

Supporting information for:**Reversible *trans-cis* photoisomerization of new pyrrolidene heterocyclic imines**

Paulo J. Coelho^{a,*}, M. Cidália R. Castro^b, M. Manuela M. Raposo^{b*}

^a *Centro de Química-Vila Real, Universidade de Trás-os-Montes e Alto Douro, 5001-801 Vila Real, Portugal.*

^b *Centro de Química, Universidade do Minho, Campus de Gualtar, 4710-057 Braga, Portugal.*

List of Contents

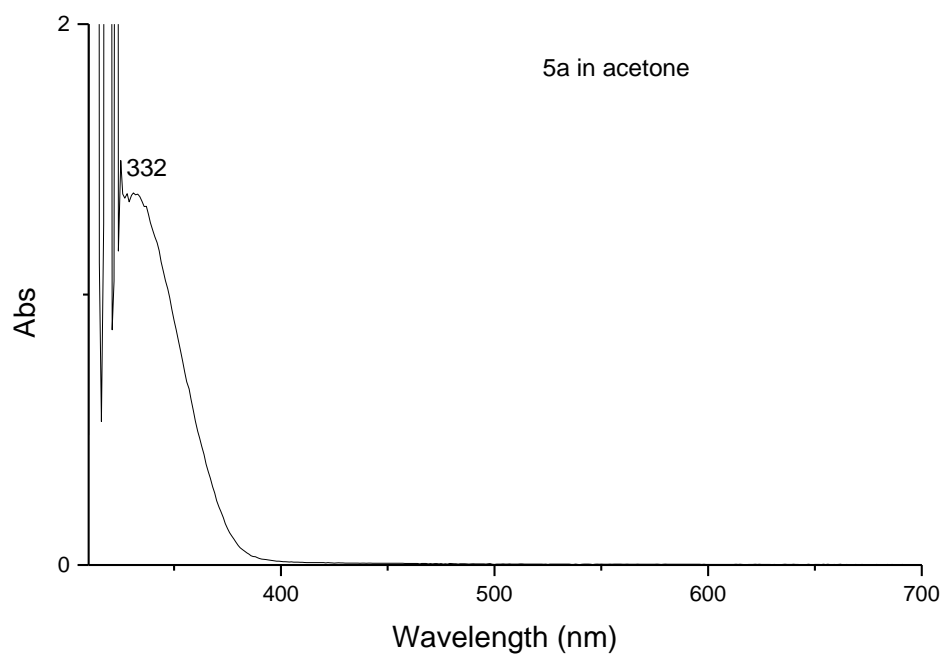
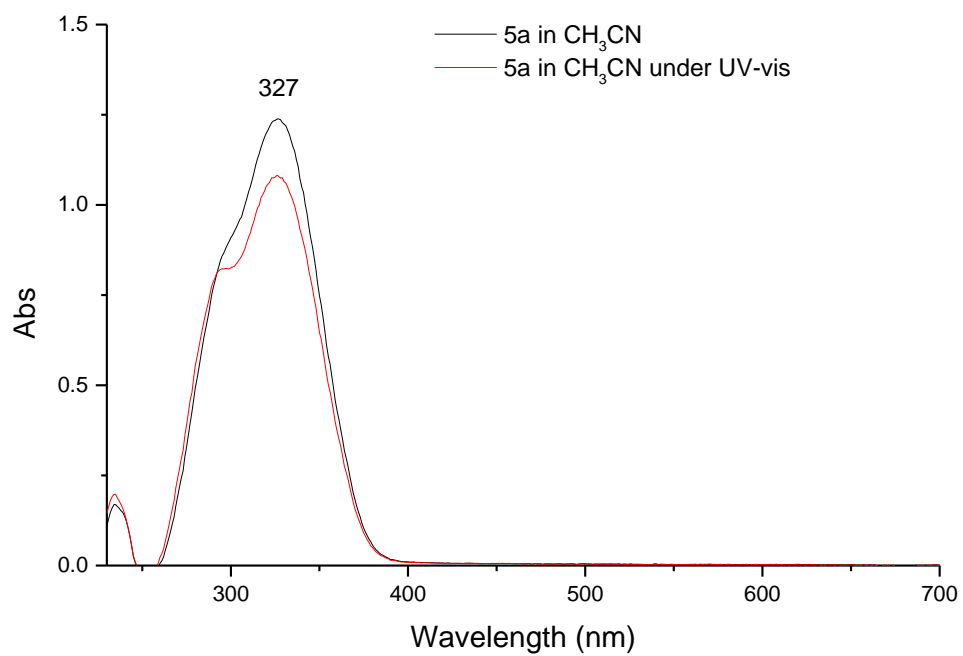
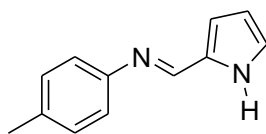
1. UV-vis spectra of imines 5-7	2
2. ¹ H and ¹³ C NMR spectra of compounds 5-6 and 7	11
3. IR spectra of compounds 5-6 and 7	24
4. Mass spectra of compounds 5-6 and 7	28

* Corresponding author Tel.: +351 259 350284; Fax: +351 259 350480; e-mail address: pcoelho@utad.pt

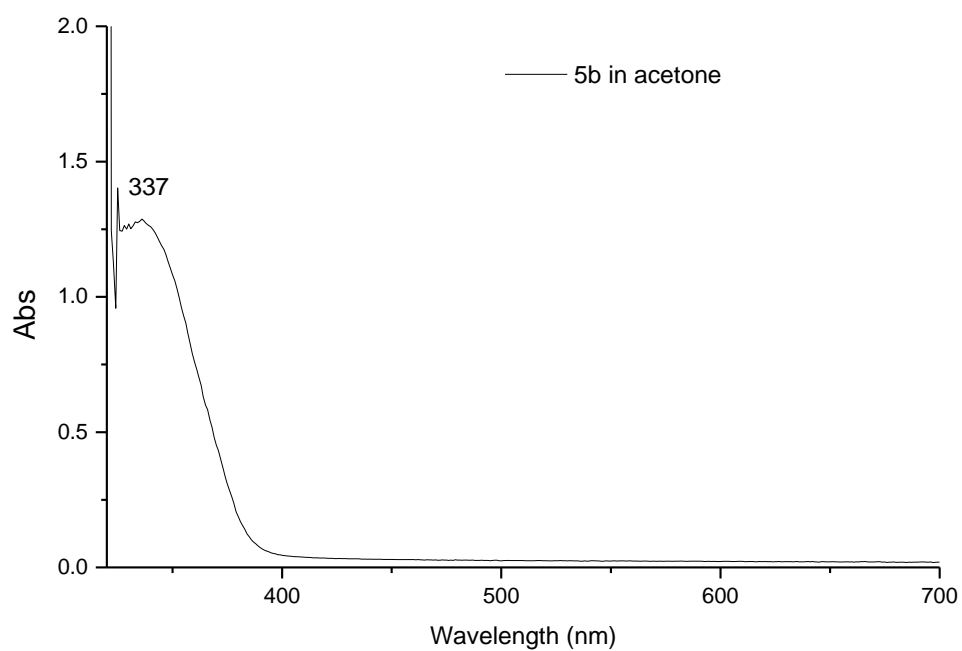
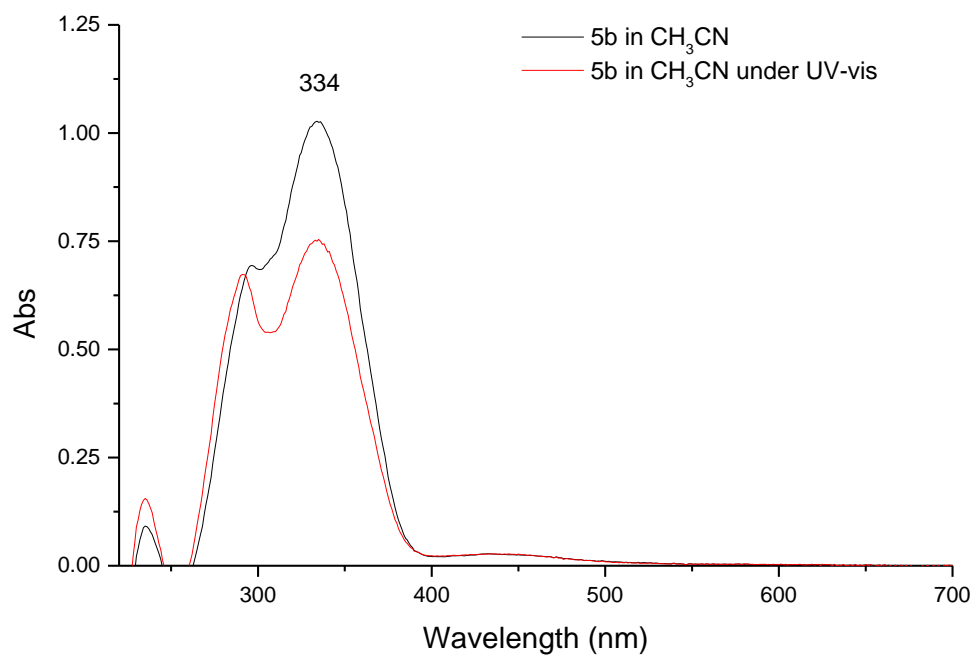
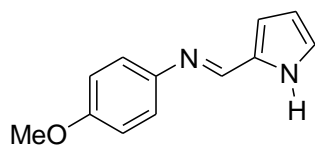
* Corresponding author Tel.: +351 253 604381; Fax: 253 604382; e-mail address: mfox@quimica.uminho.pt

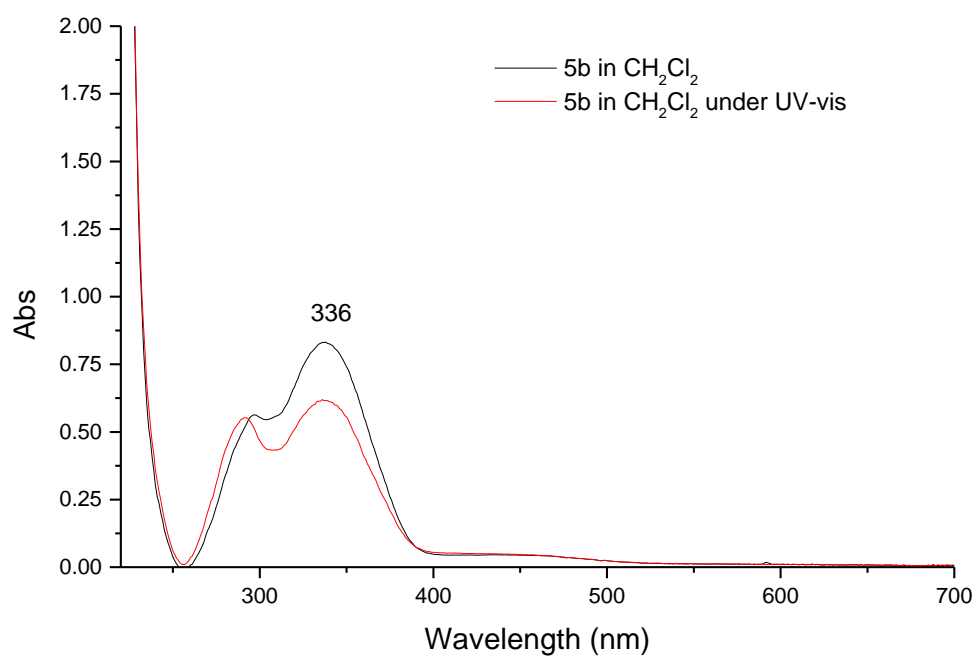
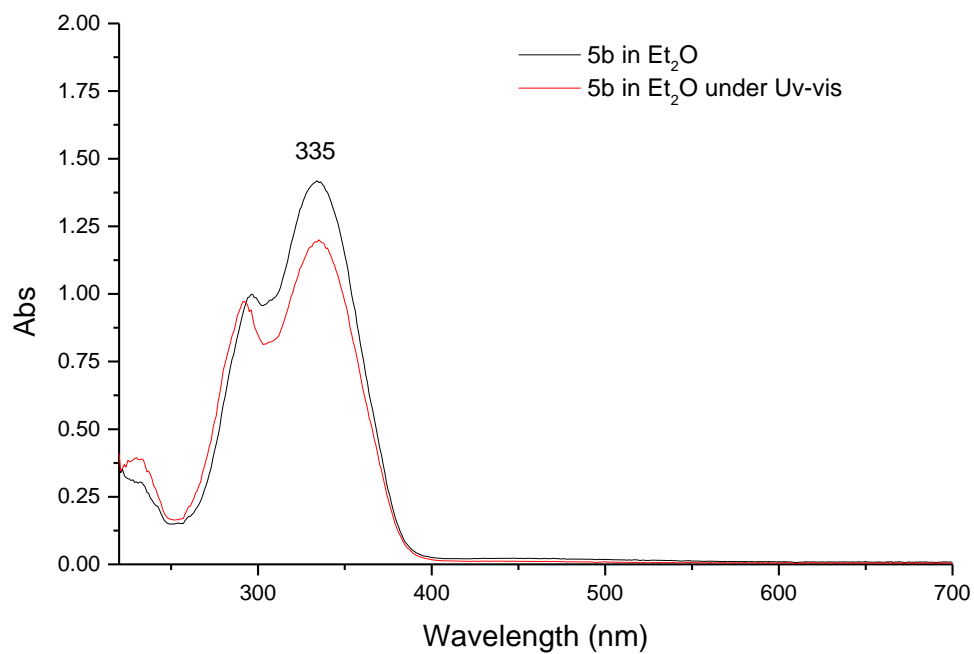
1. UV/vis Spectra of compounds 5-7 in different solvents

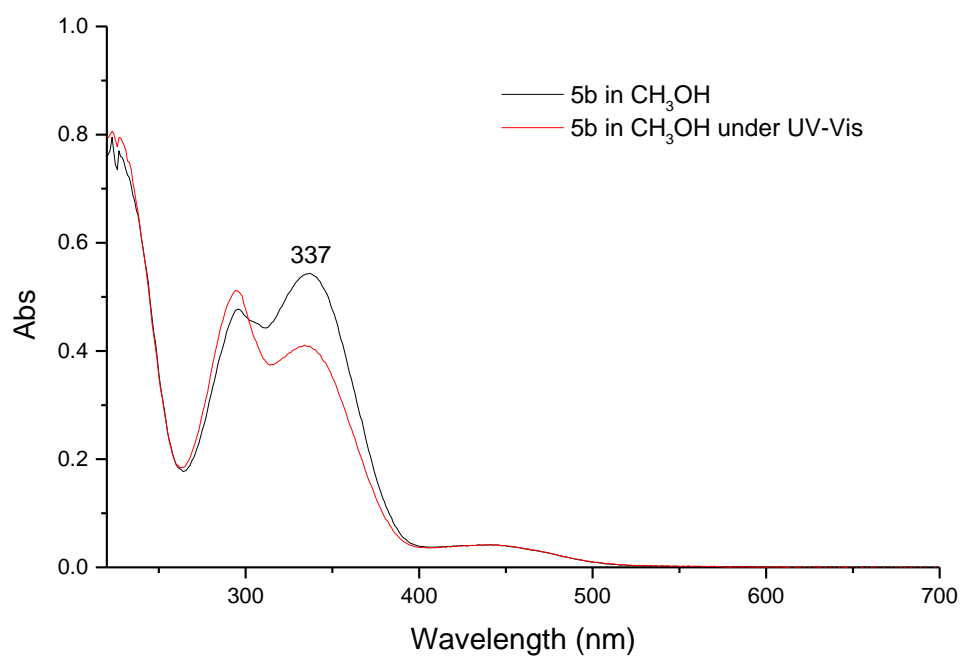
1.1. Imine 5a



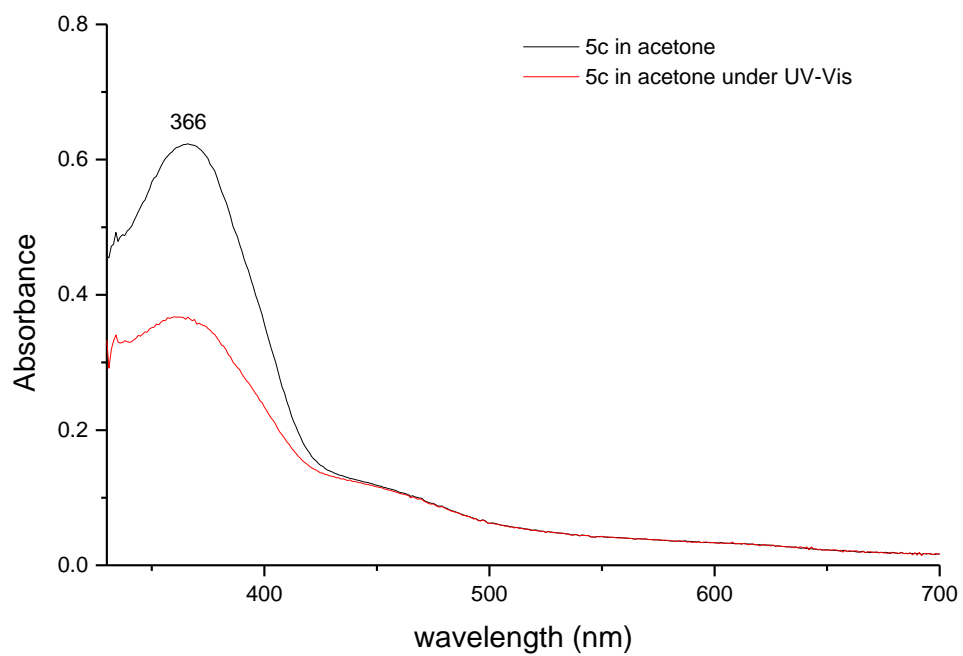
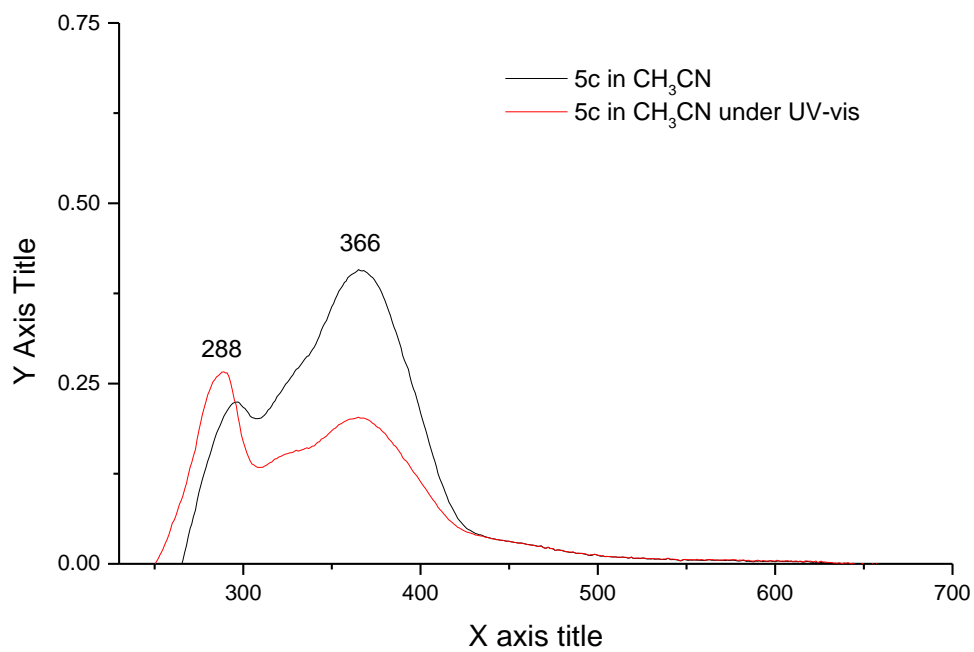
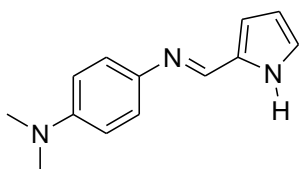
1.2. Imine 5b



