Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

New 2-(Aryl/Heteroaryl)-6-(Morpholin-4-yl/Pyrrolidin-1-yl)-(4-Trifluoromethyl)quinolines: Synthesis via Buchwald–Hartwig Amination, Photophysics, and Biomolecular Binding Properties

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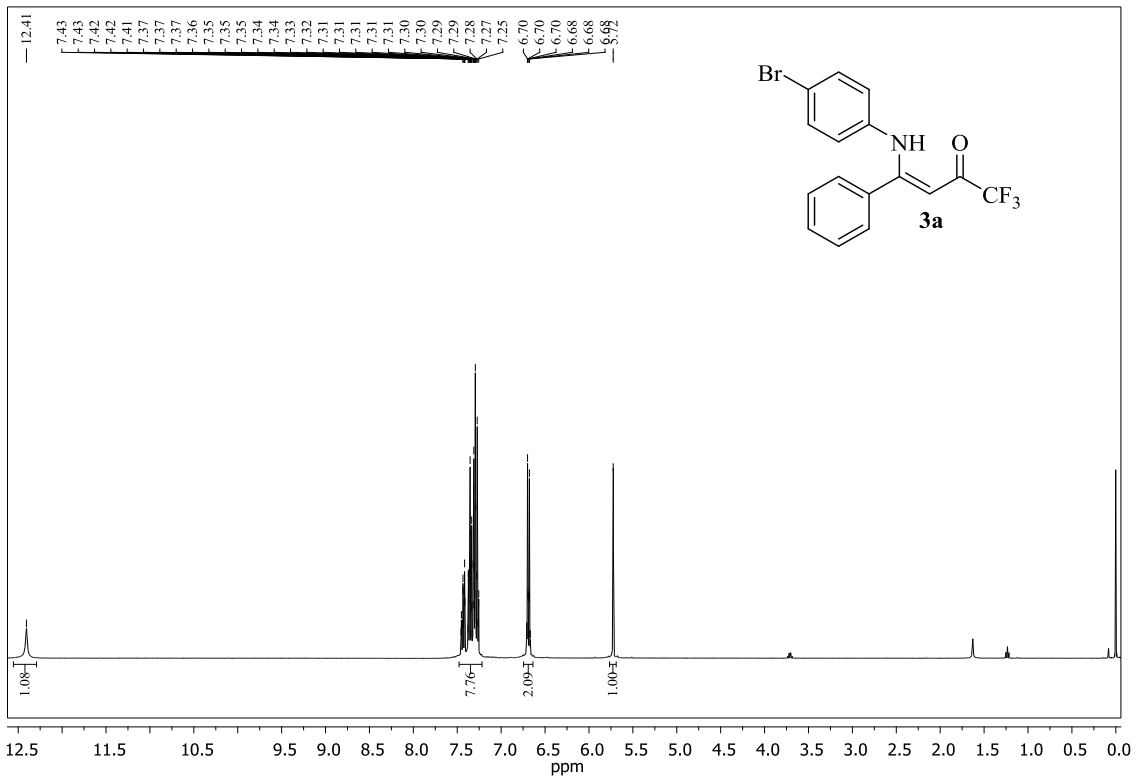
Contents: Crystallographic data, NMR, UV-vis electronic absorption and Emission fluorescence spectral data.

(a)



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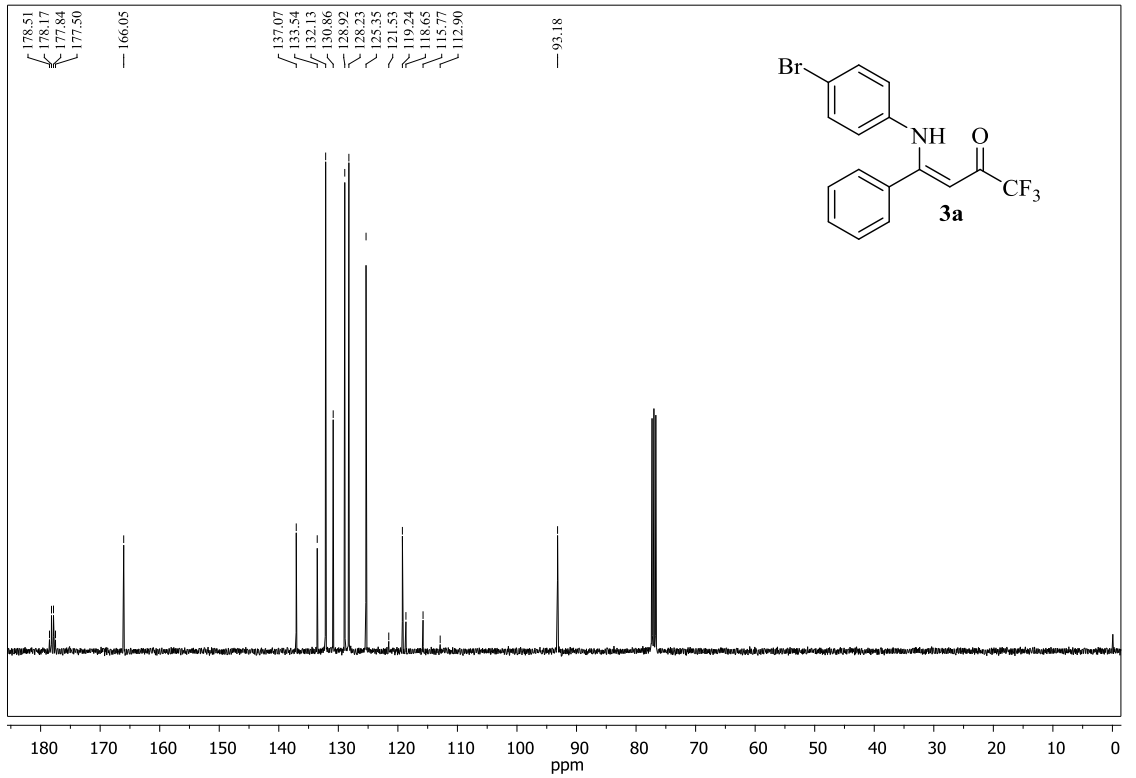
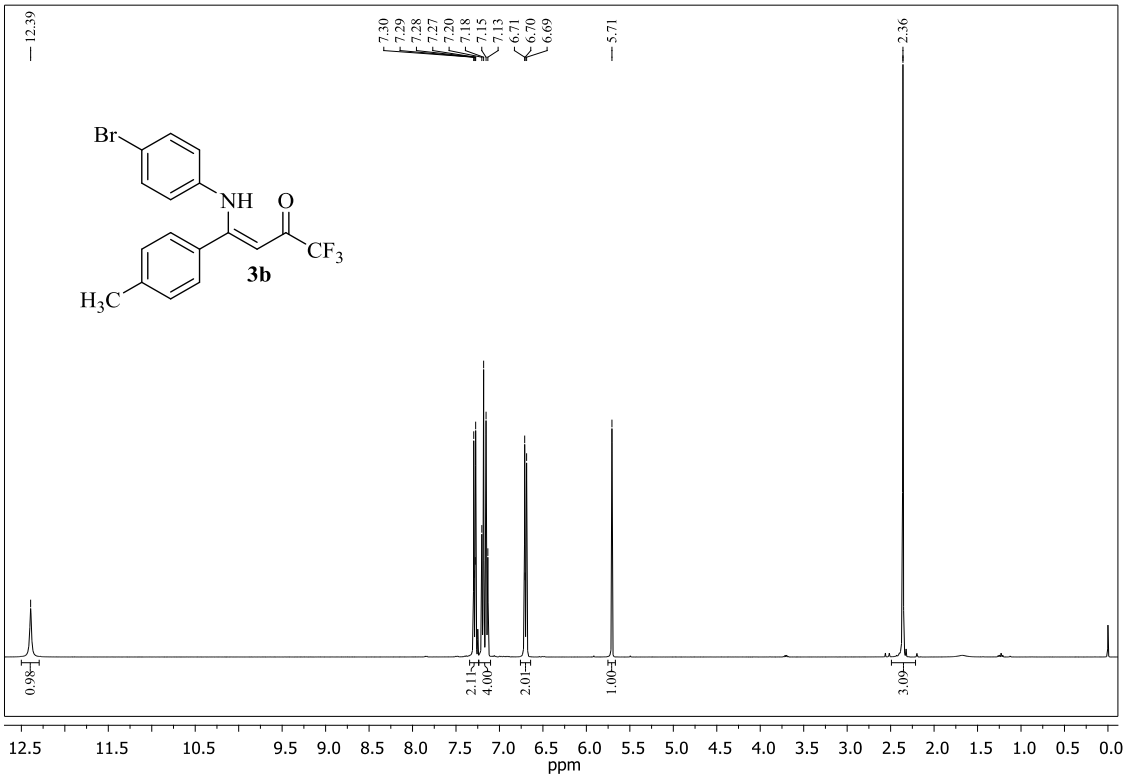


Figure 1. (a)^{1}H and (b)^{13}C NMR for compound **3a** in $CDCl_3$.

