. Algorith
C20 H23 N O4	341.1627	341.1633	96.95	1.69	341.1628	7.35	Find By Formula

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass error (ppm)	*Obs. m/z*	Find Cpds Algorith
C20 H23 N O4	341.1627	341.1633	96.95	1.69	341.1628	Find By Formula



MS Zoomed Spectrum

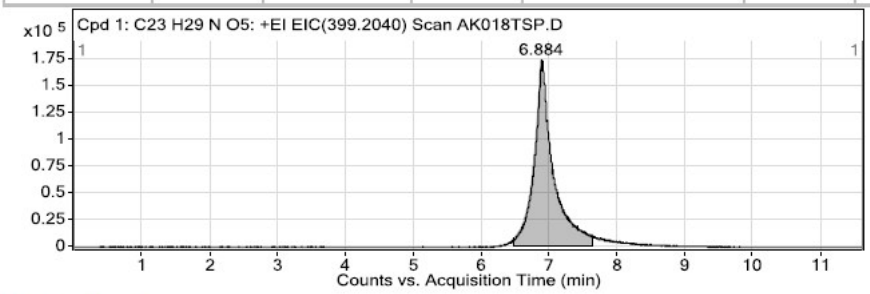


Data File	AK018TSP.D	**Sample Name**	
Position	1	**Instrument Name**	GCQTOF
Operator Name		**Acq Method**	ORGANICA_EI_4G_TSP.M
Acquired Time	7/27/2016 1:17:49 PM	**IRM Calibration Status**	Success
DA Method	UA.m	**Comment**	

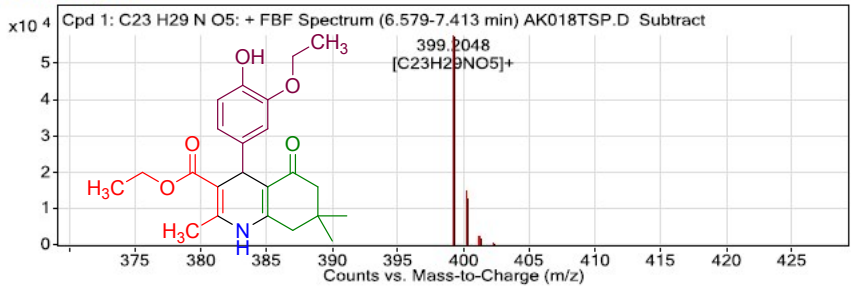
Compound Table

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass Error (ppm)	Obs. m/z	Ret.T	Find Comp. Algorith
C23 H29 N O5	399.2046	399.2053	96.53	1.9	399.2048	6.884	Find By Formula

Tgt Formula	Tgt Mass	Obs. Mass	Tgt Score	Mass error (ppm)	*Obs. m/z*	Find Cpds Algorith
C23 H29 N O5	399.2046	399.2053	96.53	1.9	399.2048	Find By Formula



MS Zoomed Spectrum

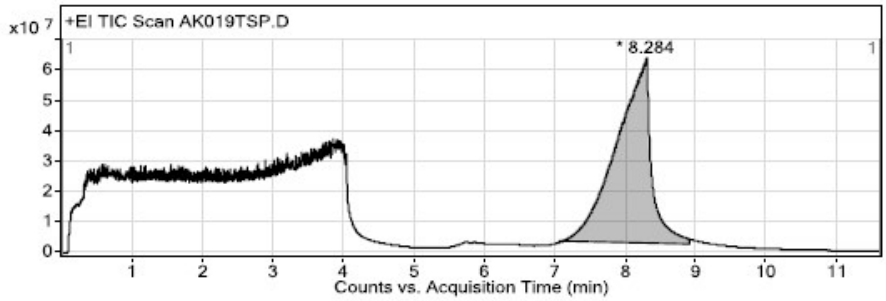


Data Filename	AK019TSP.D	**Sample Name**	
Sample Type		**Position**	1
Instrument Name	GCQTOF	**User Name**	
Acq Method	ORGANICA_EI_4G_TSP.M	**Acquired Time**	7/27/2016 1:41:10 PM
IRM Calibration Status	Success	**DA Method**	UA.m
Comment			