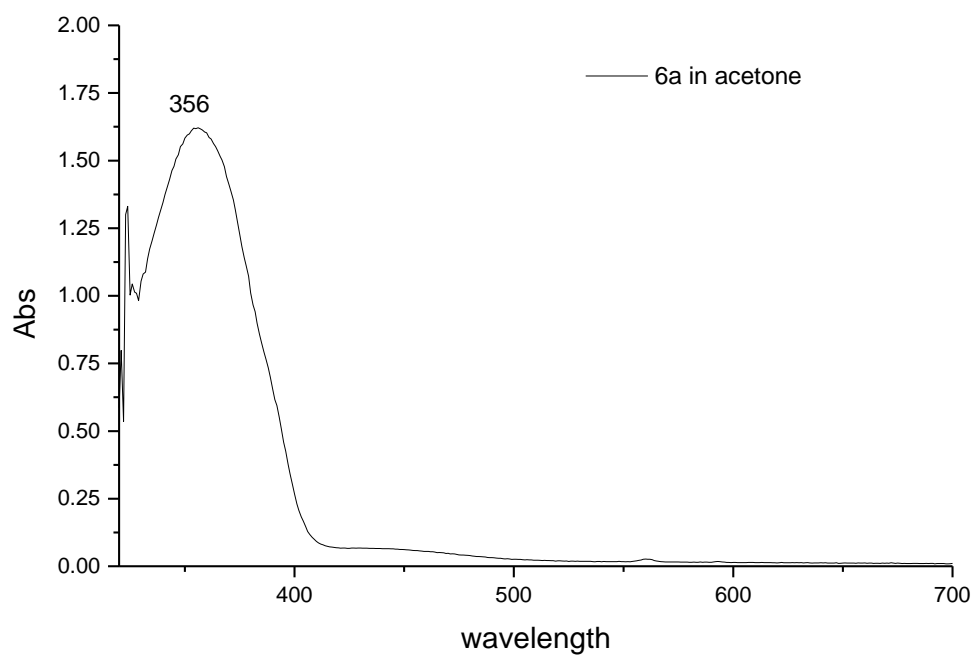
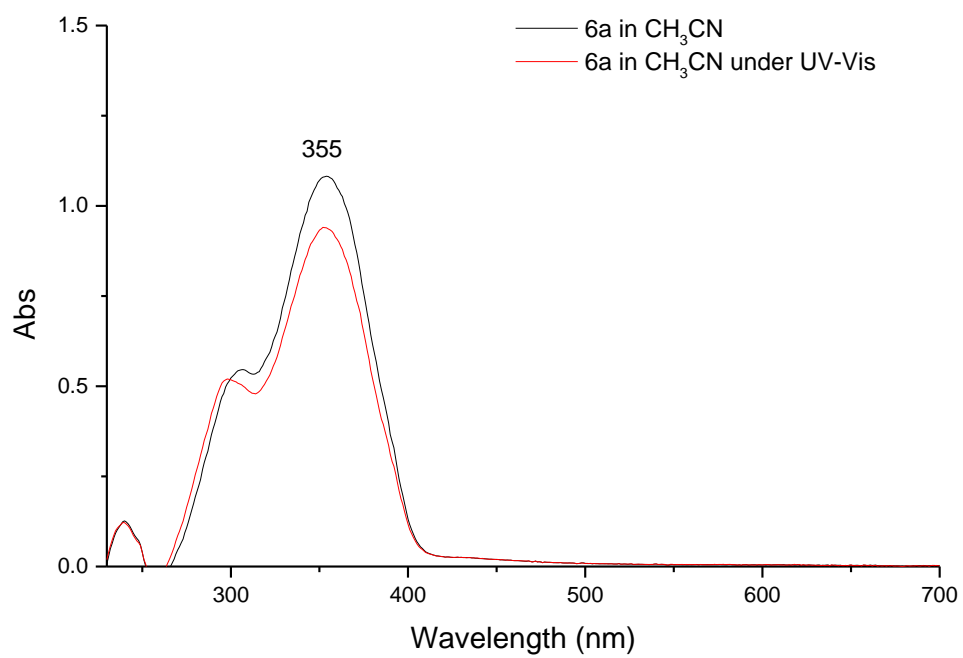
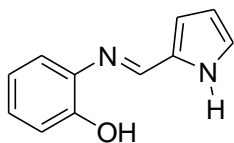




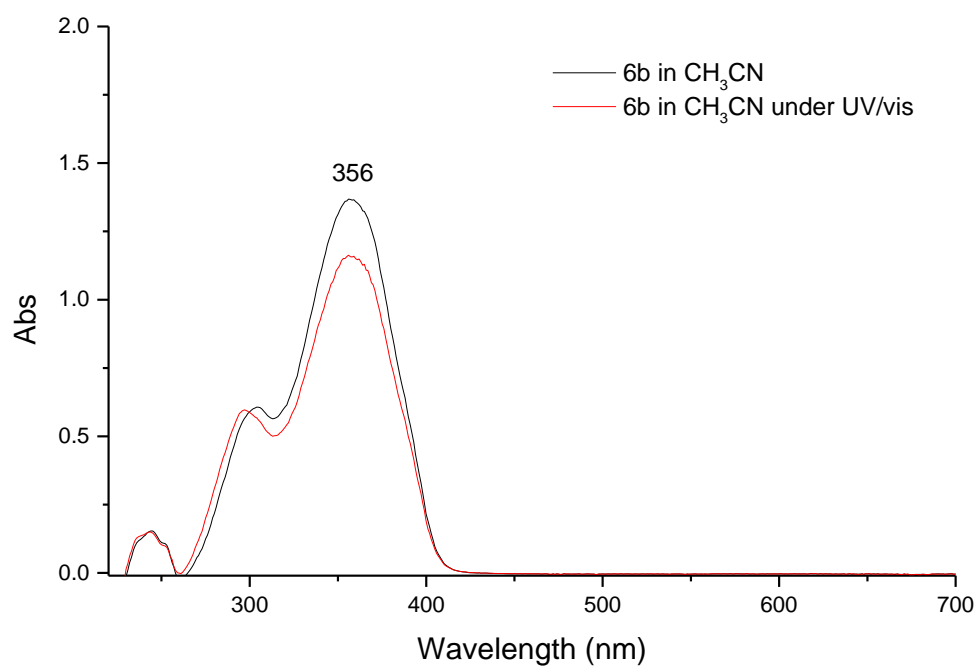
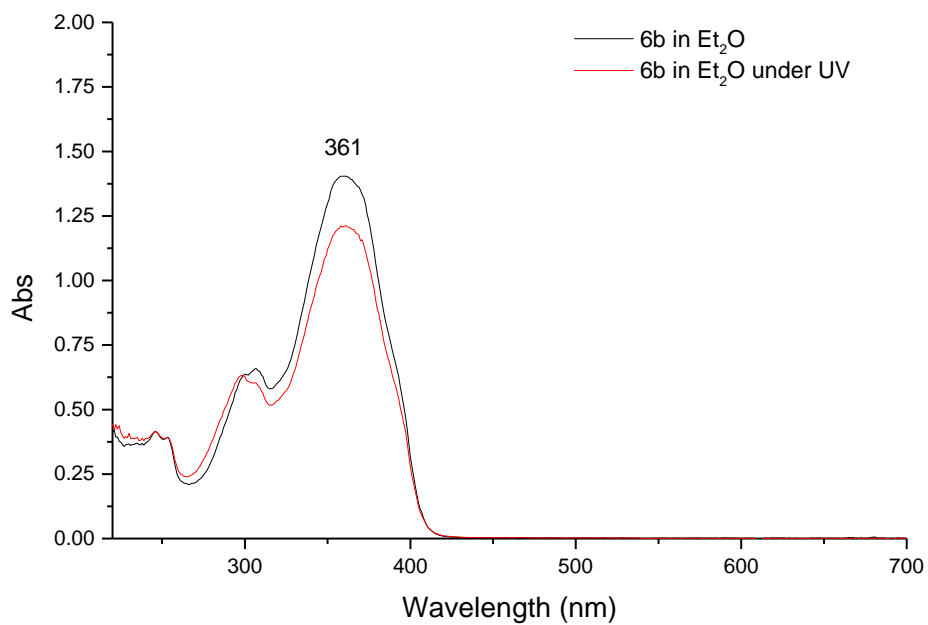
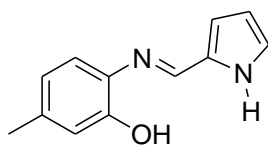
1.3. Imine 5c

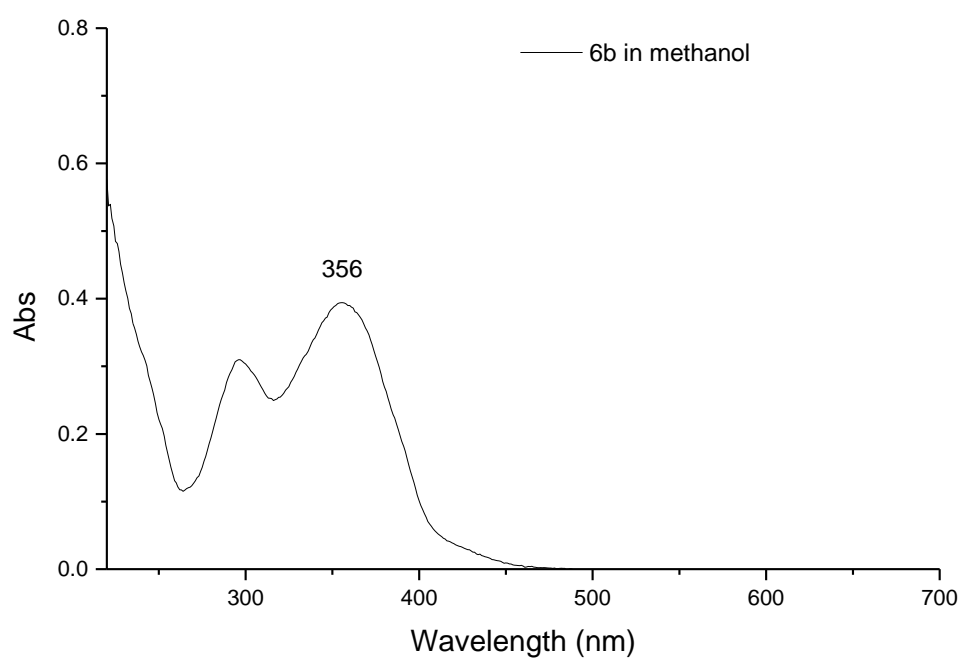
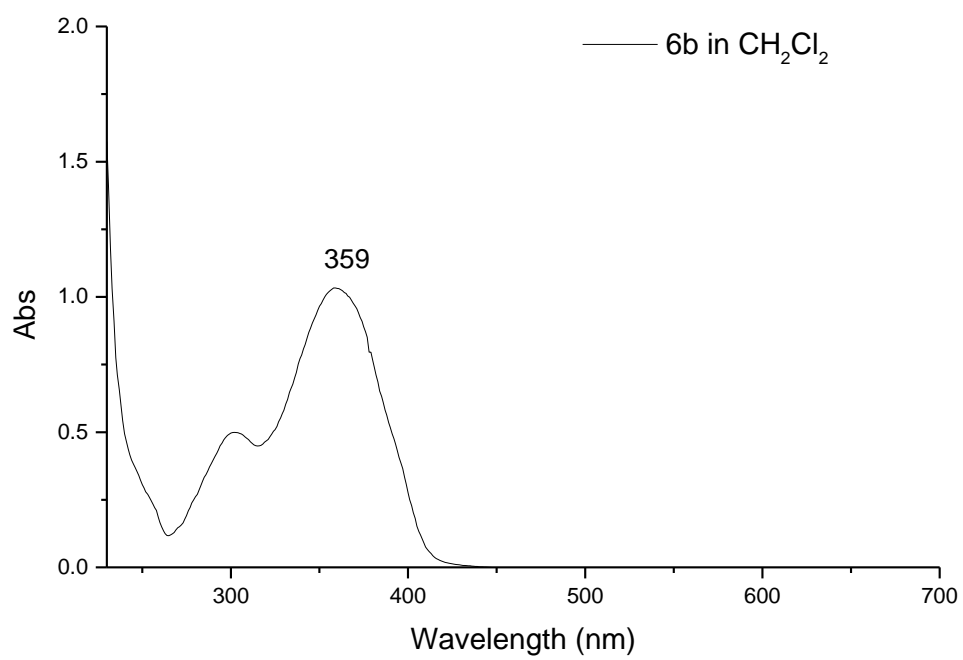