(a)



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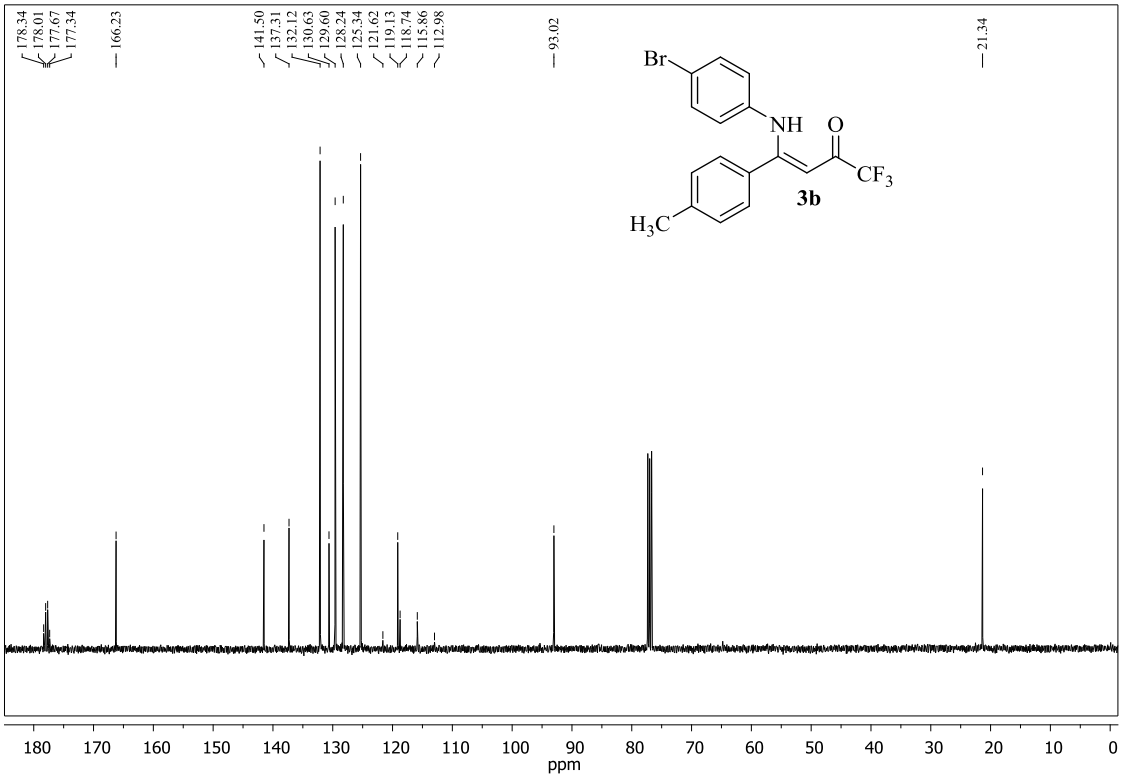
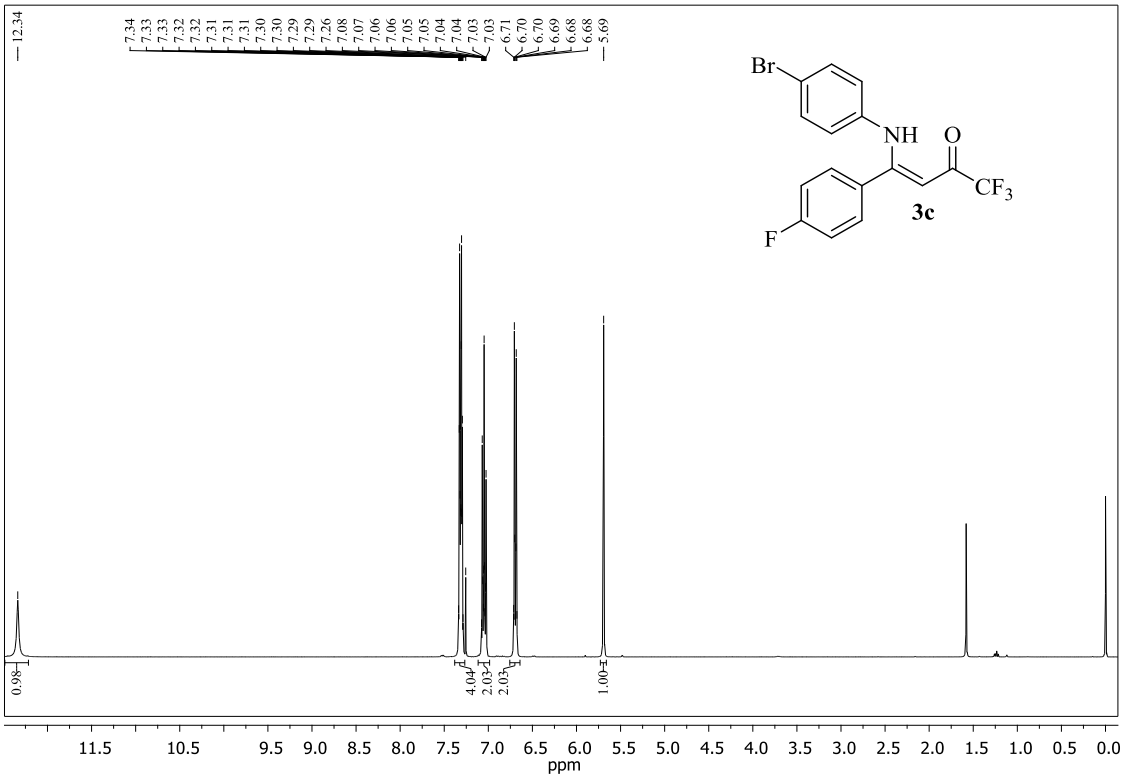


Figure 2. (a)^{1}H and (b)^{13}C NMR for compound **3b** in $CDCl_3$.

(a)



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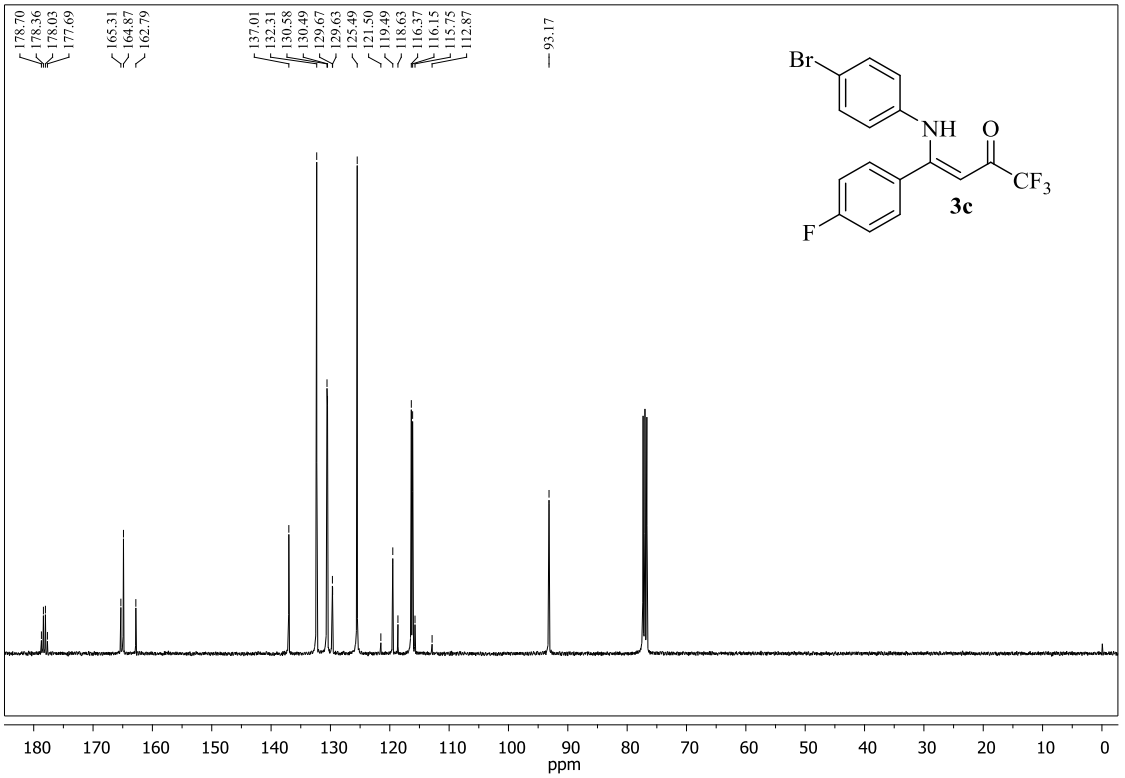
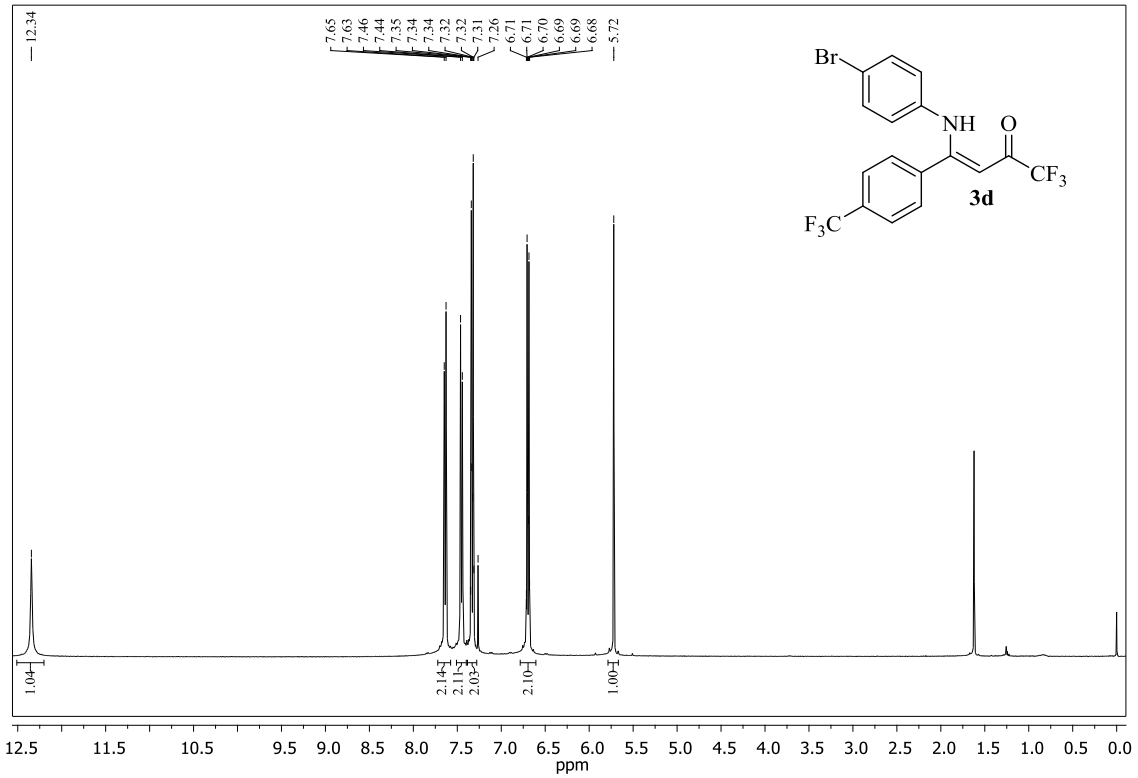


Figure 3.(a)^{1}H and (b)^{13}C NMR for compound **3c** in $CDCl_3$.