Expected Barcode		**Sample Amount**	
Dual Inj Vol		**TuneName**	atunes.ei.tune.xml
TunePath	D:\MassHunter\GCMS\1\7200\	**TuneDateStamp**	7/27/2016 11:39:36 AM
MSFirmwareVersion	G.7200.01.13	**OperatorName**	
RunCompletedFlag	True	**Acquisition SW Version**	MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013 Copyright © 1989-2013 Agilent Technologies, Inc.

User Chromatograms

Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** EI

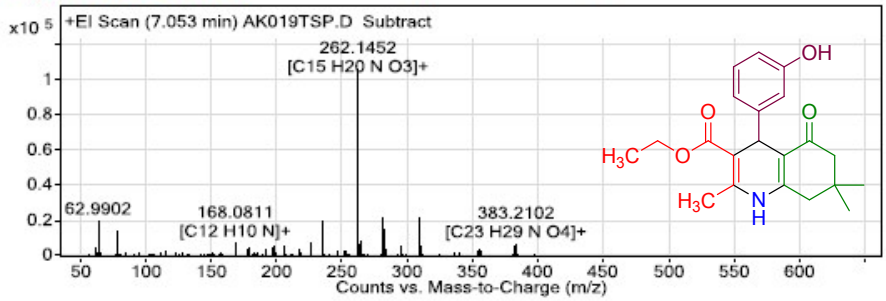


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	7.053	8.284	8.916	61197703.77	2131638407	100

User Spectra

Spectrum Source Peak (1) in "+ TIC Scan - AK019TSP.D" **Collision Energy** 0 **Ionization Mode** EI

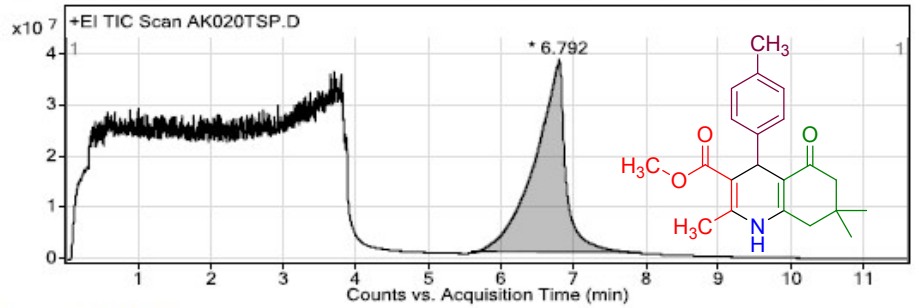


Data Filename	AK020TSP.D	**Sample Name**	
Sample Type		**Position**	1
Instrument Name	GCQTOF	**User Name**	
Acq Method	ORGANICA_EI_4G_TSP.M	**Acquired Time**	7/27/2016 2:00:49 PM
IRM Calibration Status	Success	**DA Method**	UA.m
Comment			

Expected Barcode		**Sample Amount**	
Dual Inj Vol		**TuneName**	atunes.ei.tune.xml
TunePath	D:\MassHunter\GCMS\1\7200\	**TuneDateStamp**	7/27/2016 11:57:25 AM
MSFirmwareVersion	G.7200.01.13	**OperatorName**	
RunCompletedFlag	True	**Acquisition SW Version**	MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013 Copyright © 1989-2013 Agilent Technologies, Inc.

User Chromatograms

Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** EI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	5.593	6.792	7.934	37743952.99	1123274532	100

User Spectra

Spectrum Source Peak (1) in "+ TIC Scan - AK020TSP.D" **Collision Energy** 0 **Ionization Mode** EI