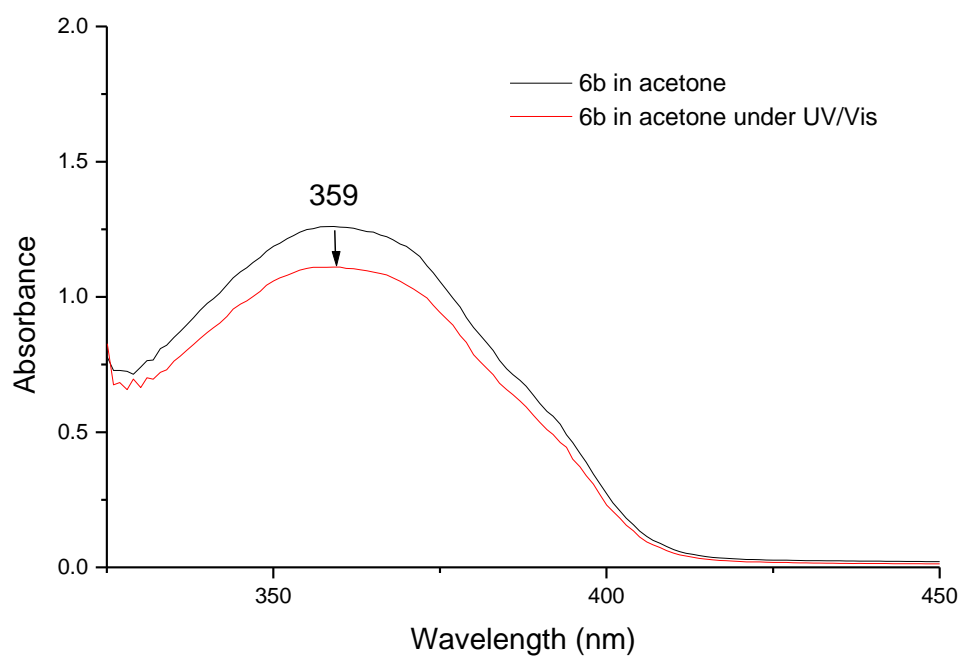
1.4. Imine 6a



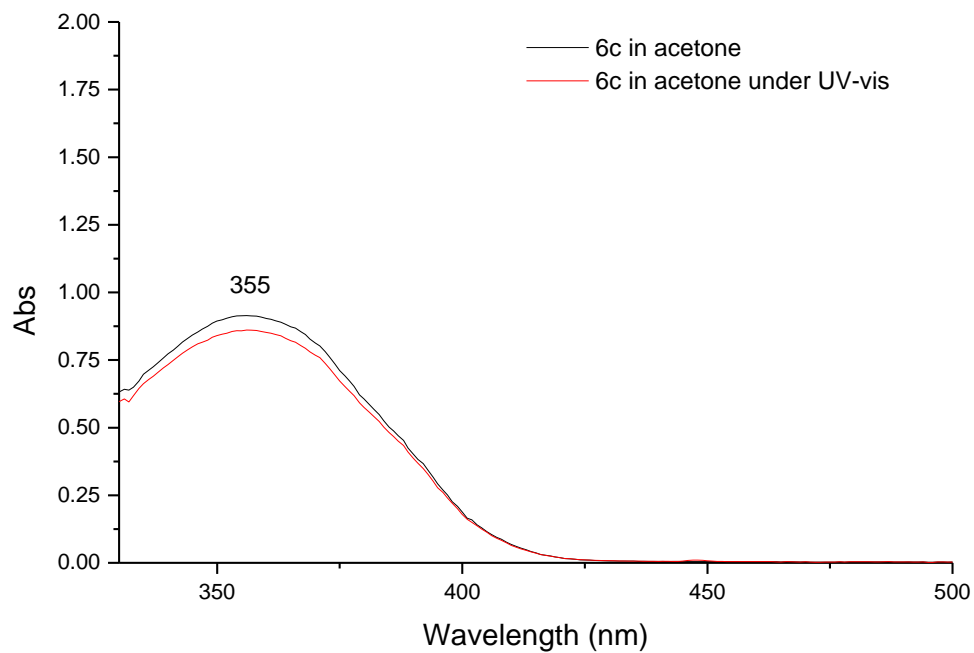
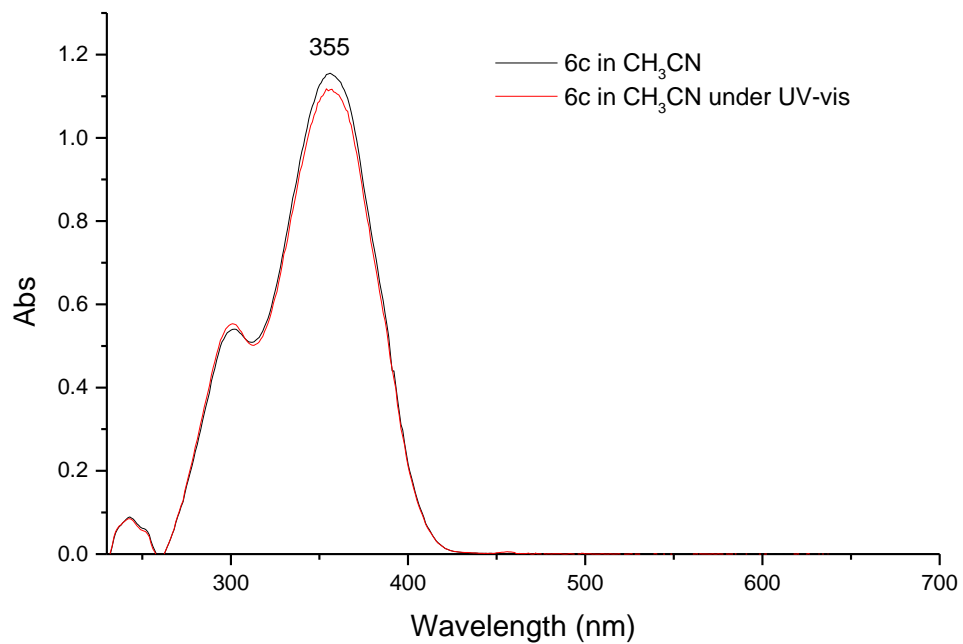
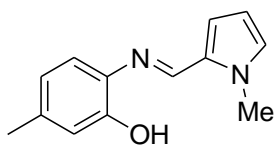
1.5. Imine 6b



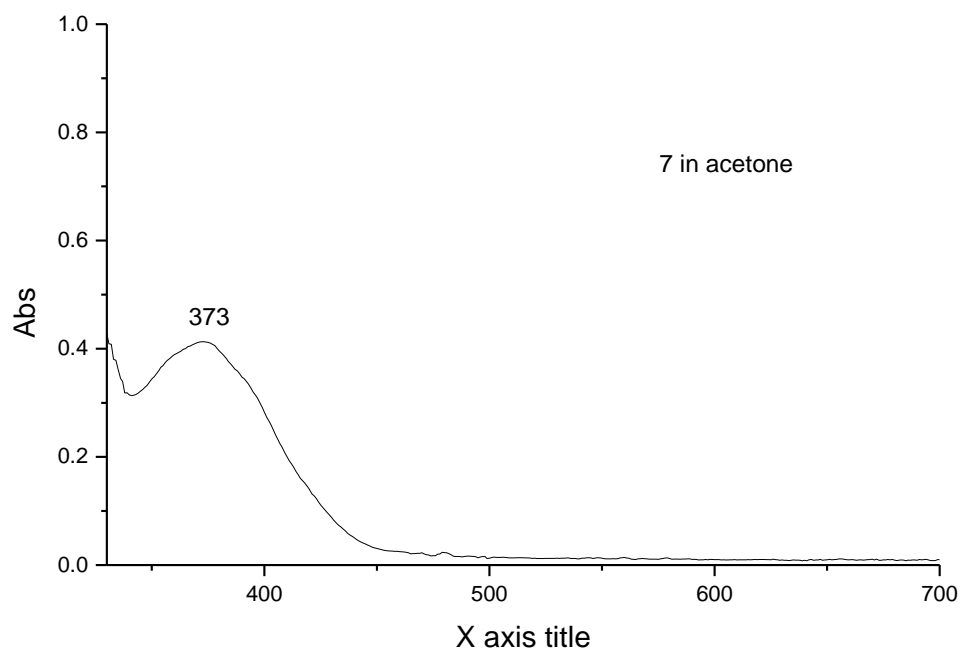
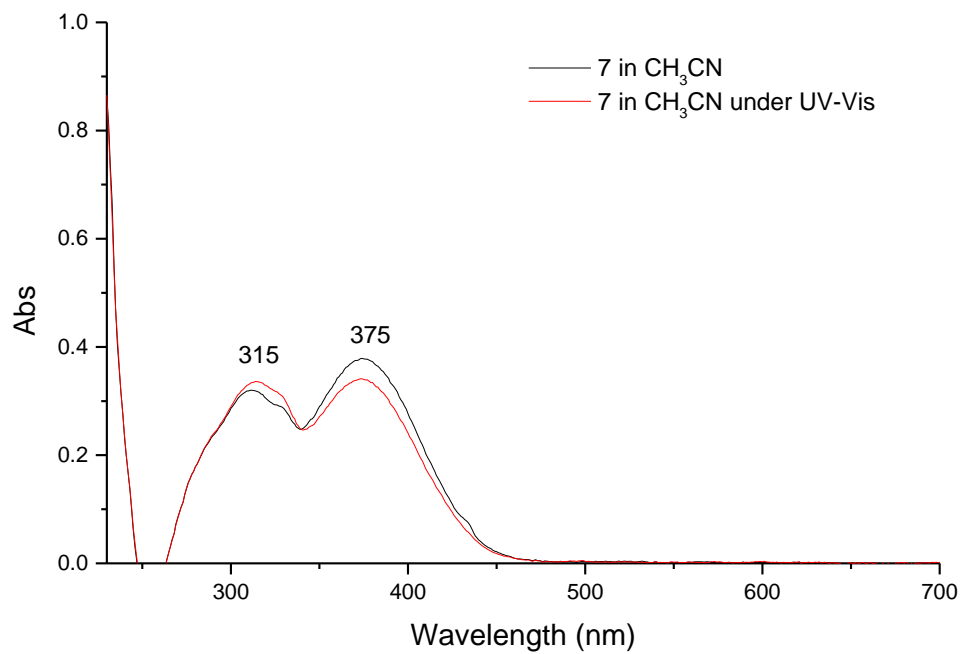
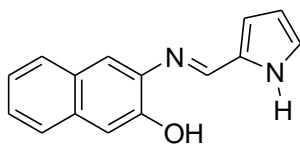




1.6. Imine 6c



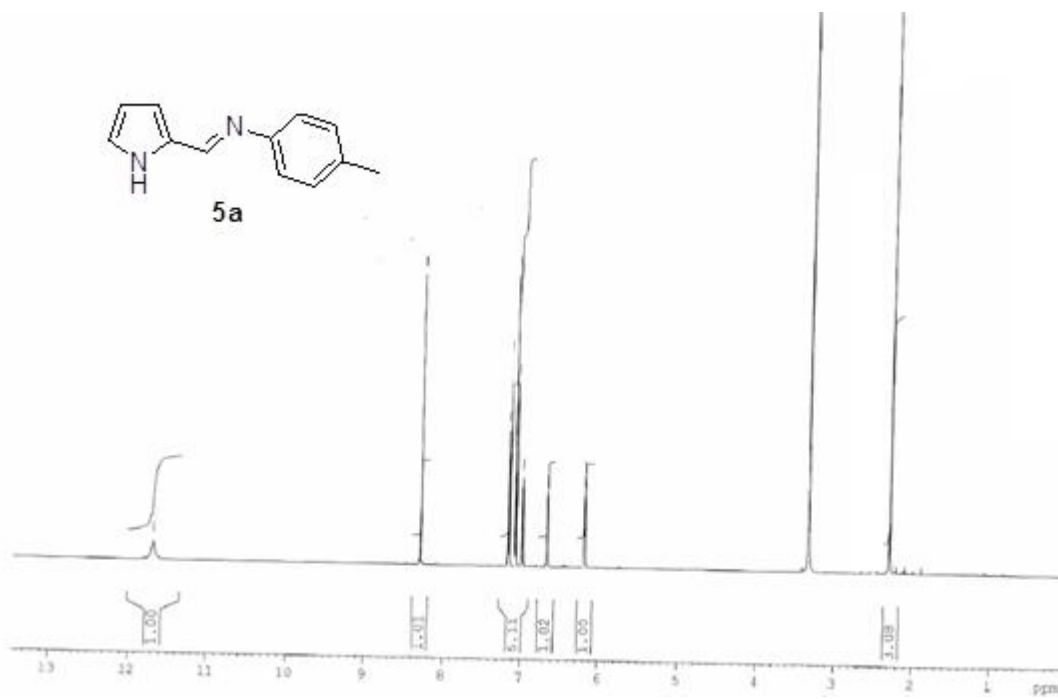
1.7. Imine 7



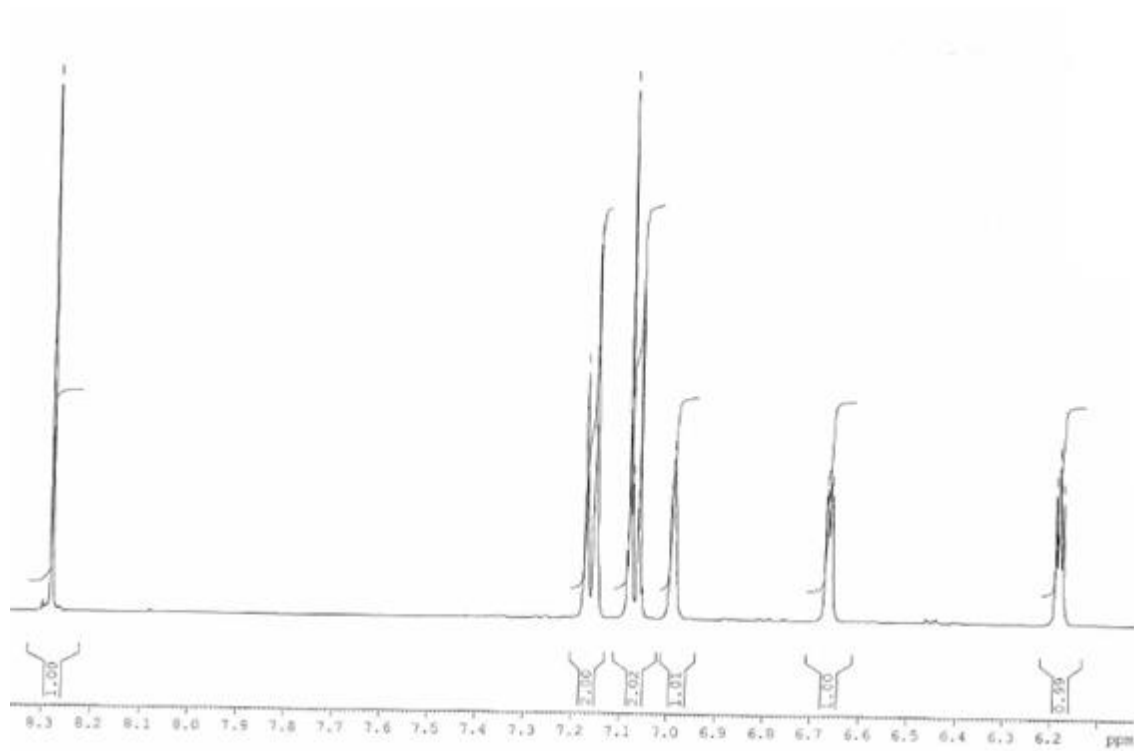
2. ^1H and ^{13}C NMR spectra of compounds 5-7

2.1. ^1H and ^{13}C NMR spectra of compound 5a.

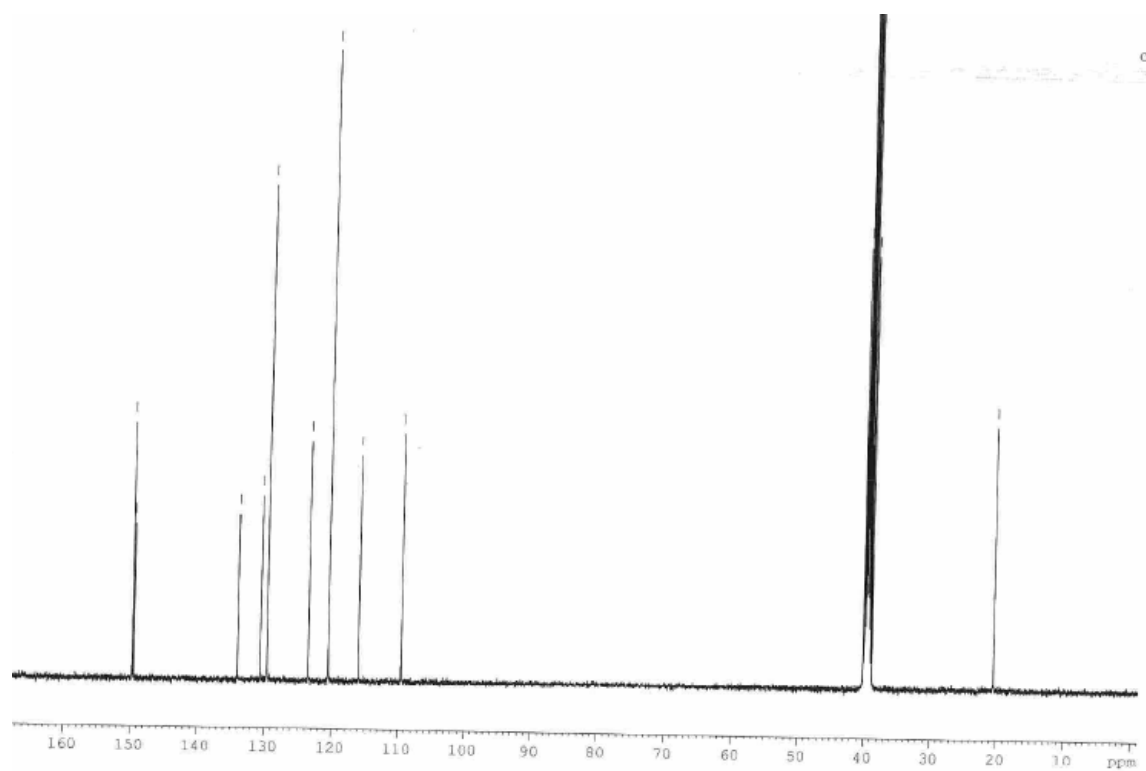
^1H NMR data for compound 5a.



Expansion of aromatic zone

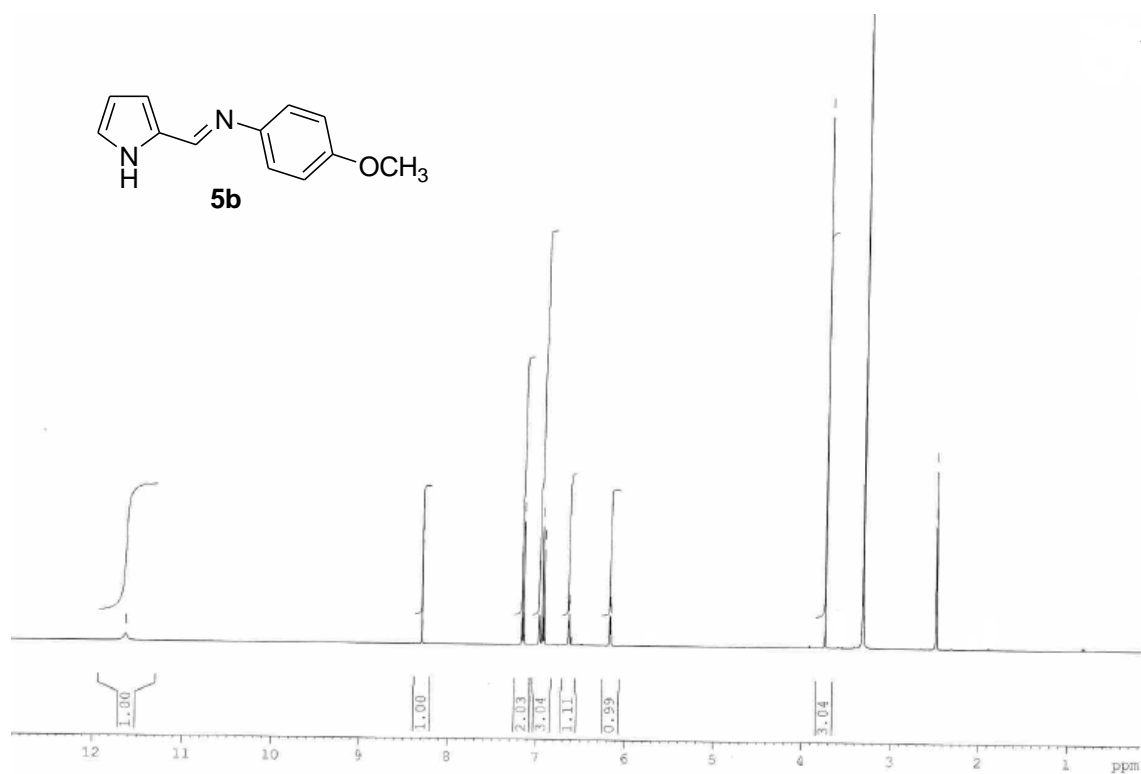


^{13}C NMR data for compound **5a**.