(a)



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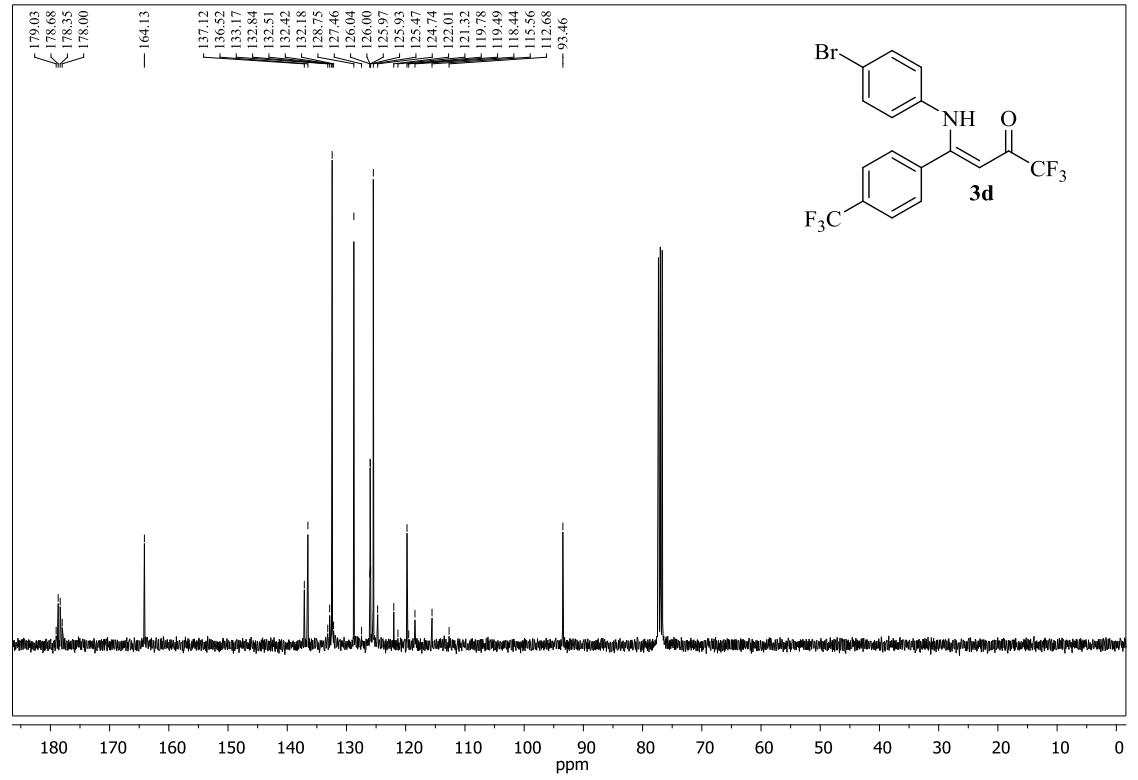
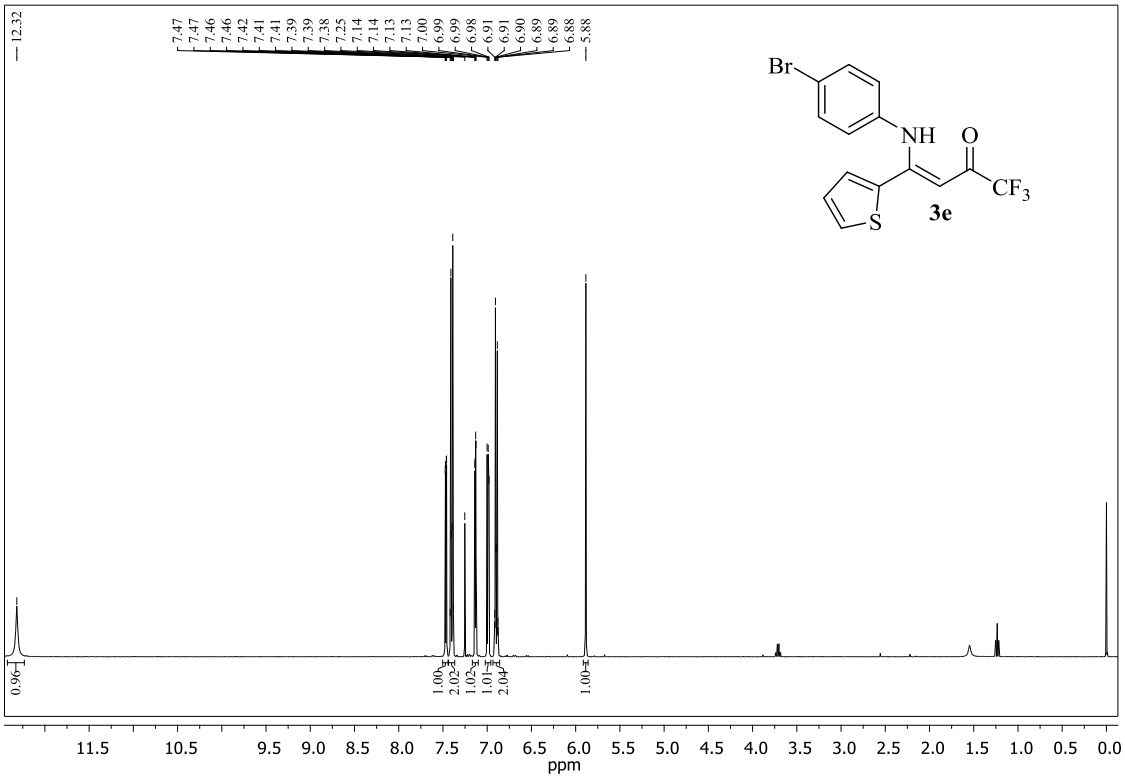


Figure 4. (a)^{1}H and (b)^{13}C NMR for compound **3d** in $CDCl_3$.

(a)



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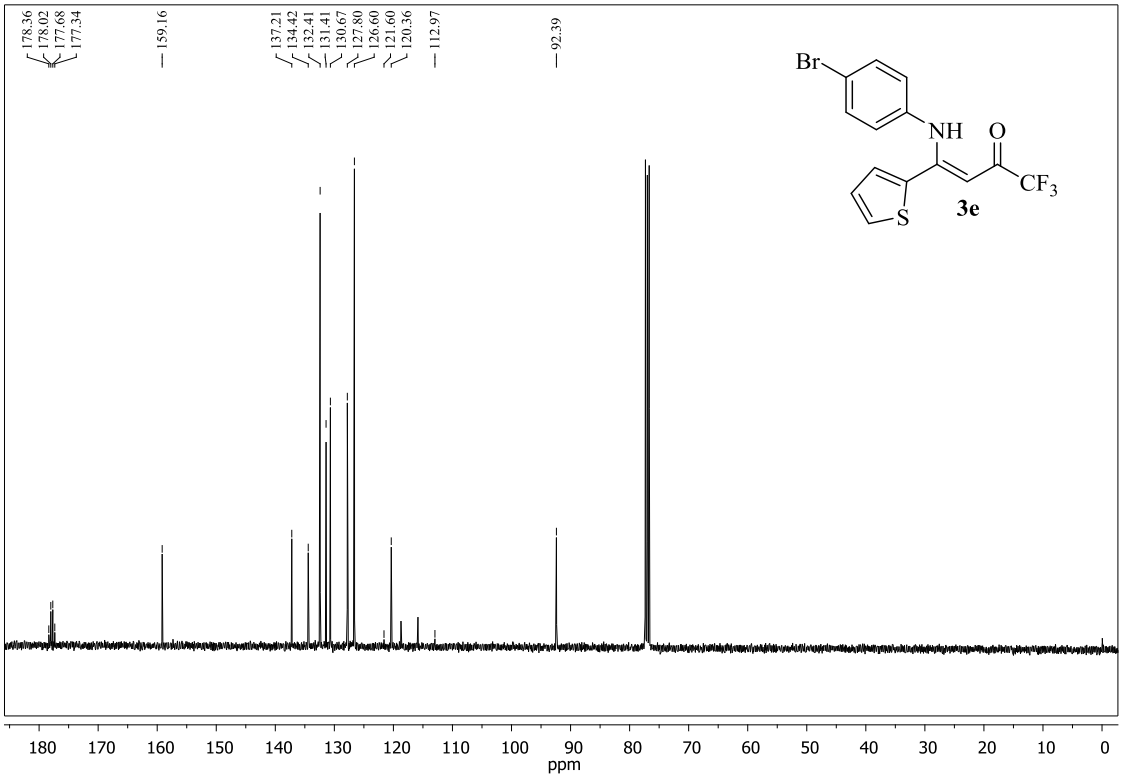
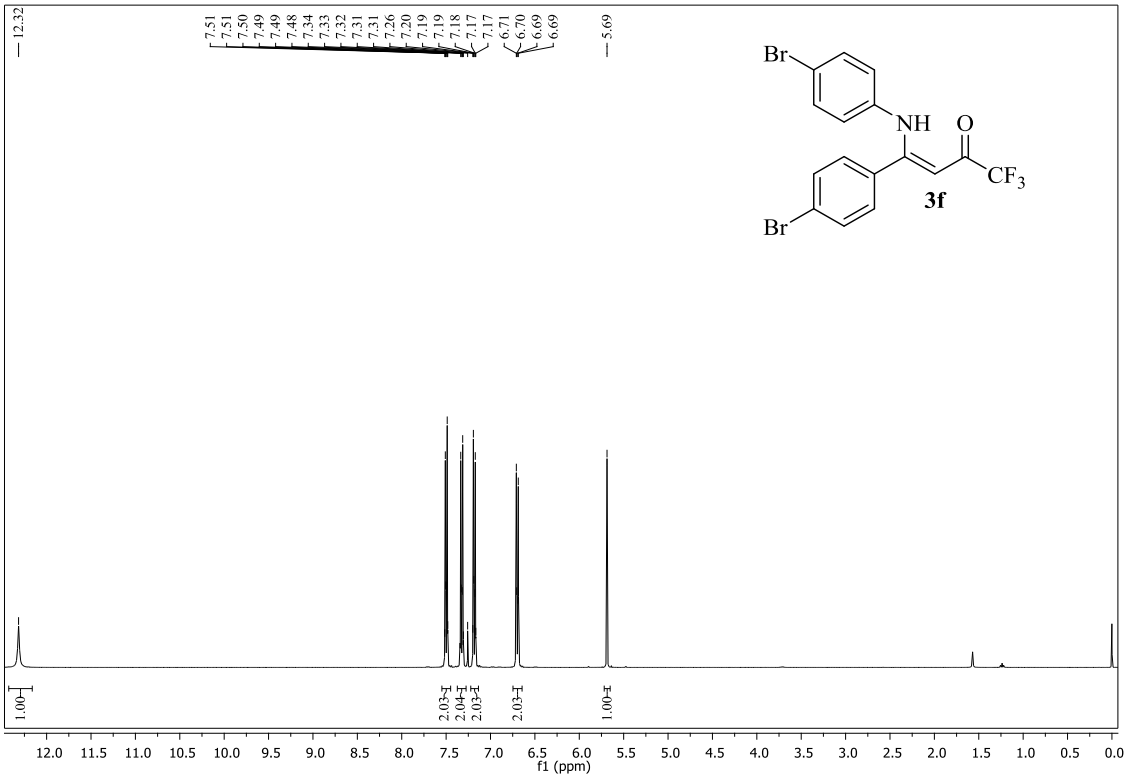


Figure 5. (a)^{1}H and (b)^{13}C NMR for compound **3e** in $CDCl_3$.

(a)



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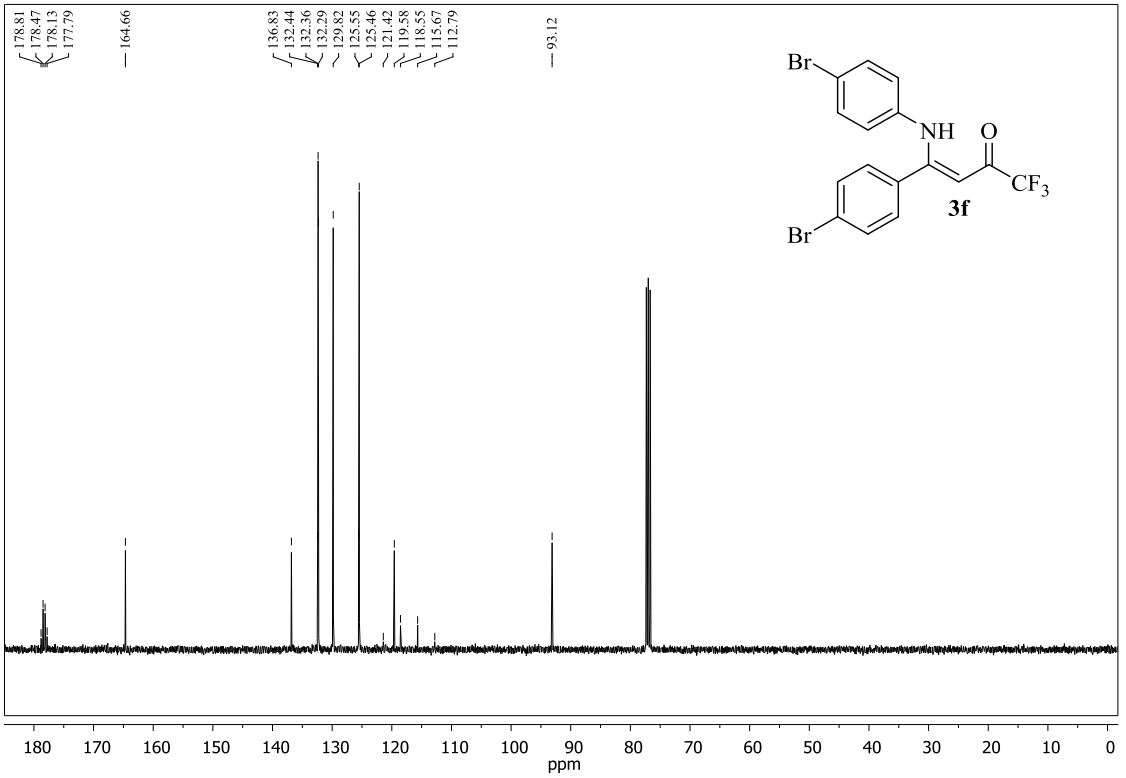
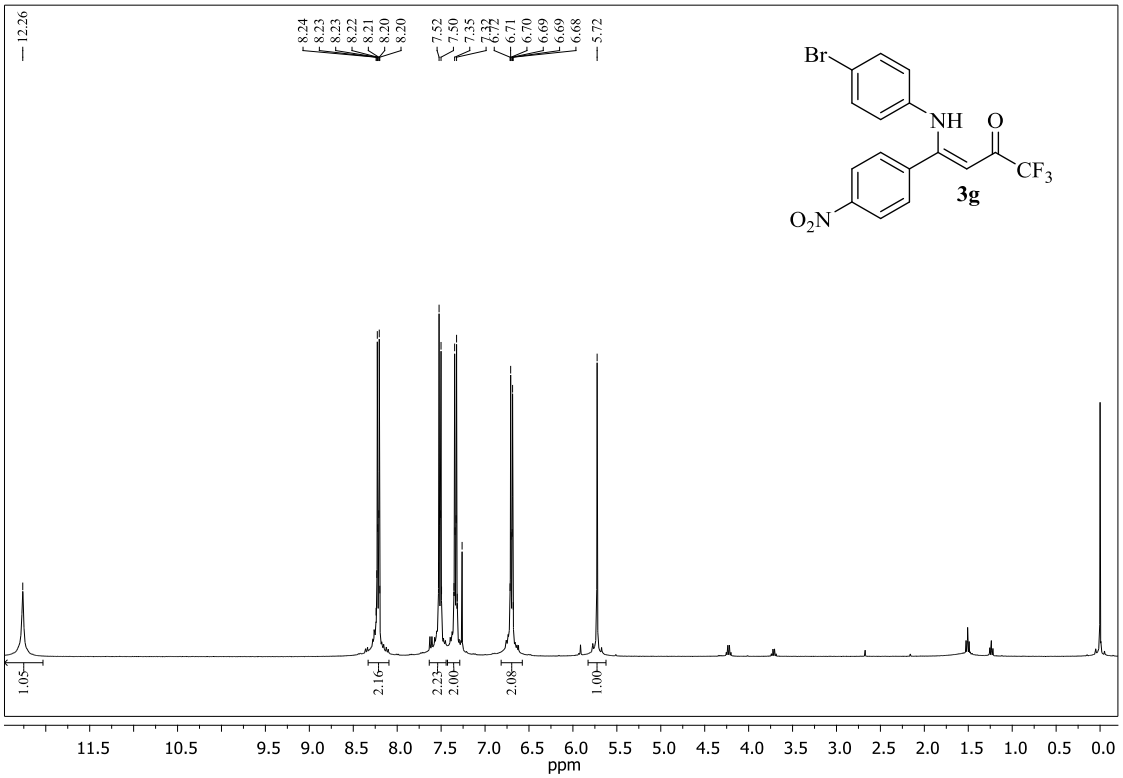


Figure 6.(a)^{1}H and (b)^{13}C NMR for compound **3f** in $CDCl_3$.

(a)



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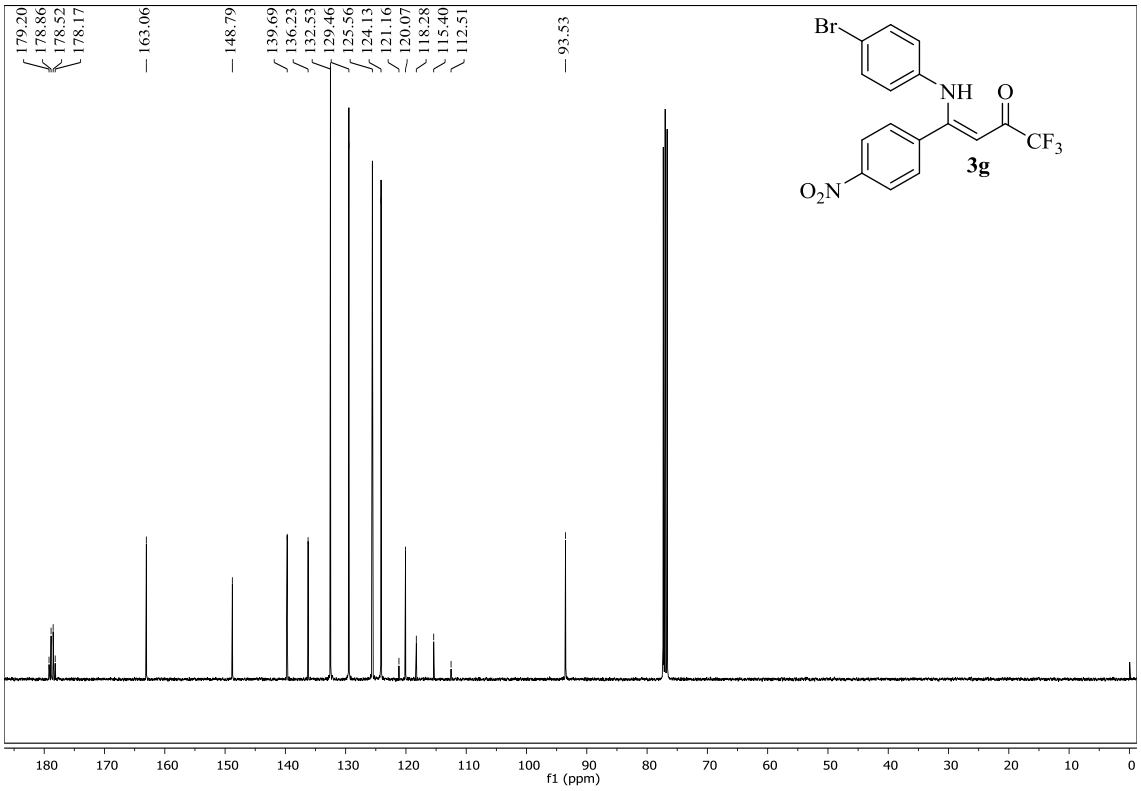
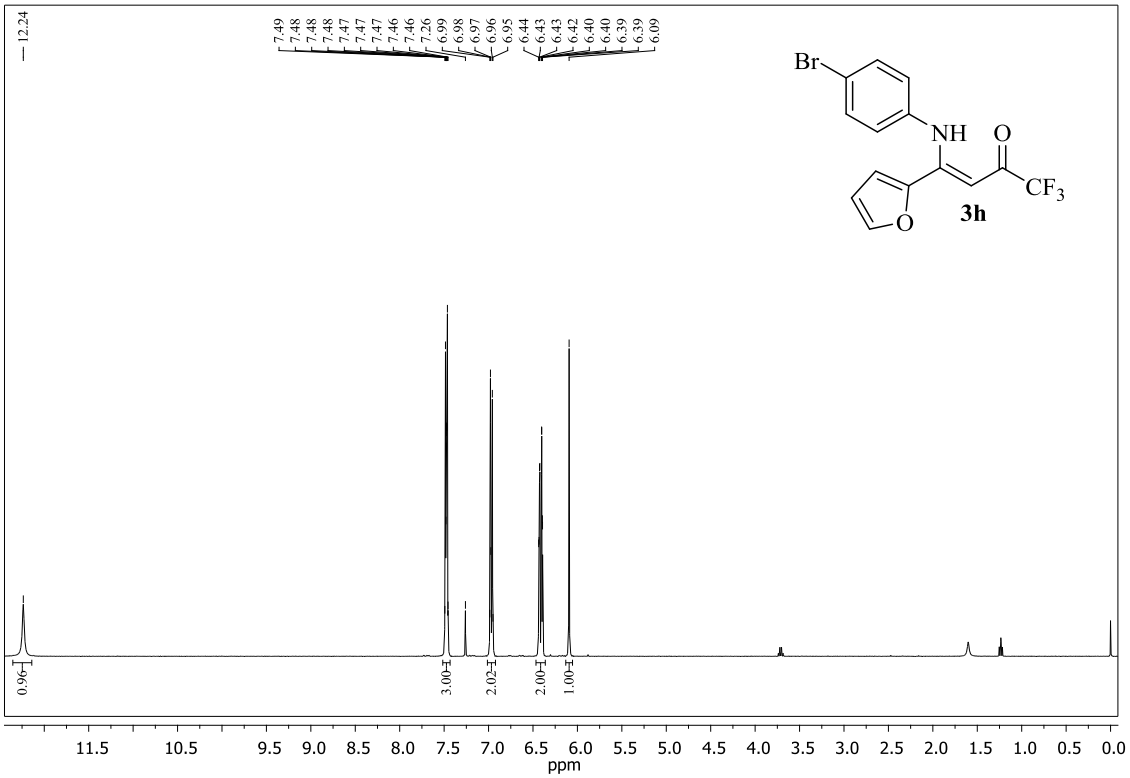