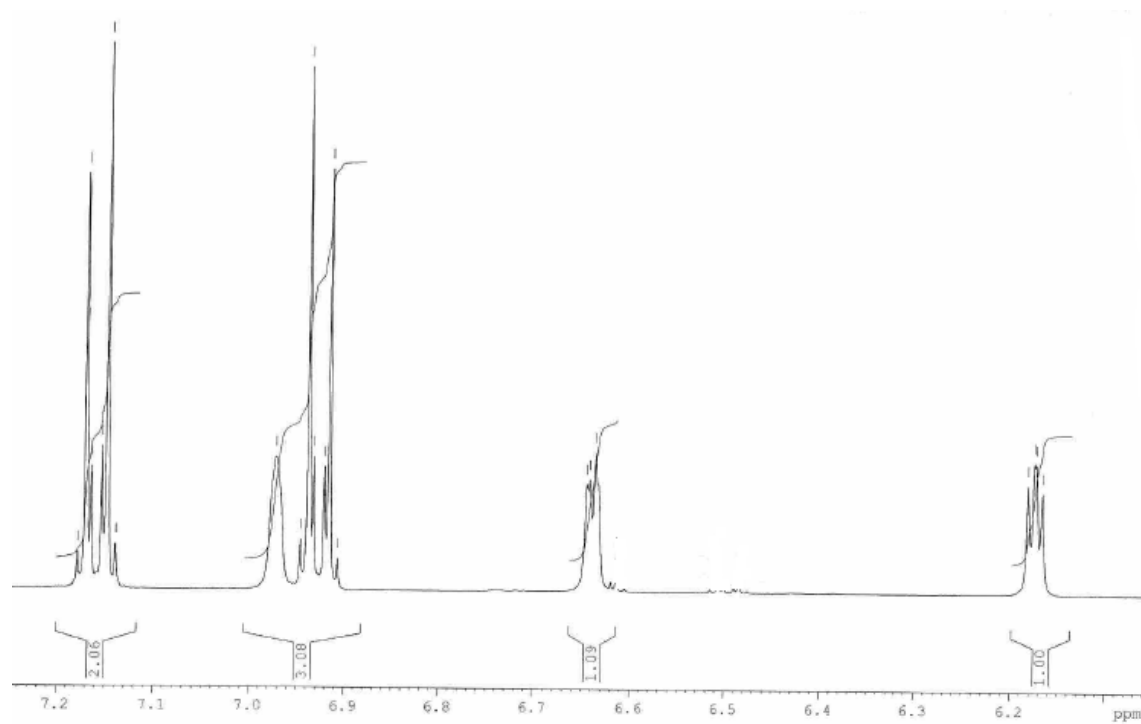


2.2. ^1H and ^{13}C NMR spectra of compound 5b.

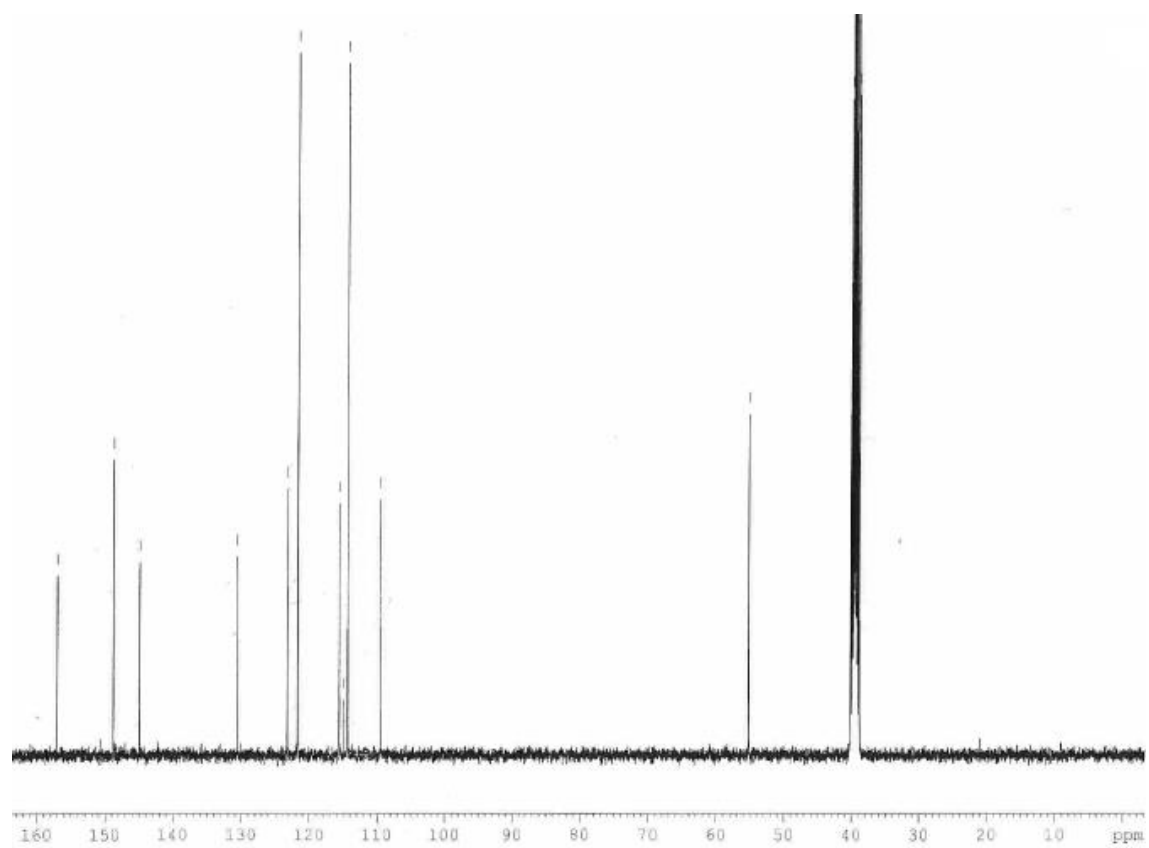
^1H NMR data for compound 5b.



Expansion of aromatic zone

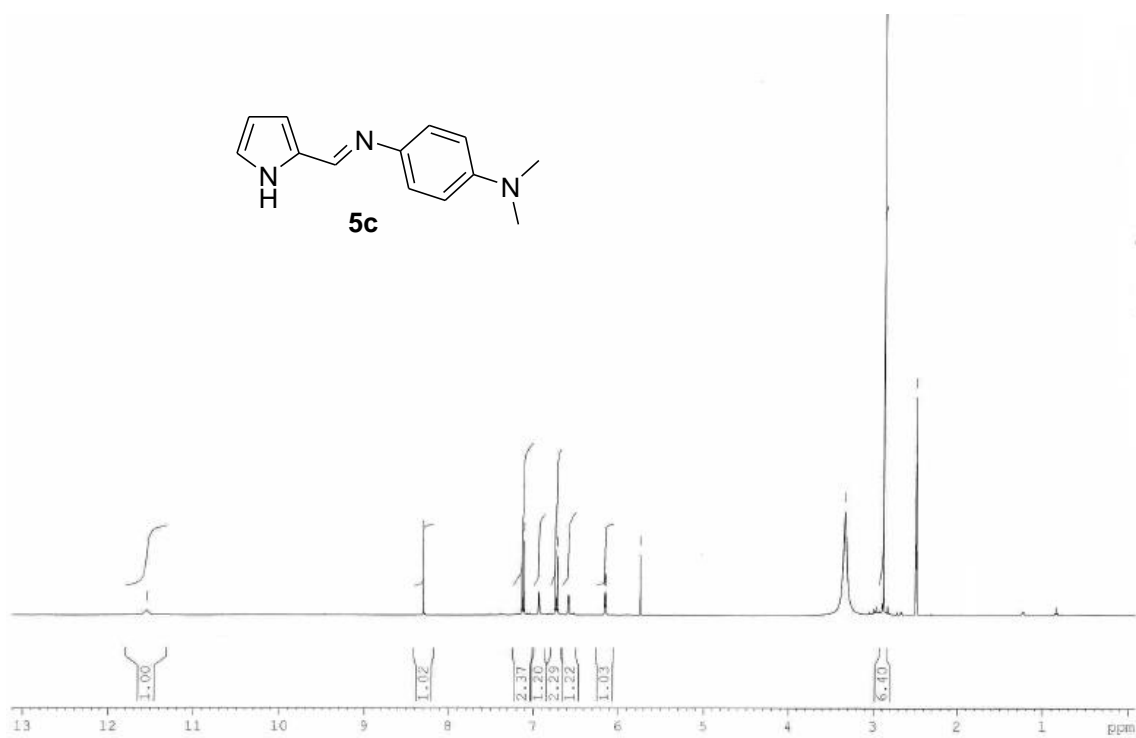


^{13}C NMR data for compound **5b**.

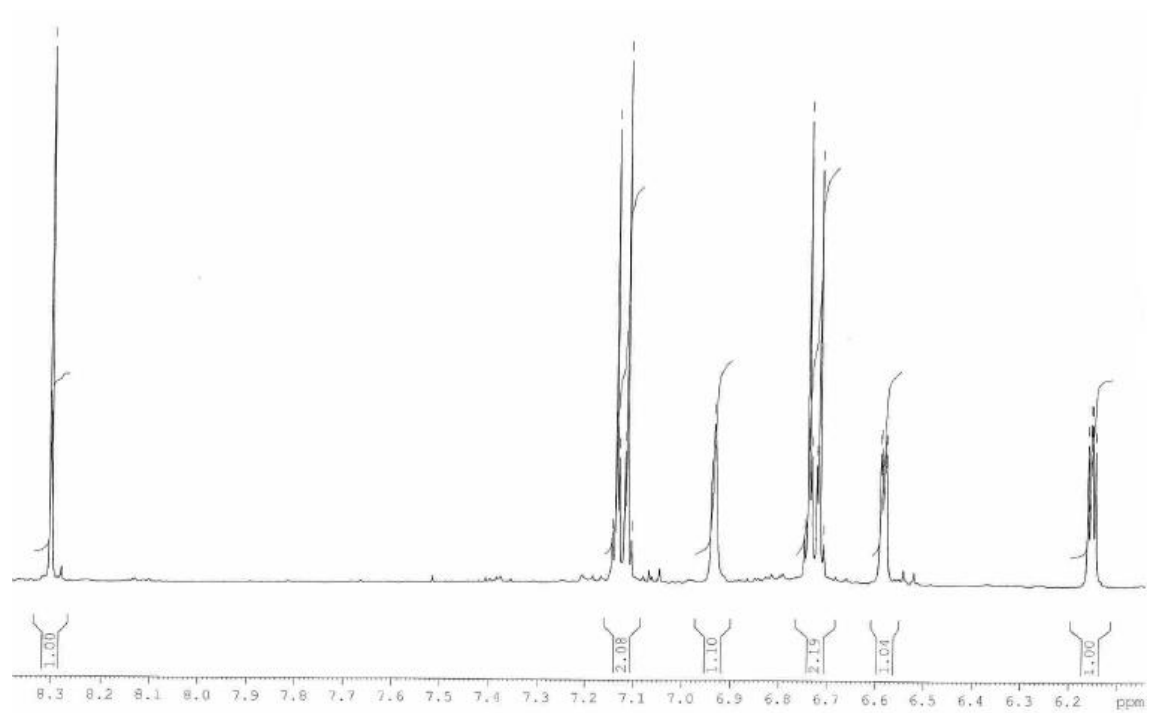


2.3. ^1H and ^{13}C NMR spectra of compound 5c.

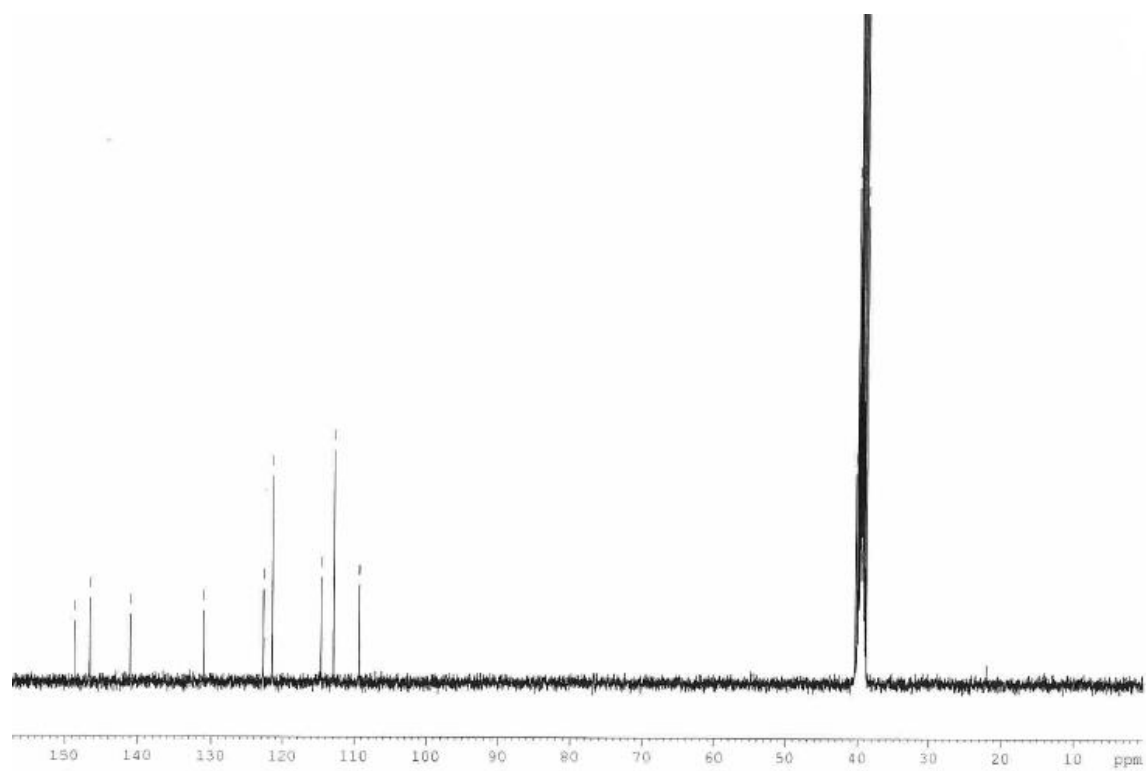
^1H NMR data for compound 5c.



Expansion of aromatic zone

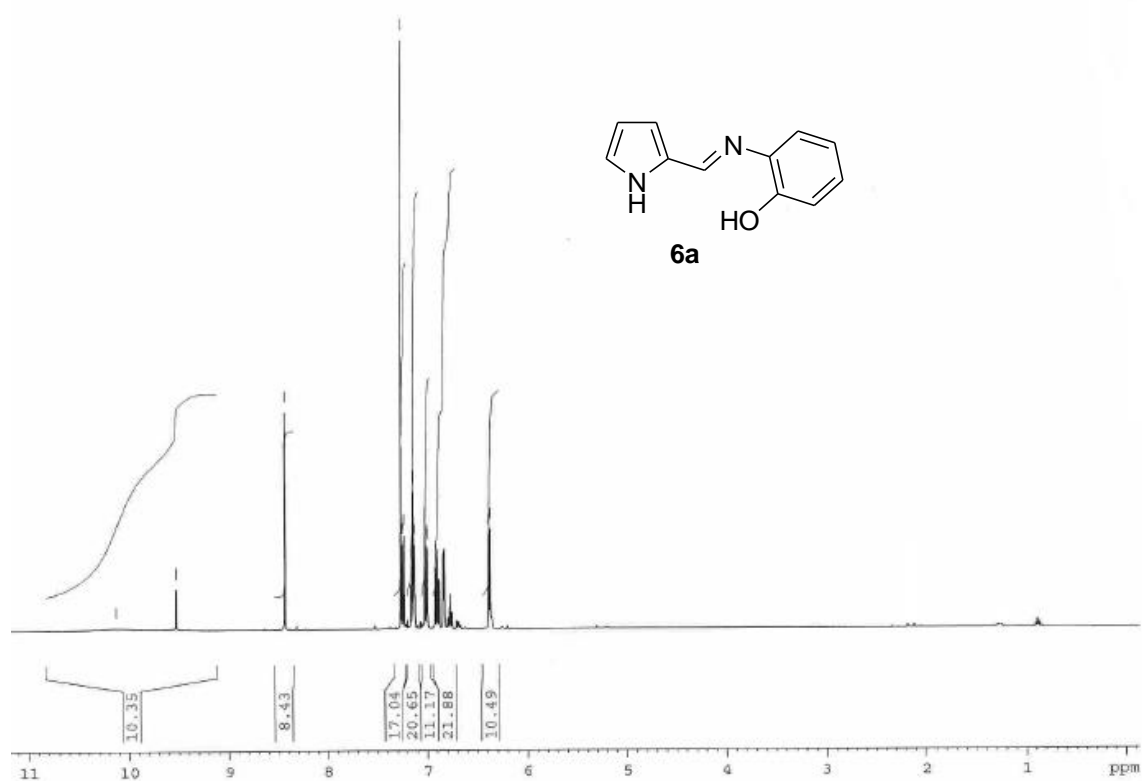


^{13}C NMR data for compound **5c**.