Figure 7. (a)^{1}H and (b)^{13}C NMR for compound **3g** in $CDCl_3$.

(a)



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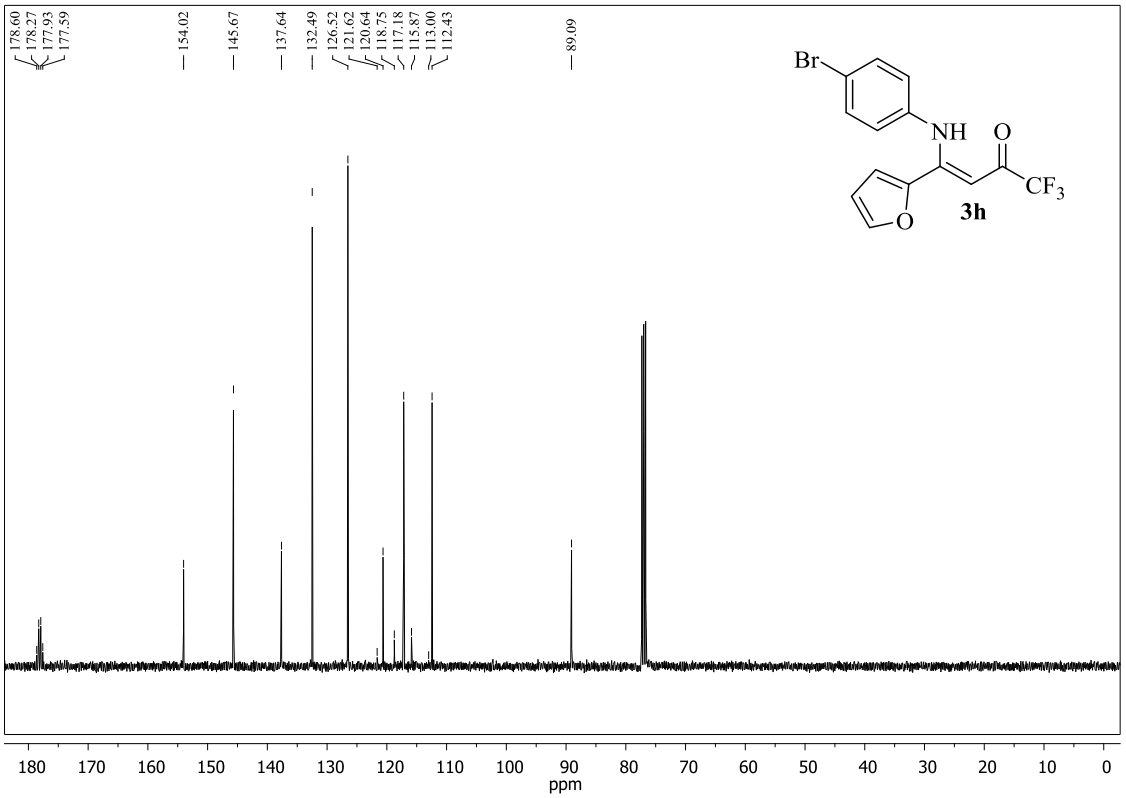
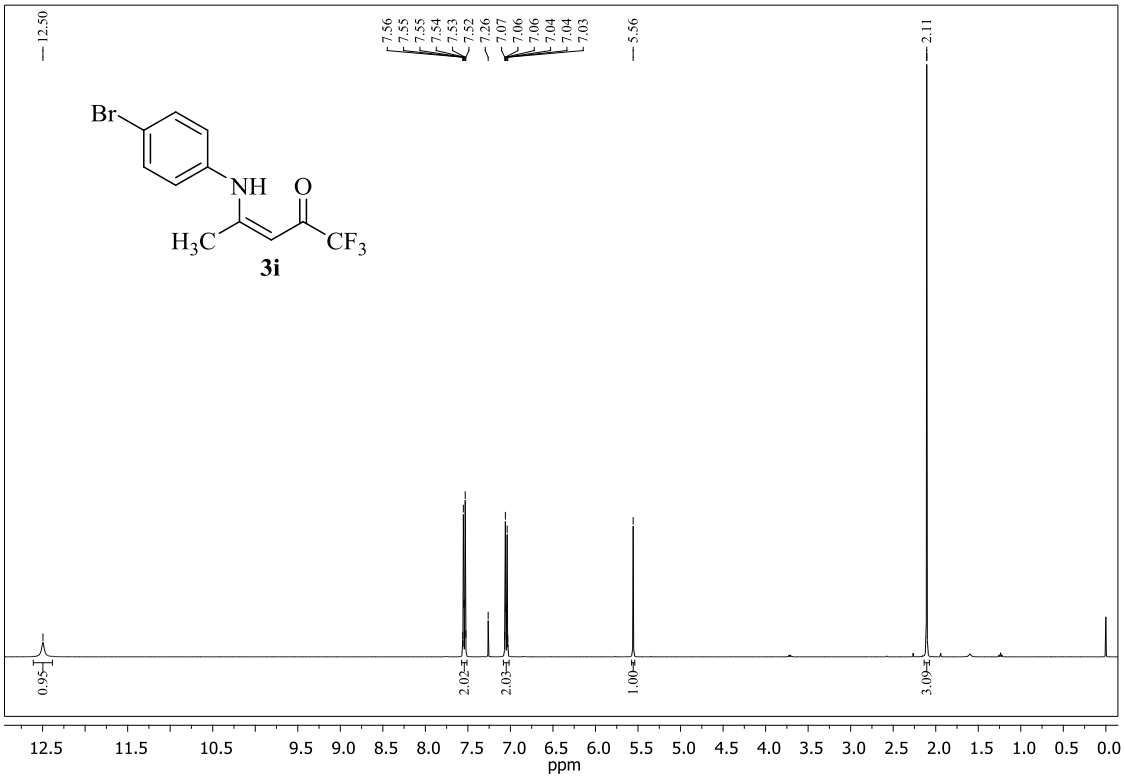


Figure 8. (a)^{1}H and (b)^{13}C NMR for compound **3h** in $CDCl_3$.

(a)



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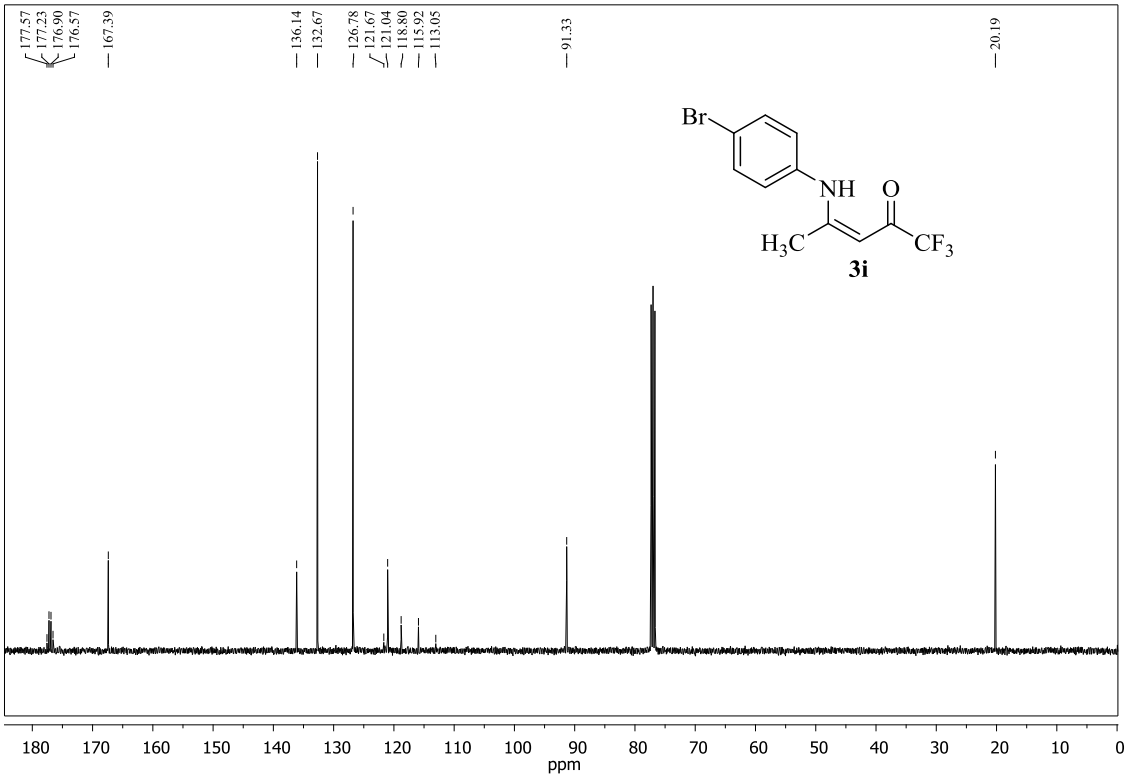


Figure 9. (a) ^{1}H and (b) ^{13}C NMR for compound **3i** in $CDCl_3$.

(a)

(b)

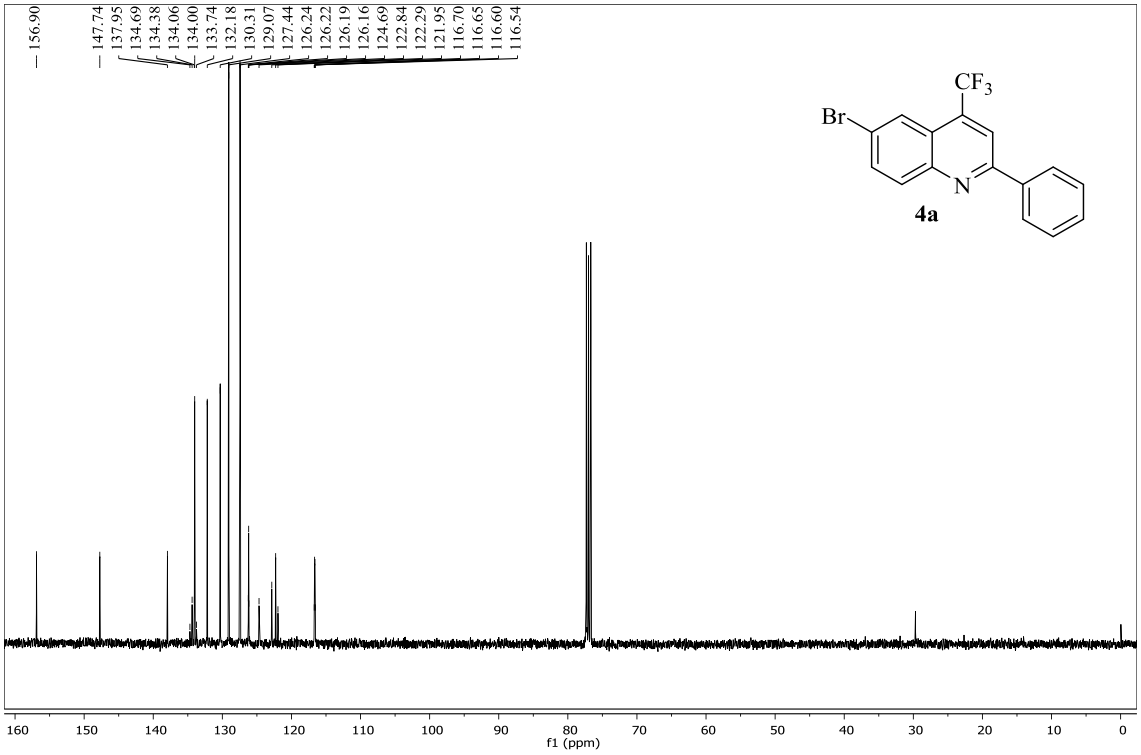
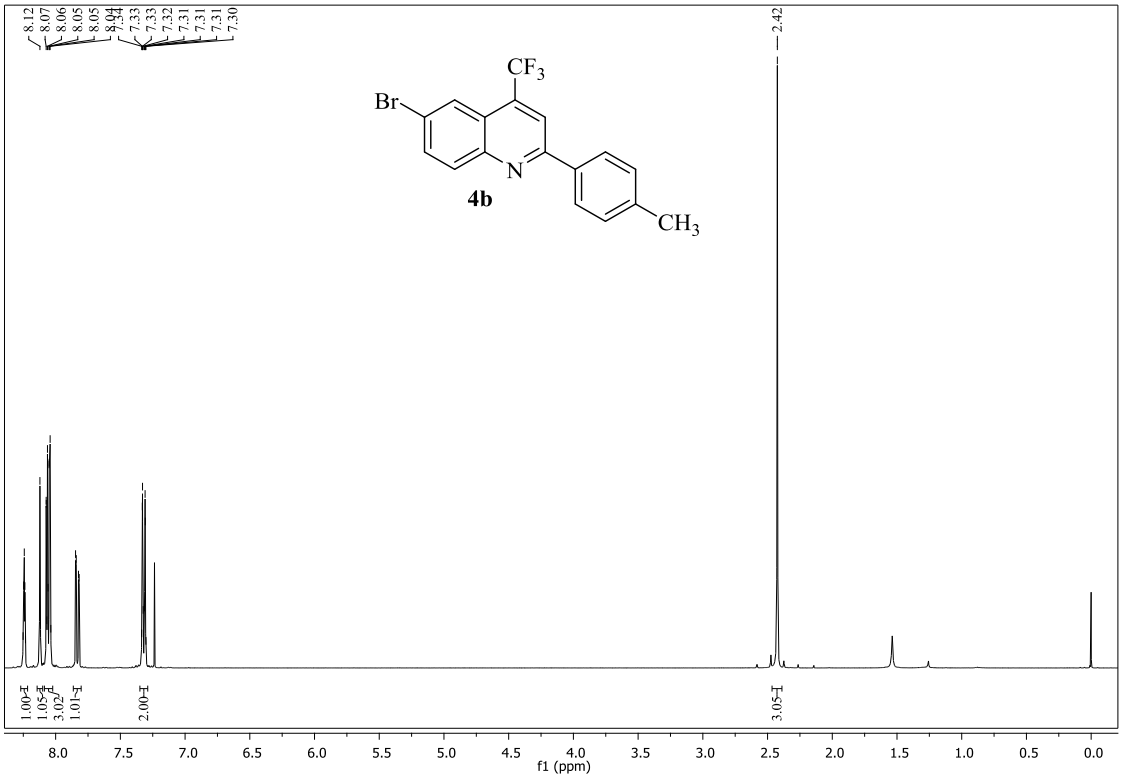


Figure 10. (a)^{1}H and (b)^{13}C NMR for compound **4a** in $CDCl_3$.

(a)



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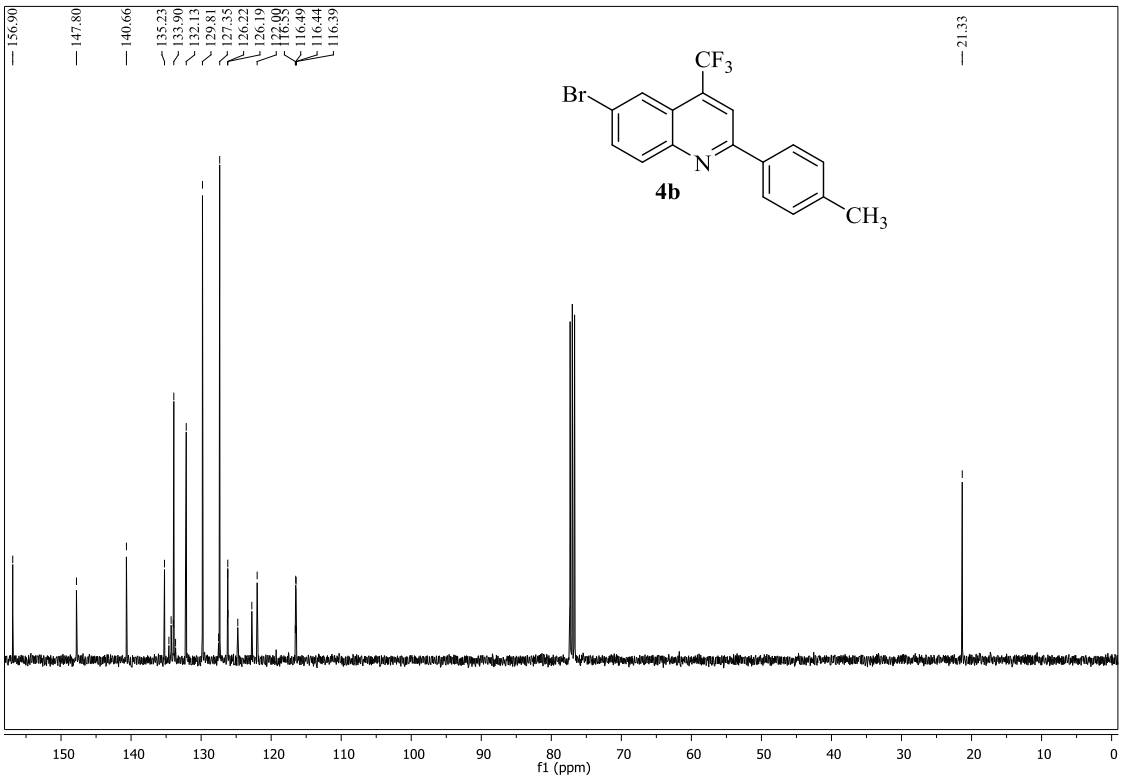
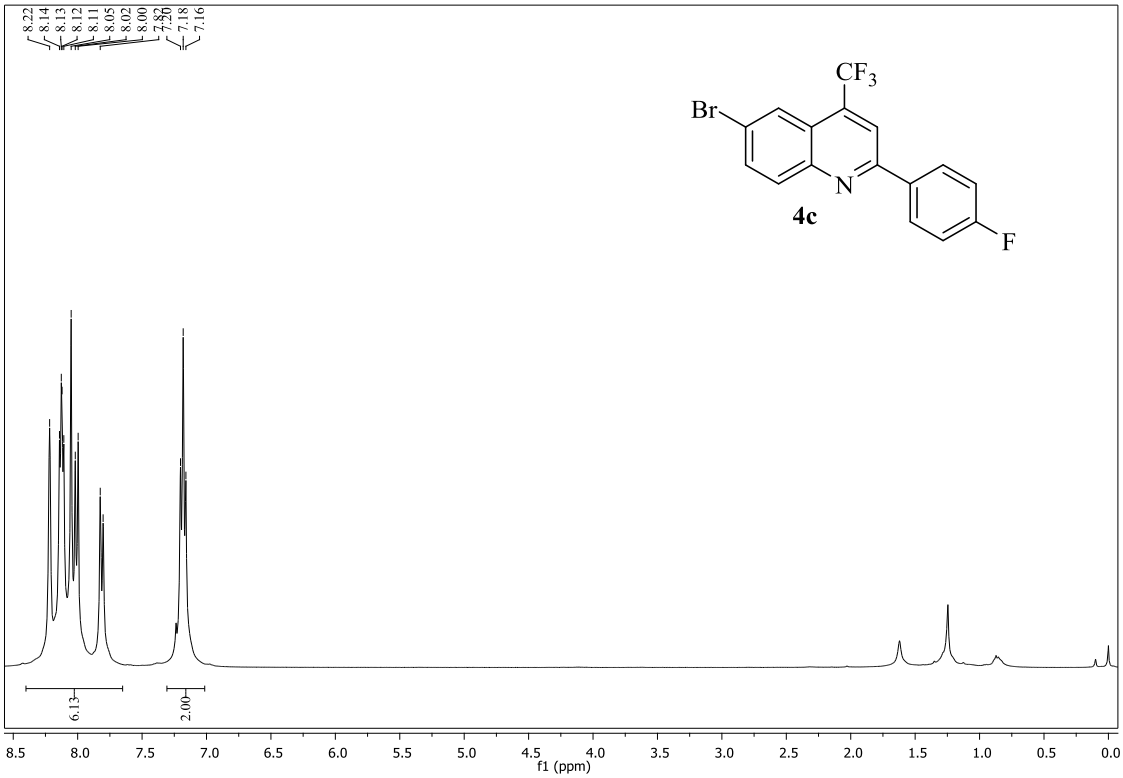