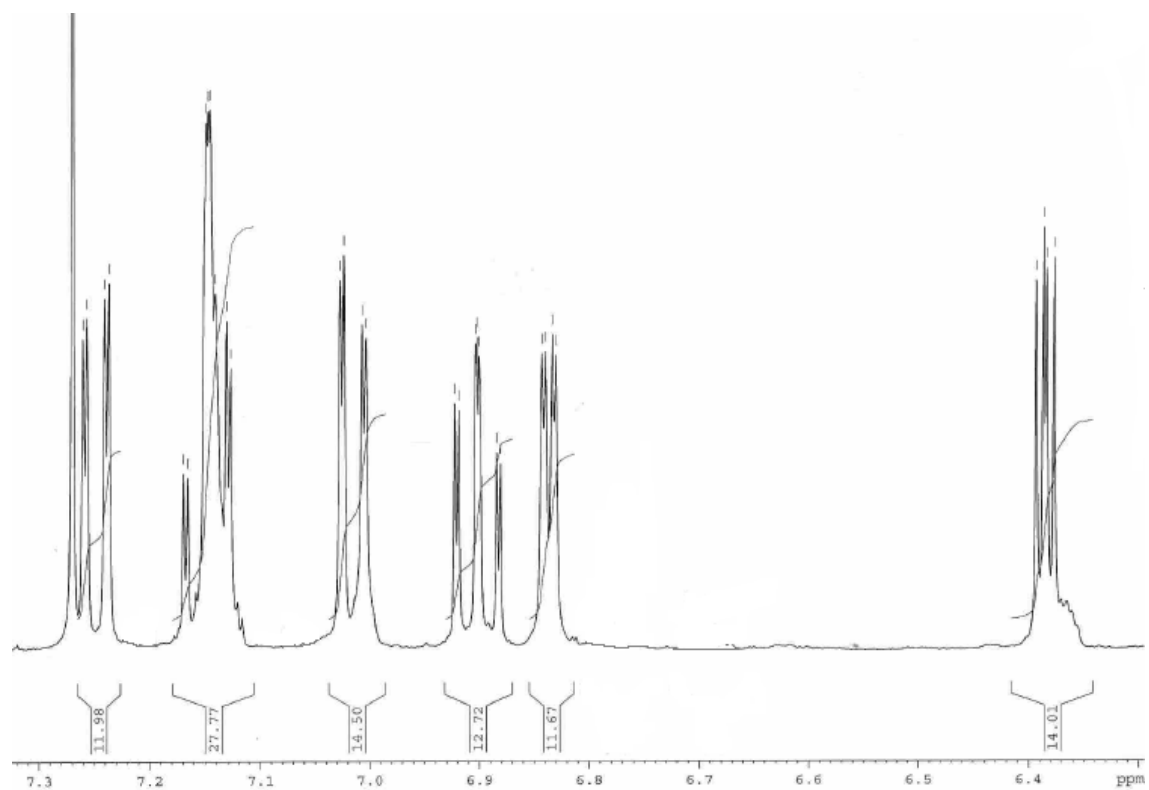


2.4. ^1H and ^{13}C NMR spectra of compound 6a.

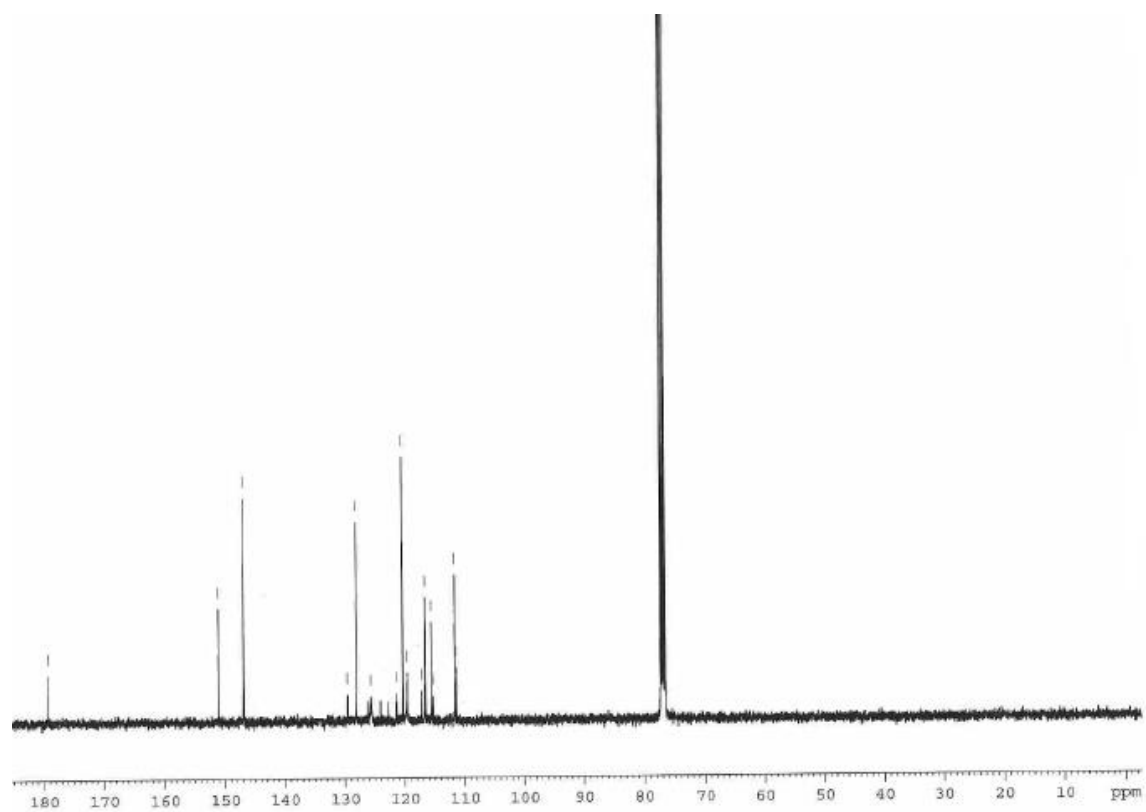
^1H NMR data for compound 6a.



Expansion of aromatic zone

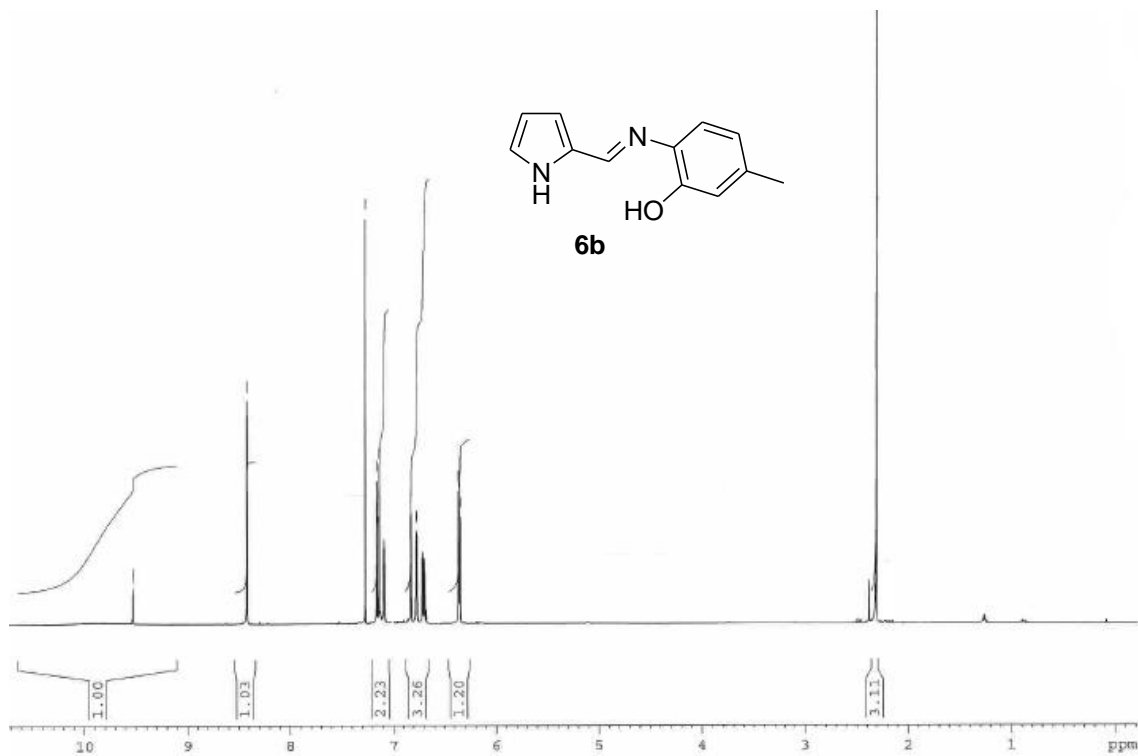


^{13}C NMR data for compound **6a**.

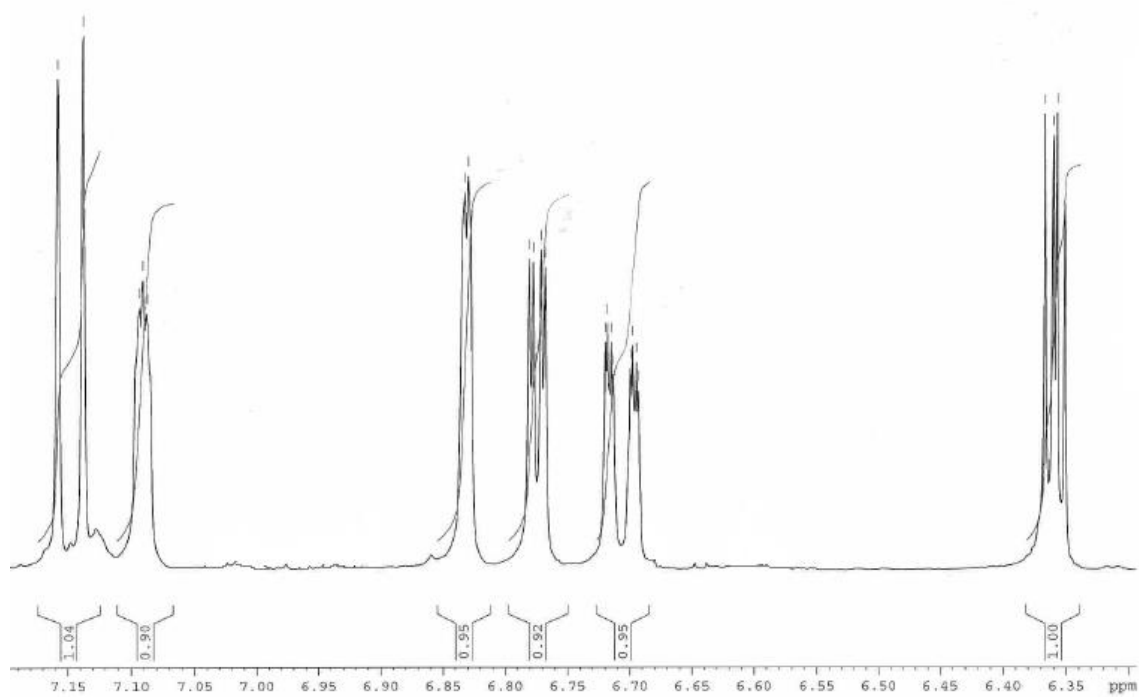


2.5. ^1H and ^{13}C NMR spectra of compound 6b.

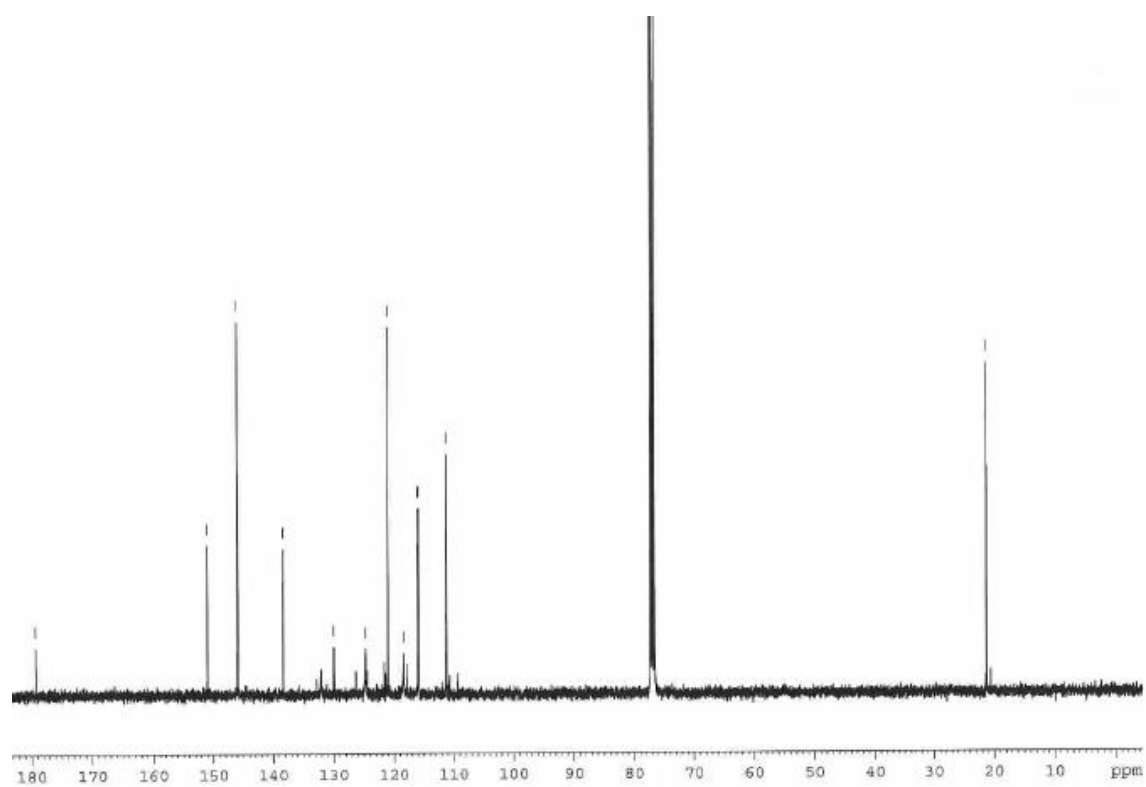
^1H NMR data for compound 6b.



Expansion of aromatic zone

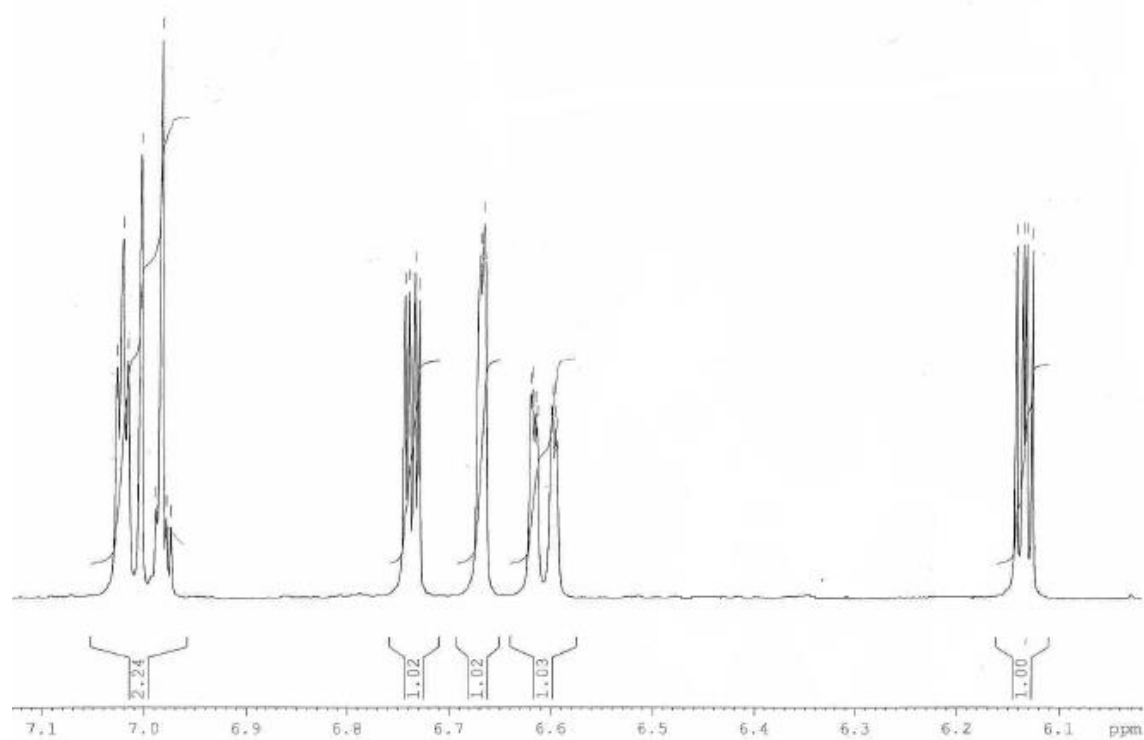
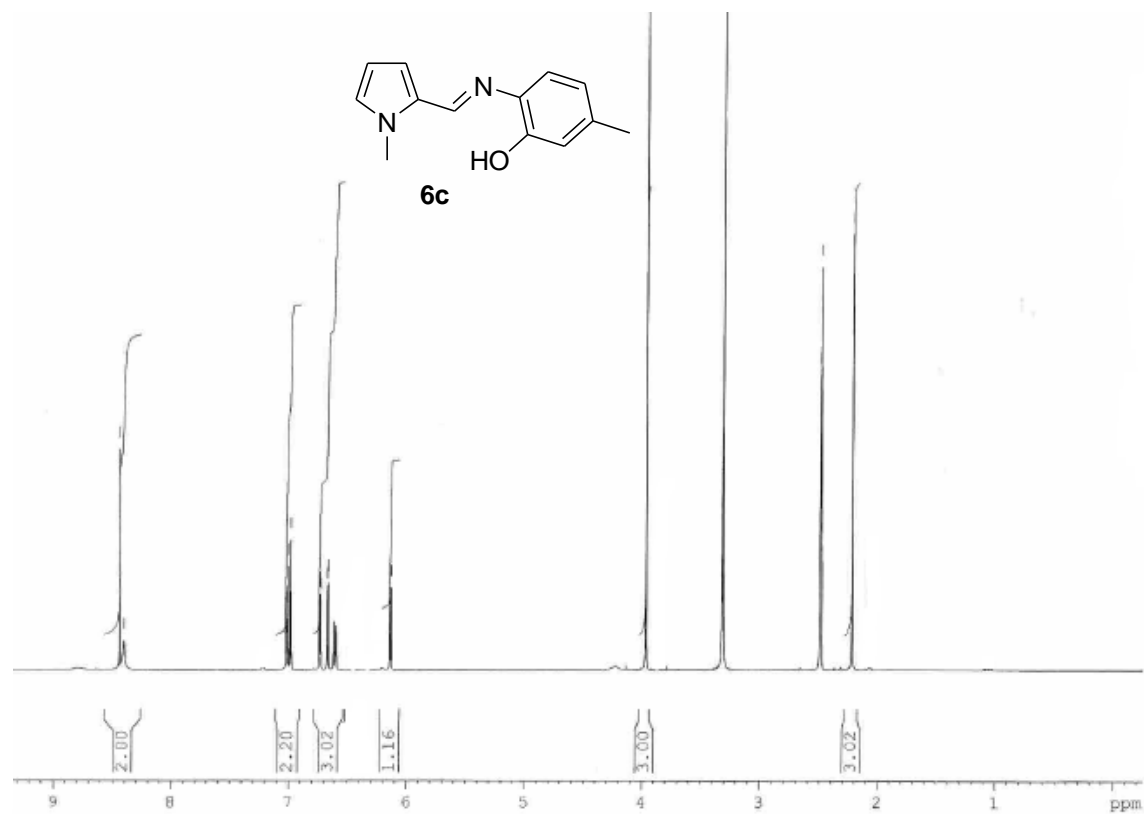


^{13}C NMR data for compound **6b**.