Figure 11.(a)^{1}H and (b)^{13}C NMR for compound **4b** in $CDCl_3$.

(a)



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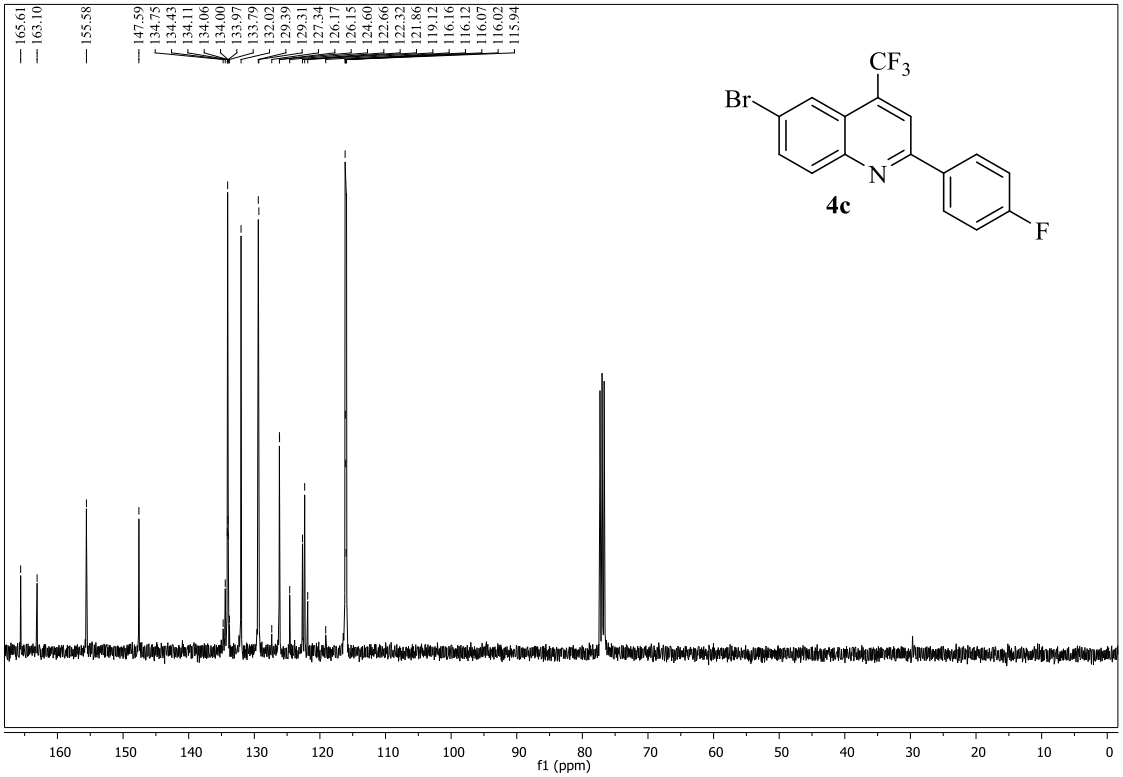
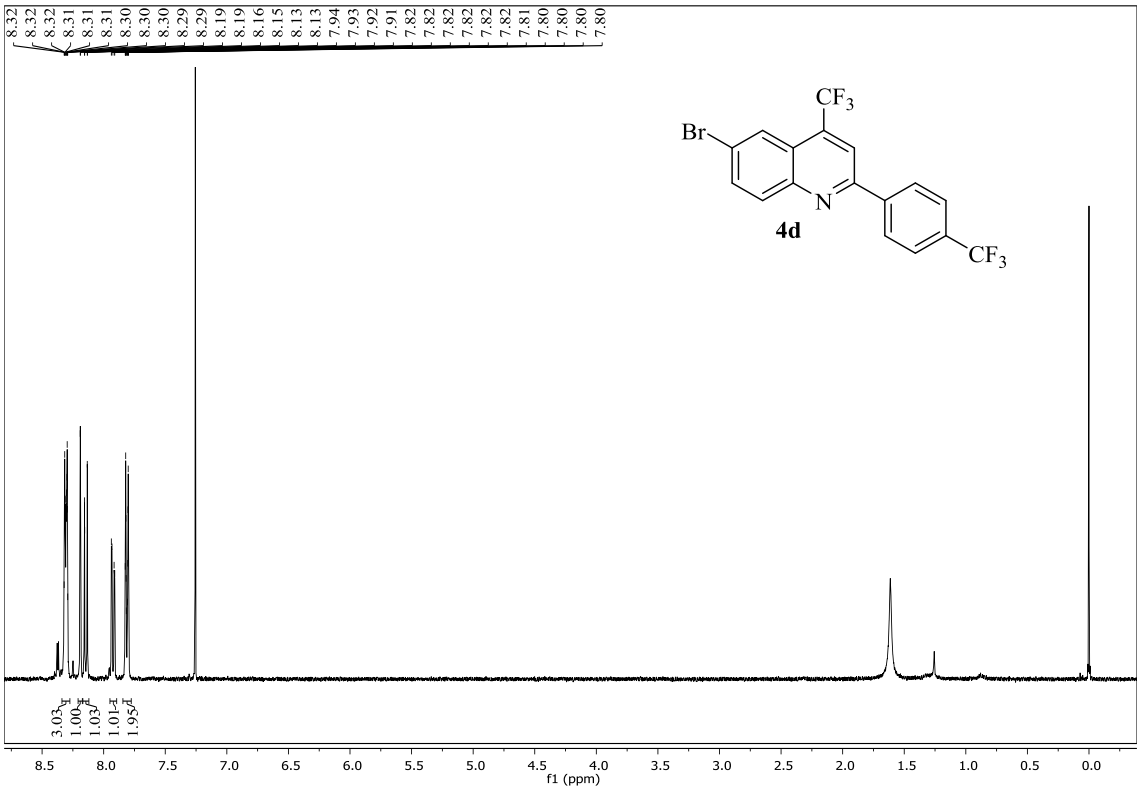


Figure 12. (a)^{1}H and (b)^{13}C NMR for compound **4c** in $CDCl_3$.

(a)