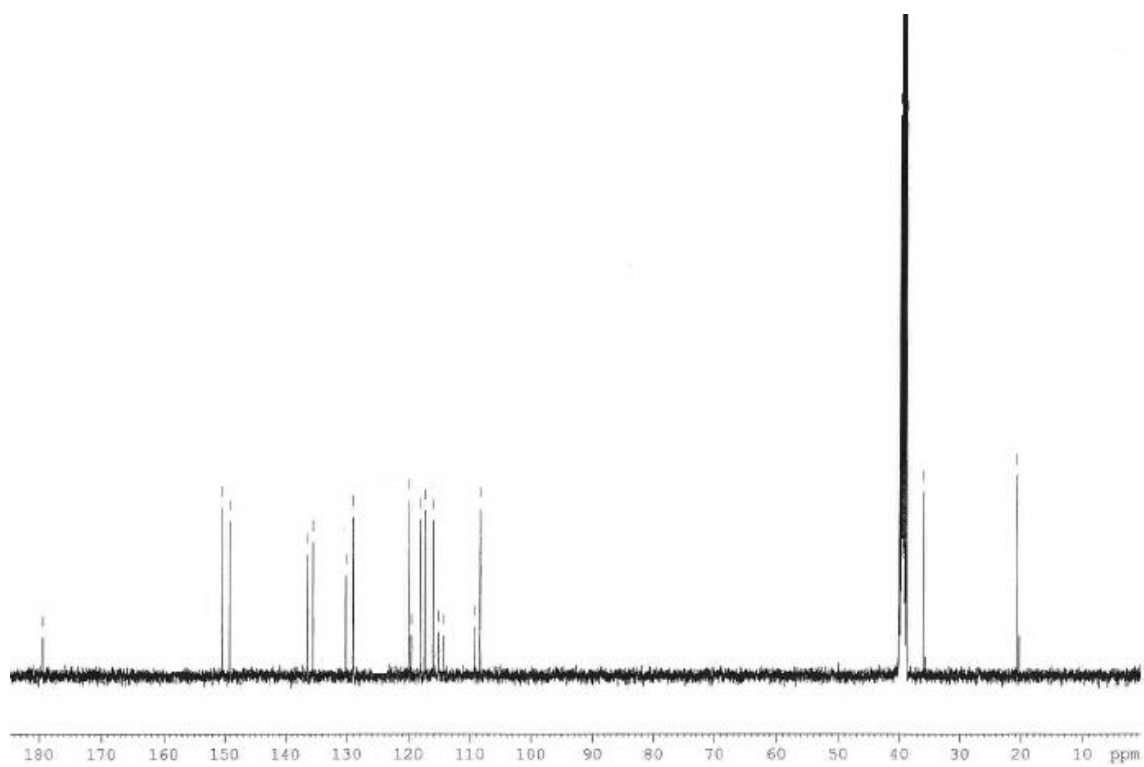


2.6. ^1H and ^{13}C NMR spectra of compound **6c**.

^1H NMR data for compound **6c**.

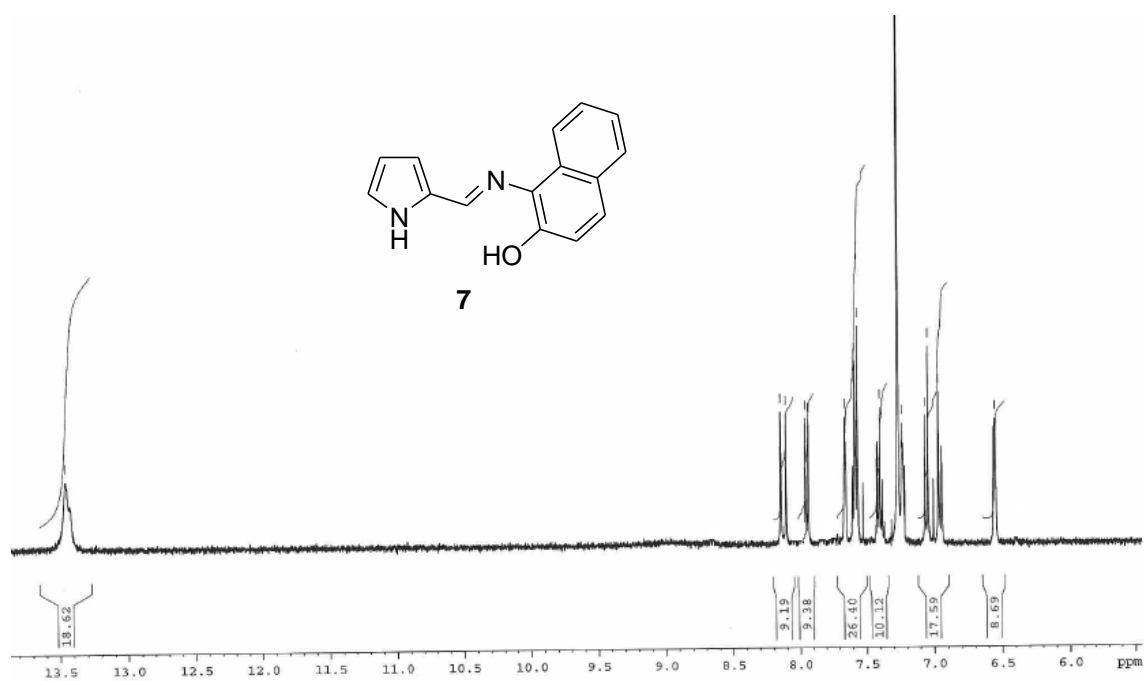


^{13}C NMR data for compound **6c**.

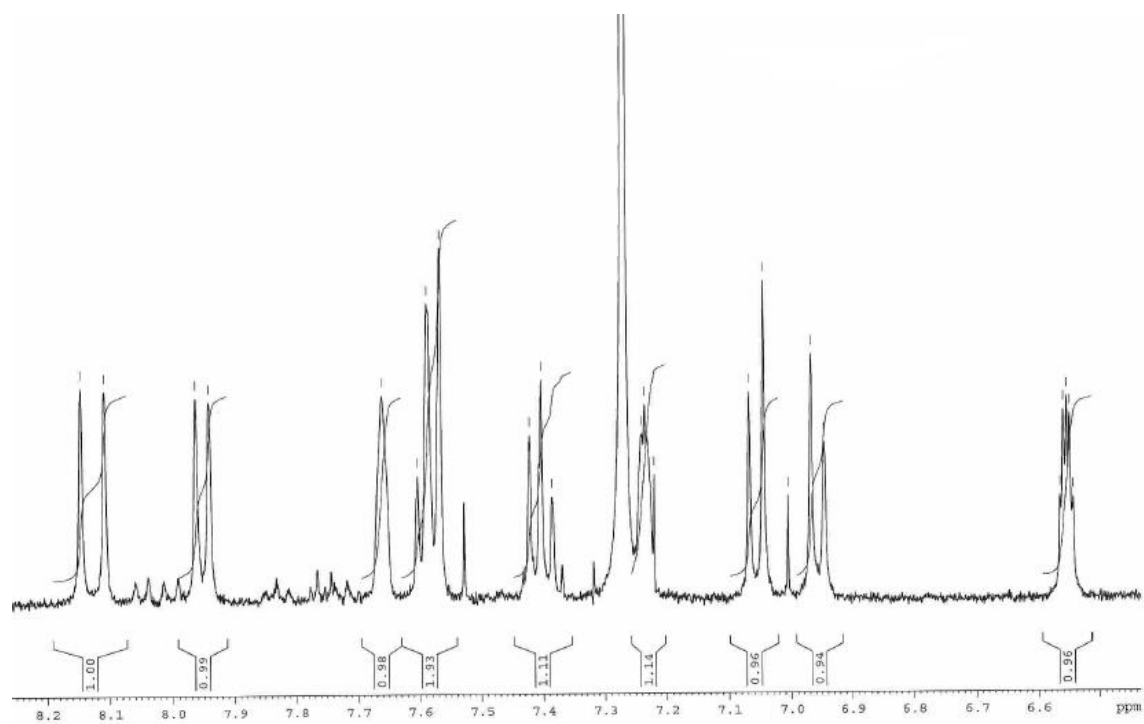


2.7. ^1H and ^{13}C NMR spectra of compound 7

^1H NMR data for compound 7 .

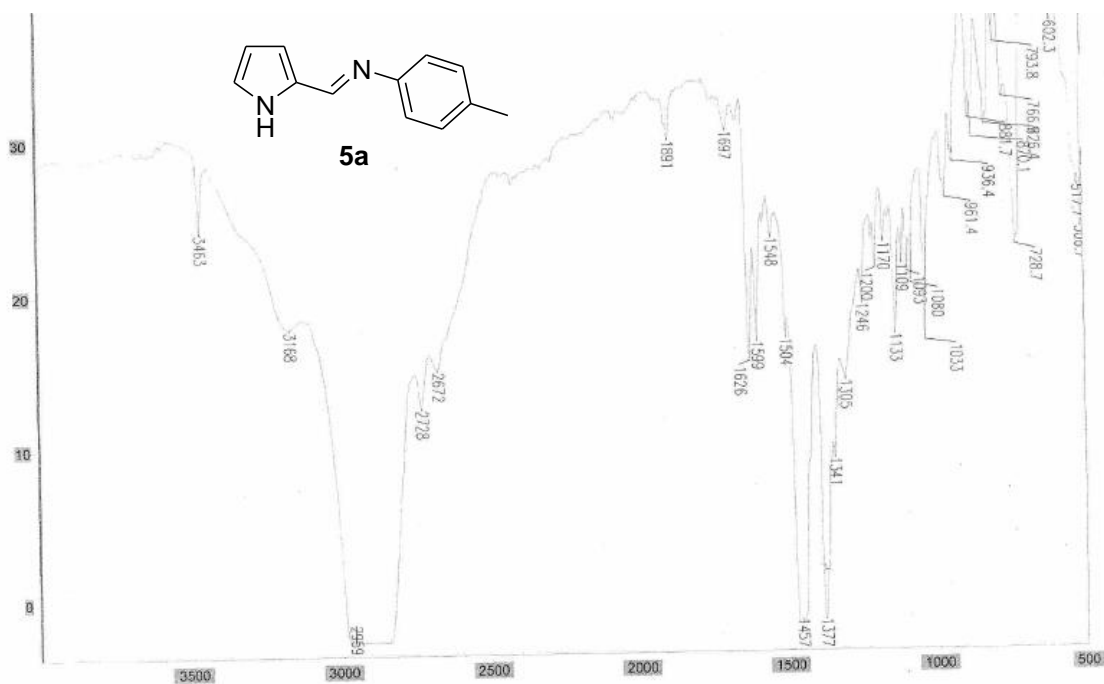


Expansion of aromatic zone

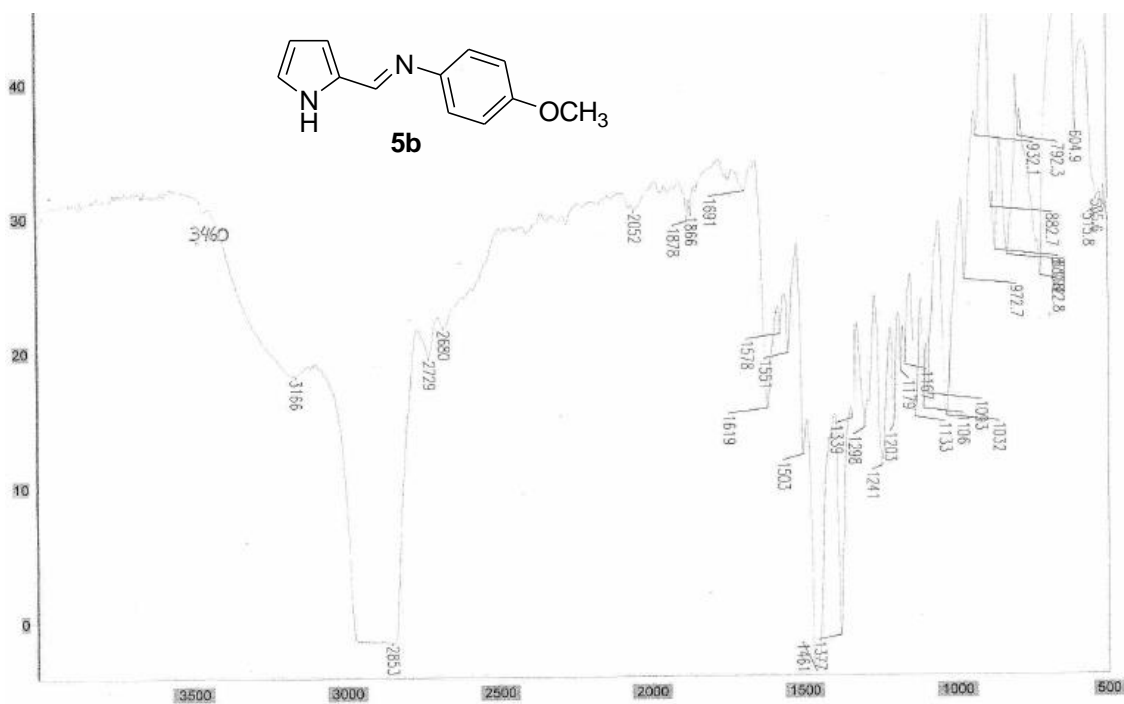


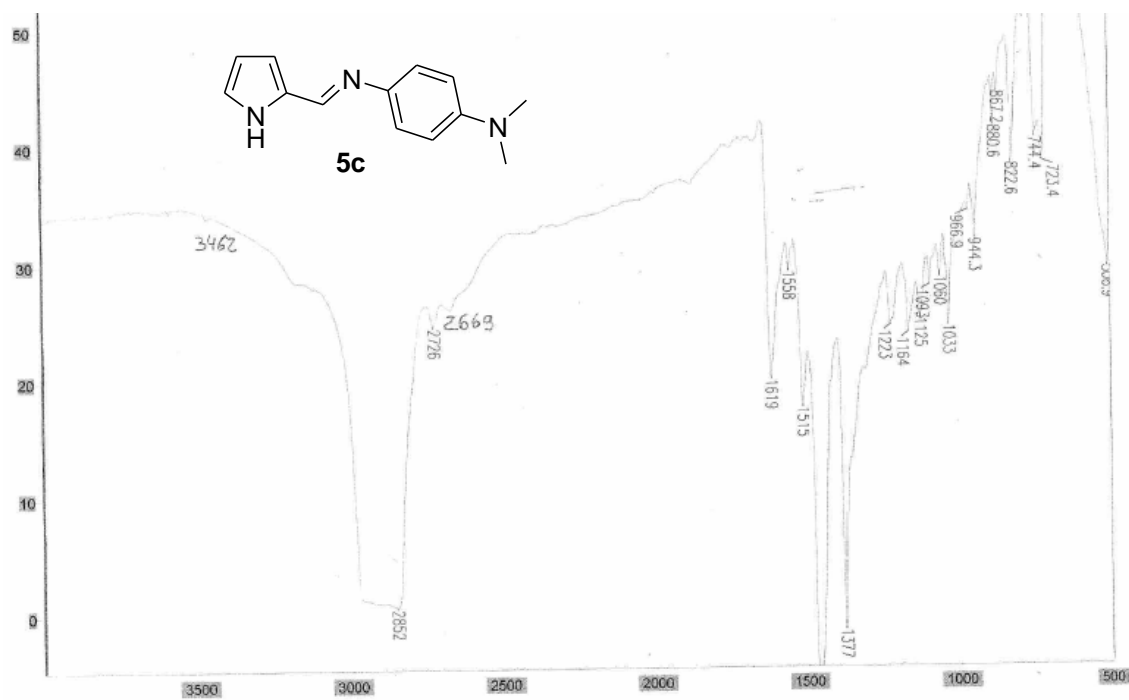
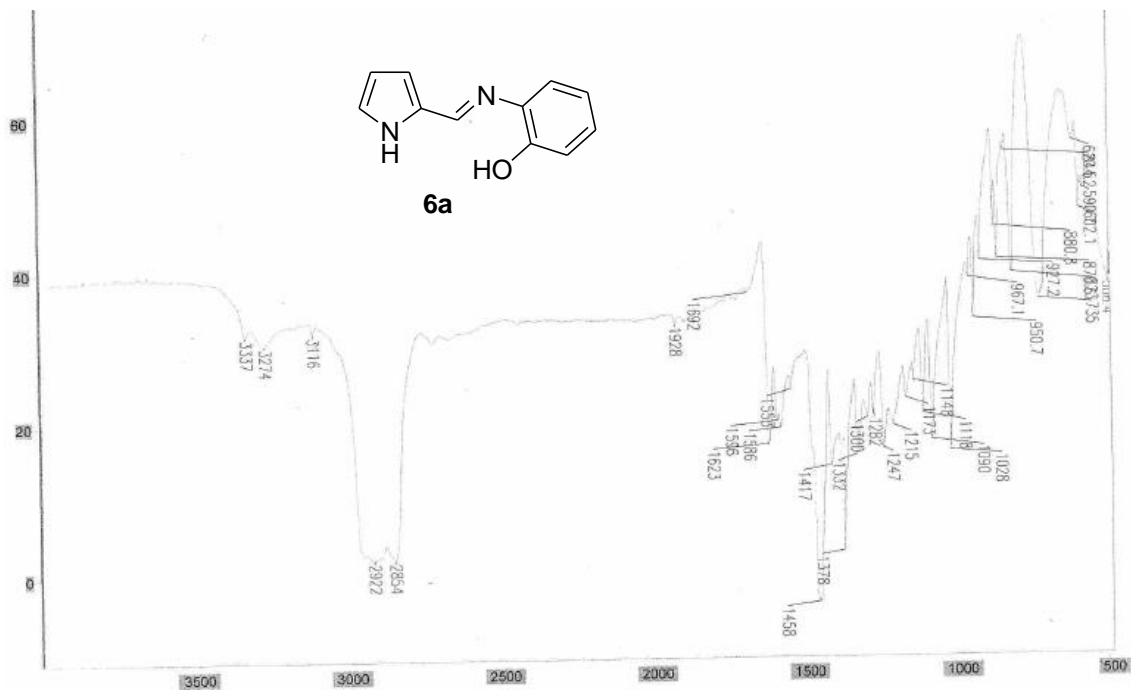
3. IR spectra of compounds 5-7.

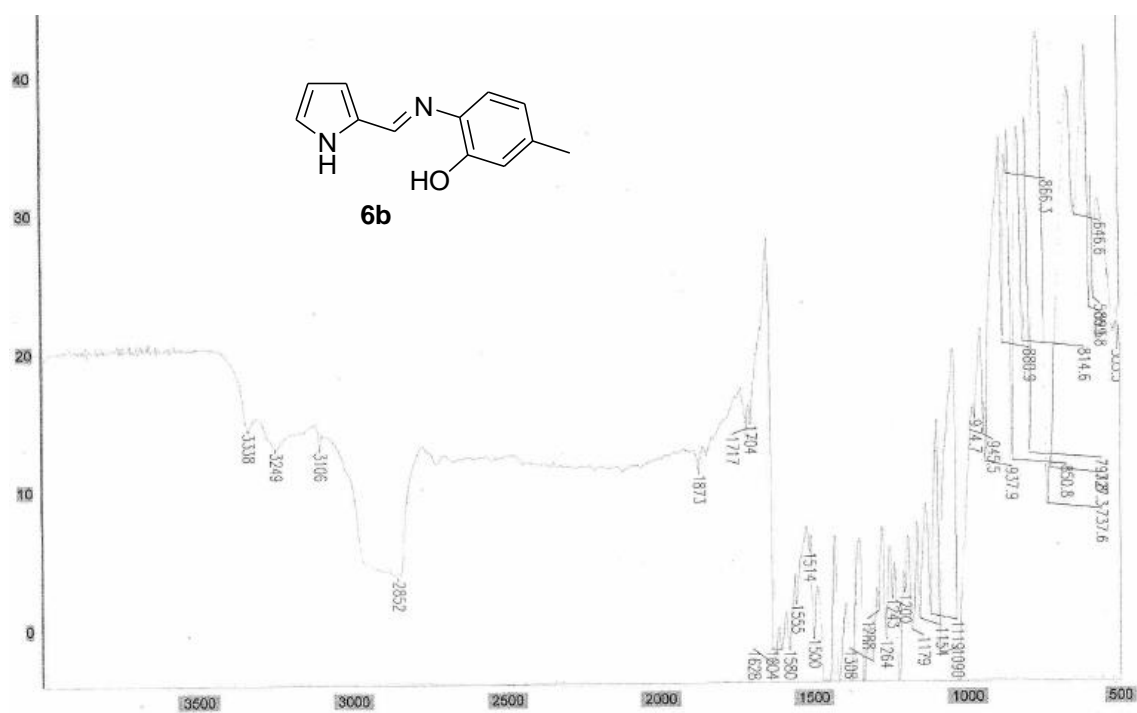
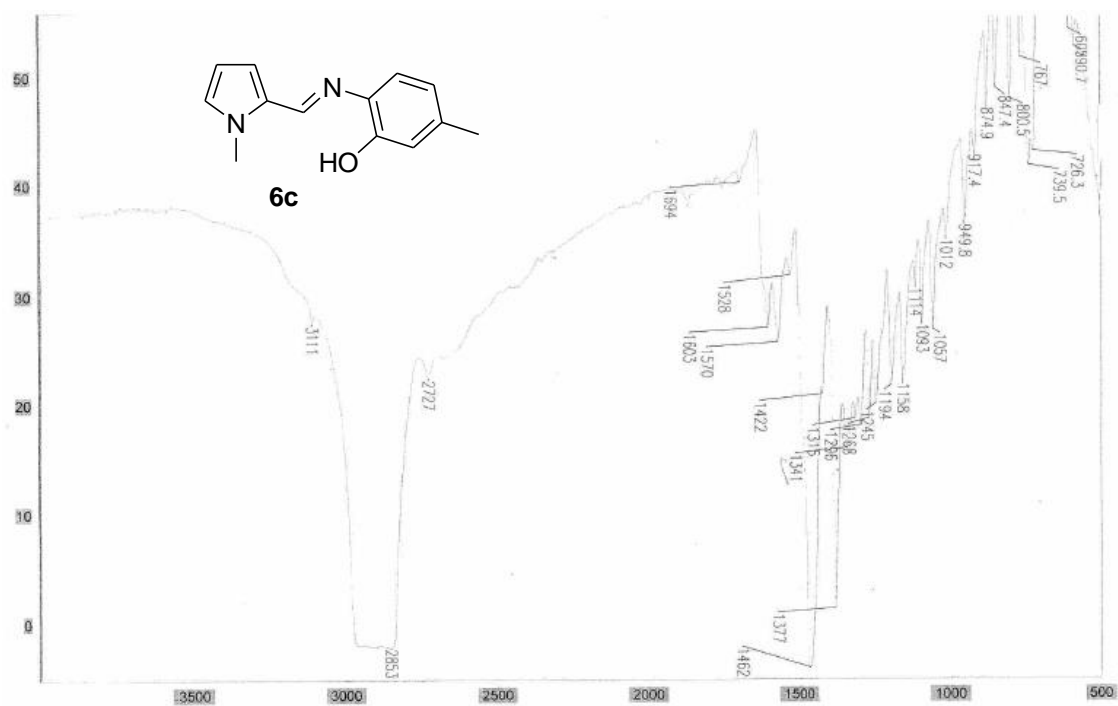
IR data for compound **5a**.



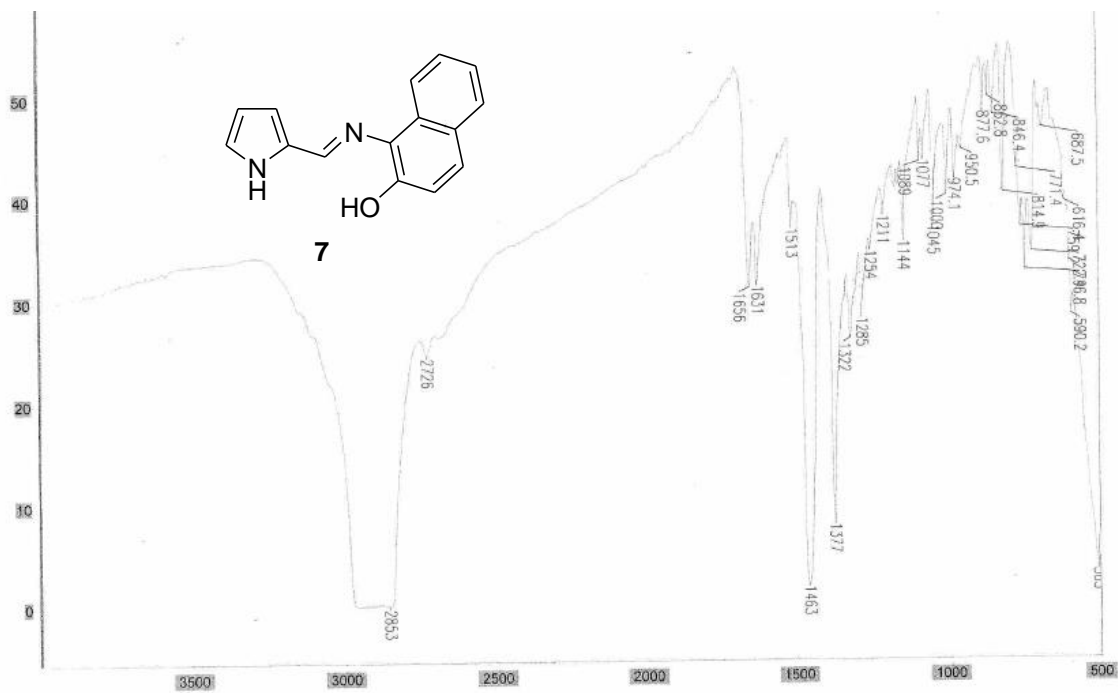
IR data for compound **5b**.



IR data for compound **5c**.IR data for compound **6a**.

IR data for compound **6b**.IR data for compound **6c**.

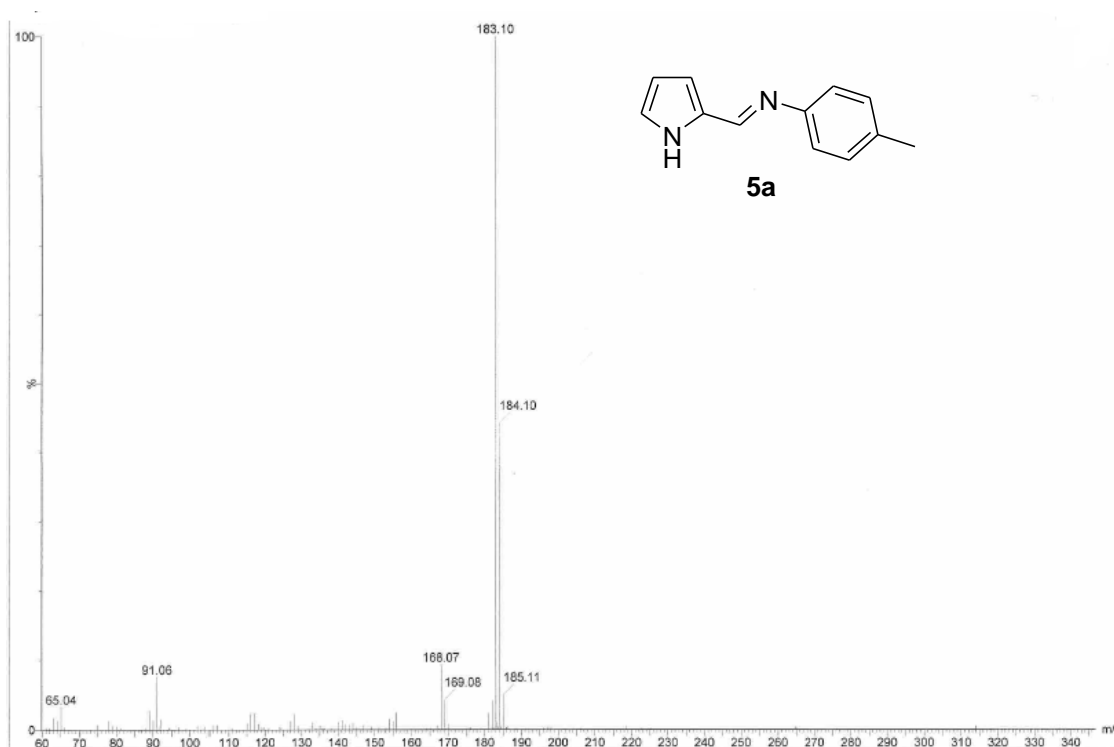
IR data for compound 7.



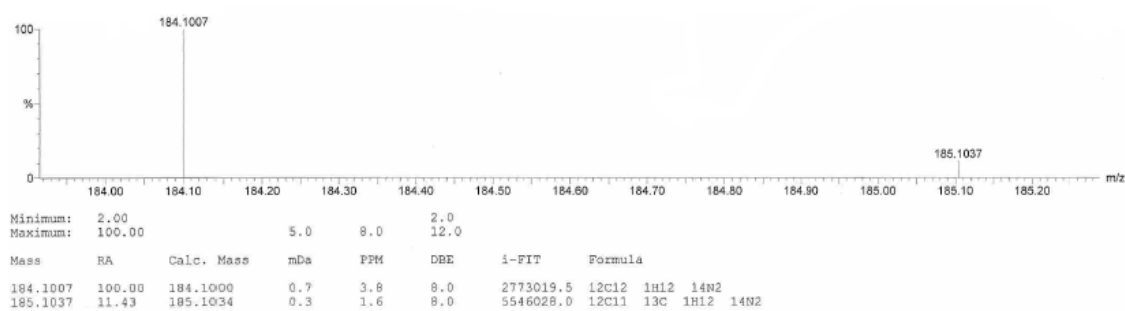
4. Mass spectra of compounds 5 and 6-7.

4.1. MS data for compound 5a.

EI (TOF) data for compound **5a**.

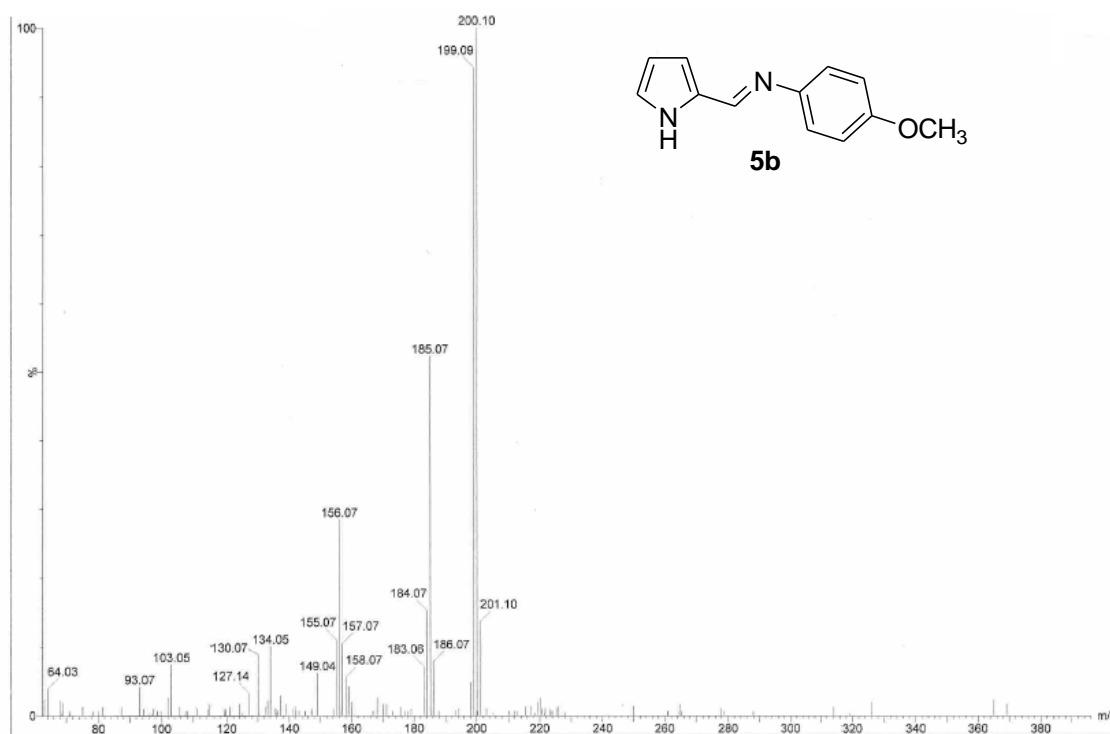


HRMS EI (TOF) data for compound **5a**.

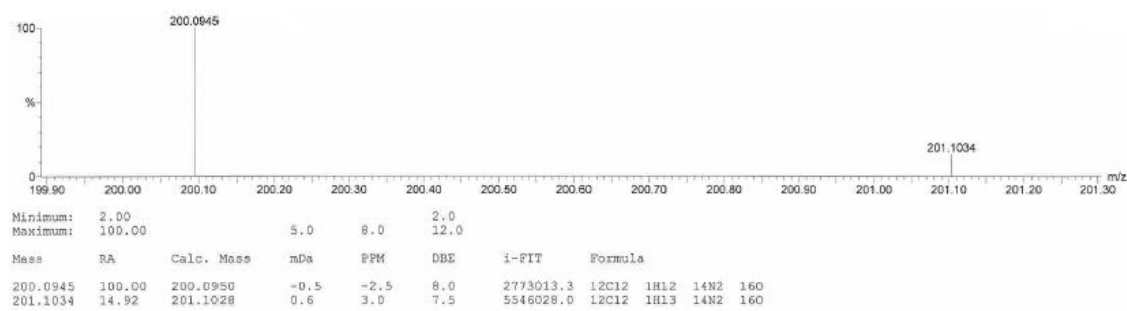


4.2. MS data for compound 5b.

EI (TOF) data for compound **5b**.

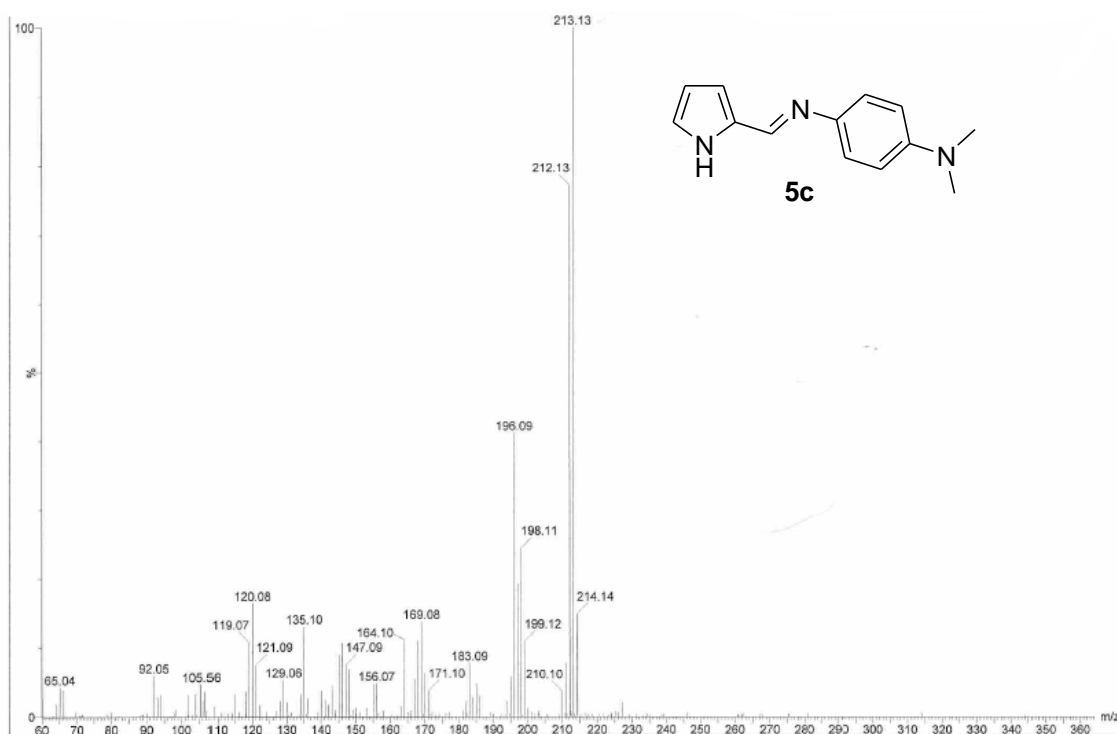


HRMS EI (TOF) data for compound **5b**.

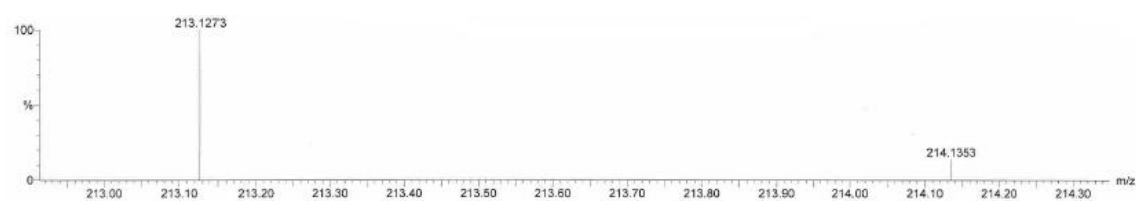


4.3. MS data for compound 5c.

EI (TOF) data for compound 5c.



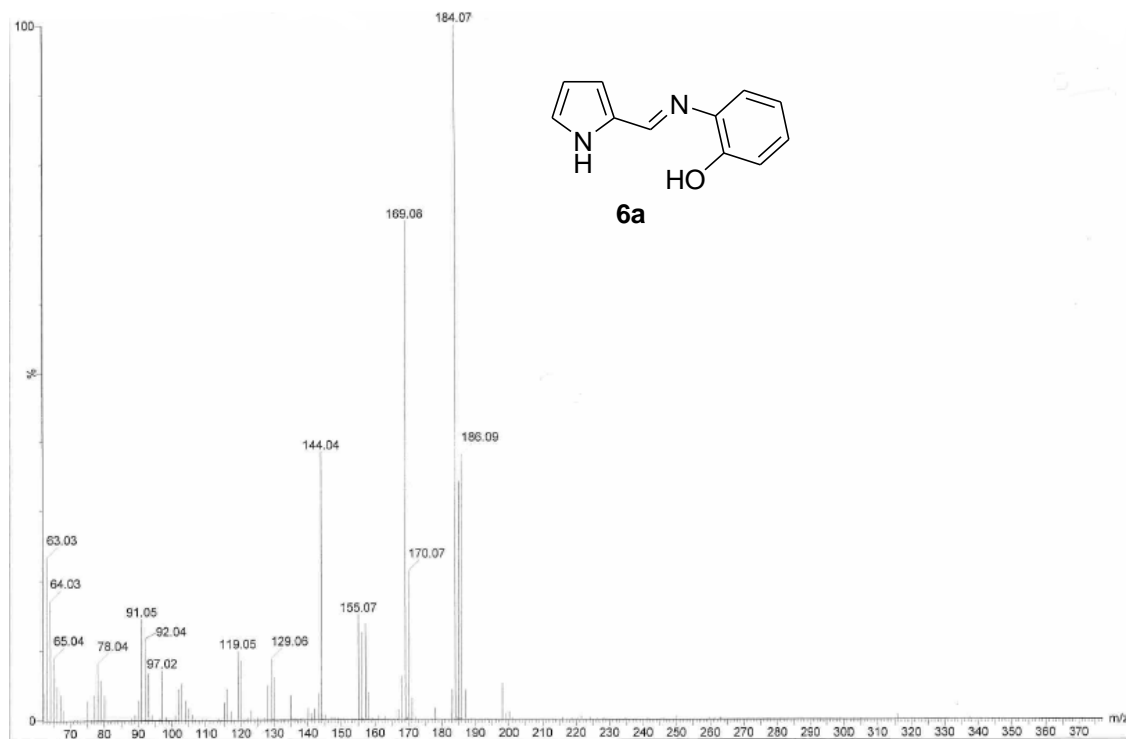
HRMS EI (TOF) data for compound 5c.



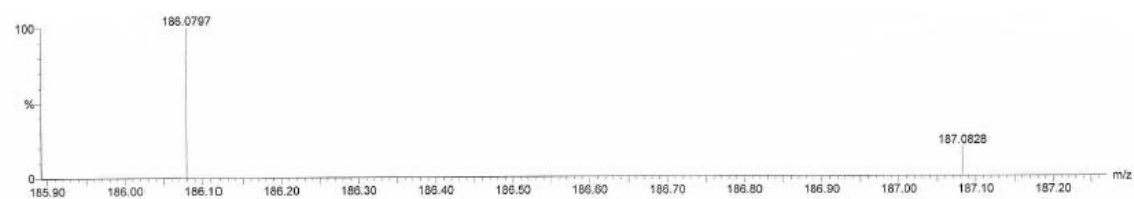
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
213.1273	100.00	213.1266	0.7	3.3	8.0	2773066.0	C ₁₂ H ₁₃ N ₃
214.1353	13.86	214.1344	0.9	4.2	7.5	5546077.5	C ₁₂ H ₁₄ N ₃

4.4. MS data for compound 6a.

EI (TOF) data for compound 6a.



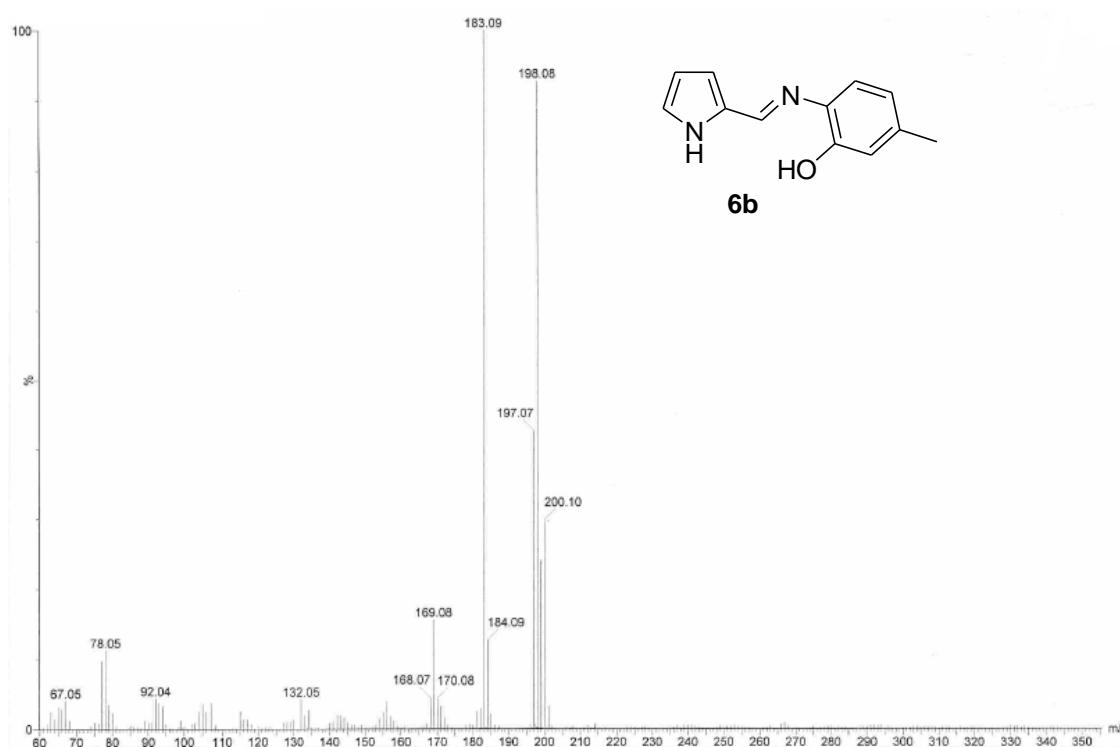
HRMS EI (TOF) data for compound 6a.



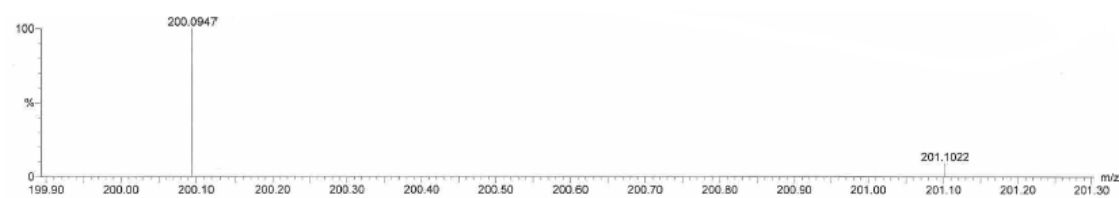
Mass	RA	Calc. Mass	mDa	PPM	DRE	i-FIT	Formula
186.0797	100.00	186.0793	0.4	2.1	8.0	2773013.0	C ₁₂ H ₁₀ N ₂ O
187.0828	19.36	187.0827	0.1	0.5	8.0	5546025.5	C ₁₂ H ₁₀ N ₂ O

4.5. MS data for compound 6b.

EI (TOF) data for compound **6b**.



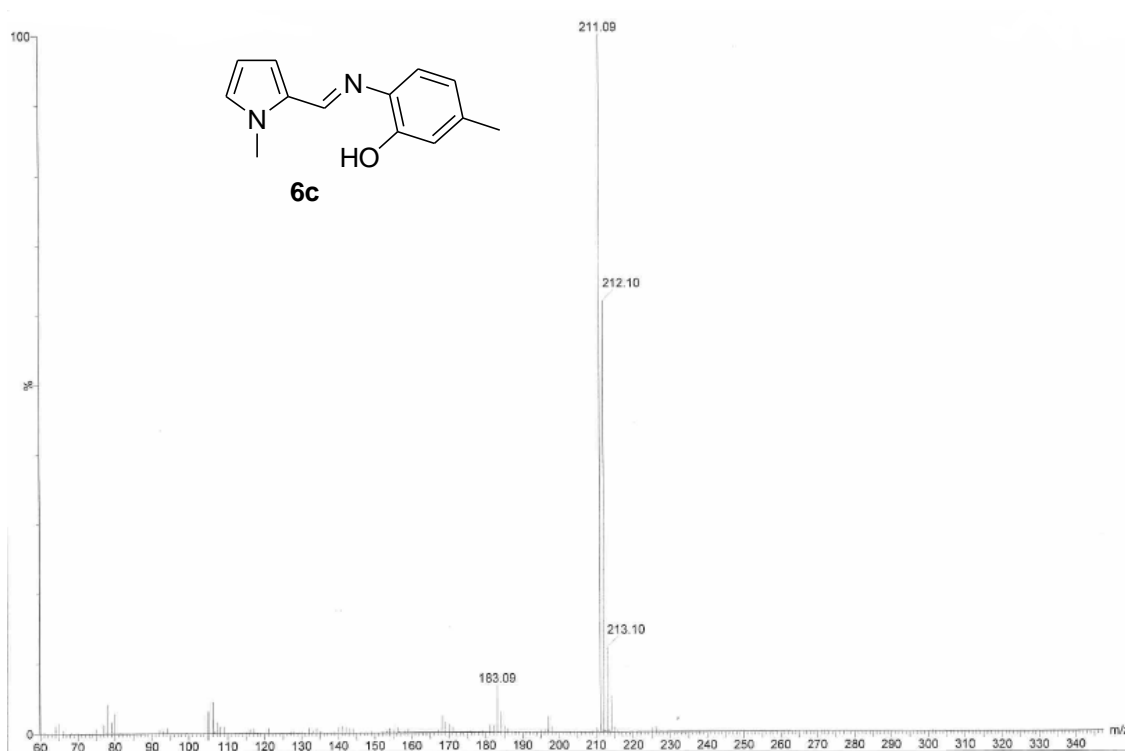
HRMS EI (TOF) data for compound **6b**.



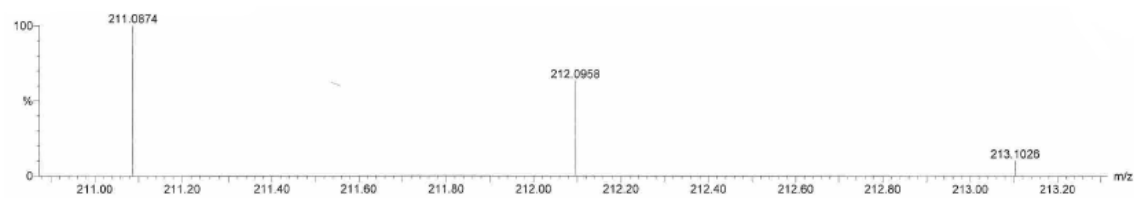
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
200.0947	100.00	200.0950	-0.3	-1.5	8.0	2780898.3	C ₁₂ H ₁₂ N ₂ O
201.1022	8.92	201.1028	-0.6	-3.0	7.5	5546926.5	C ₁₂ H ₁₃ N ₂ O

4.6. MS data for compound 6c.

EI (TOF) data for compound 6c.



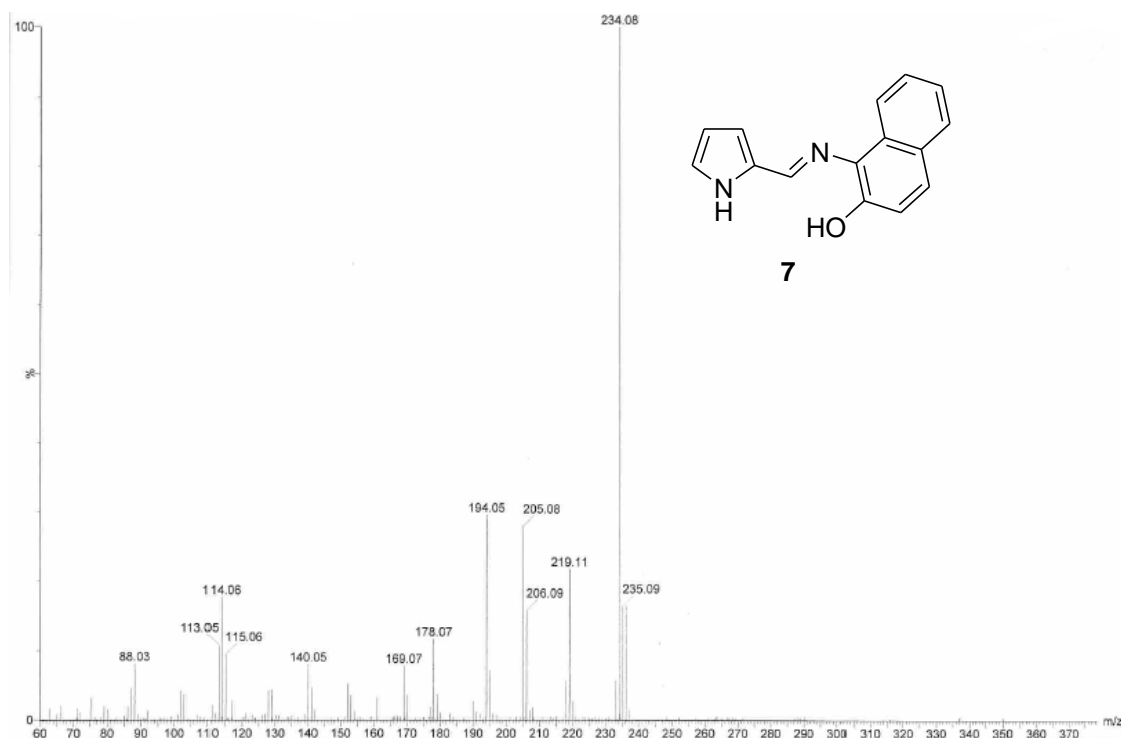
HRMS EI (TOF) data for compound 6c.



Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
211.0874	100.00	211.0871	0.3	1.4	9.5	1117.0	C ₁₂ H ₁₁ N ₂ O
212.0958	63.17	212.0950	0.8	3.8	9.0	2773618.5	C ₁₂ H ₁₂ N ₂ O
213.1026	10.10	213.1028	-0.2	-0.9	8.5	5546264.5	C ₁₂ H ₁₃ N ₂ O

4.7. MS data for compound 7.

EI (TOF) data for compound 7.



HRMS EI (TOF) data for compound 7.