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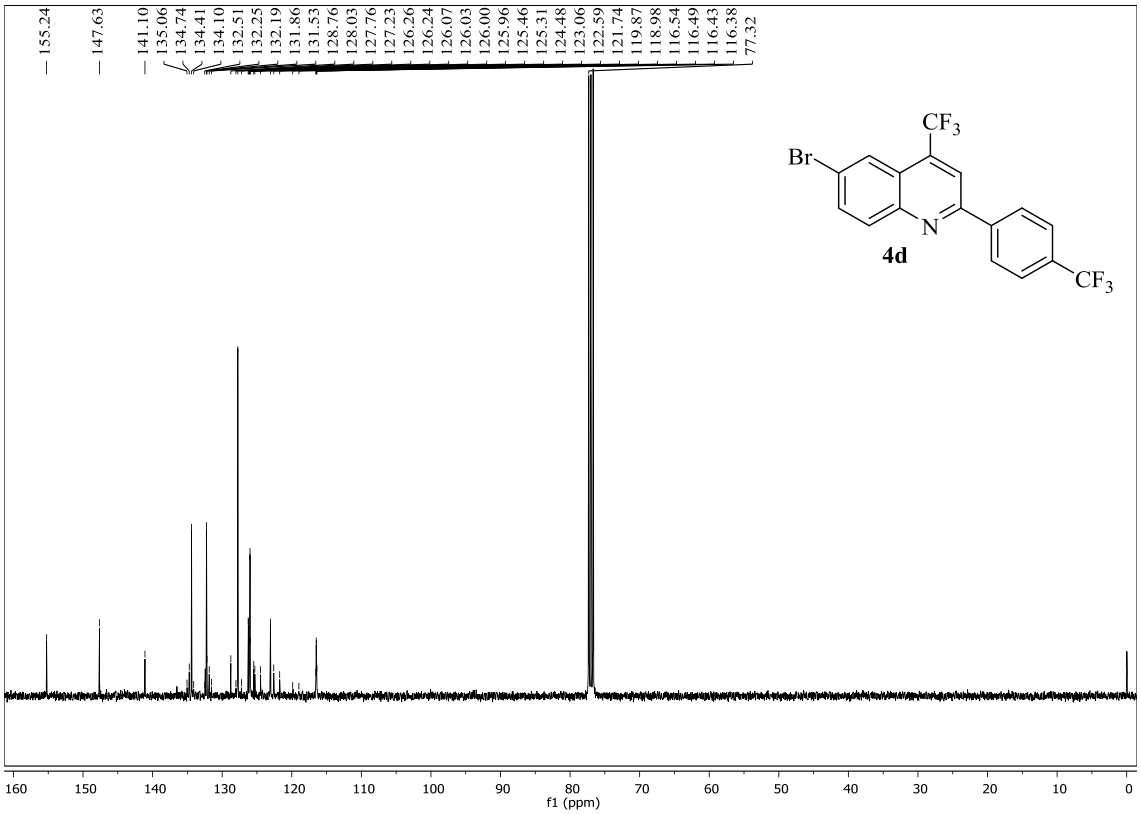
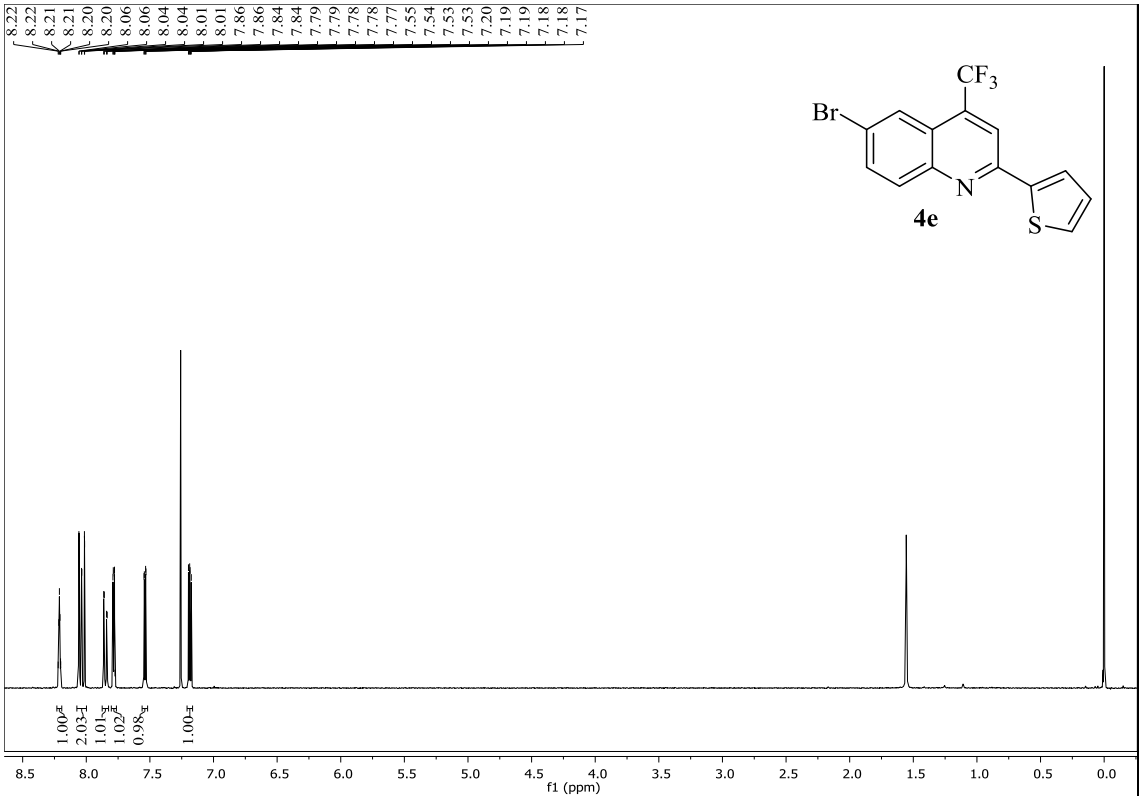


Figure 13. (a)^{1}H and (b)^{13}C NMR for compound **4d** in $CDCl_3$.

(a)



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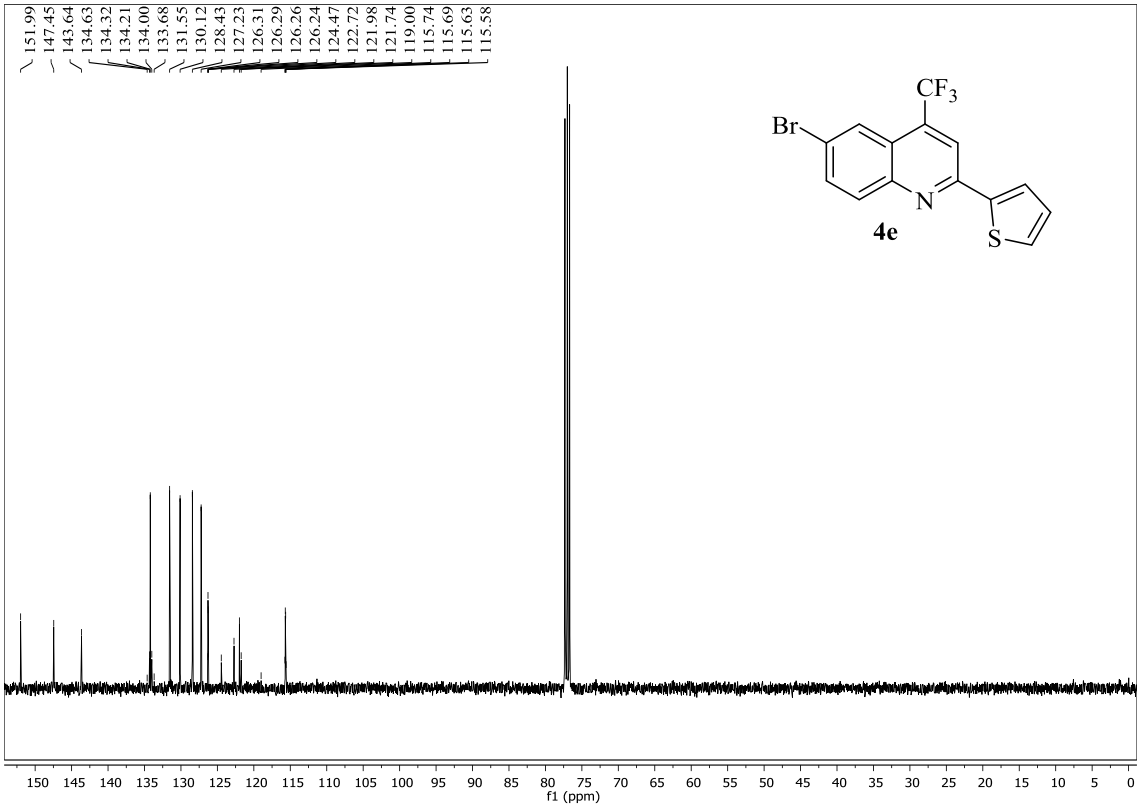
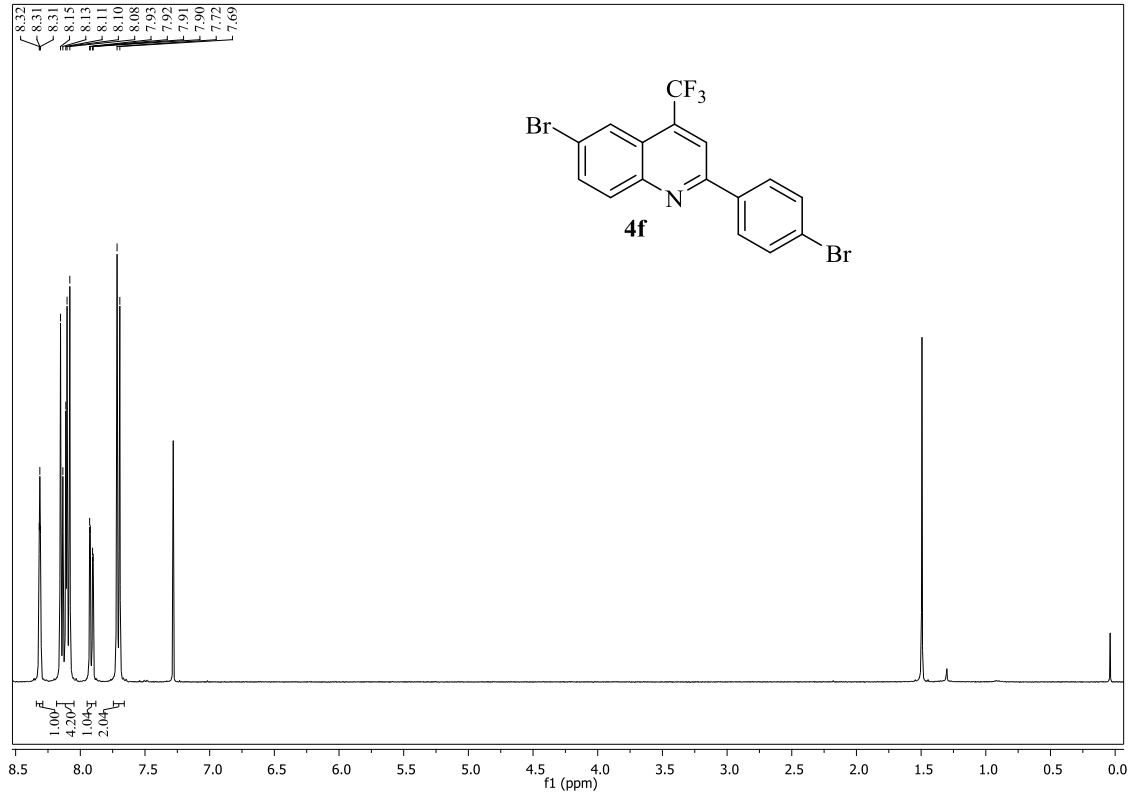


Figure 14. (a)^{1}H and (b)^{13}C NMR for compound **4e** in $CDCl_3$.

(a)



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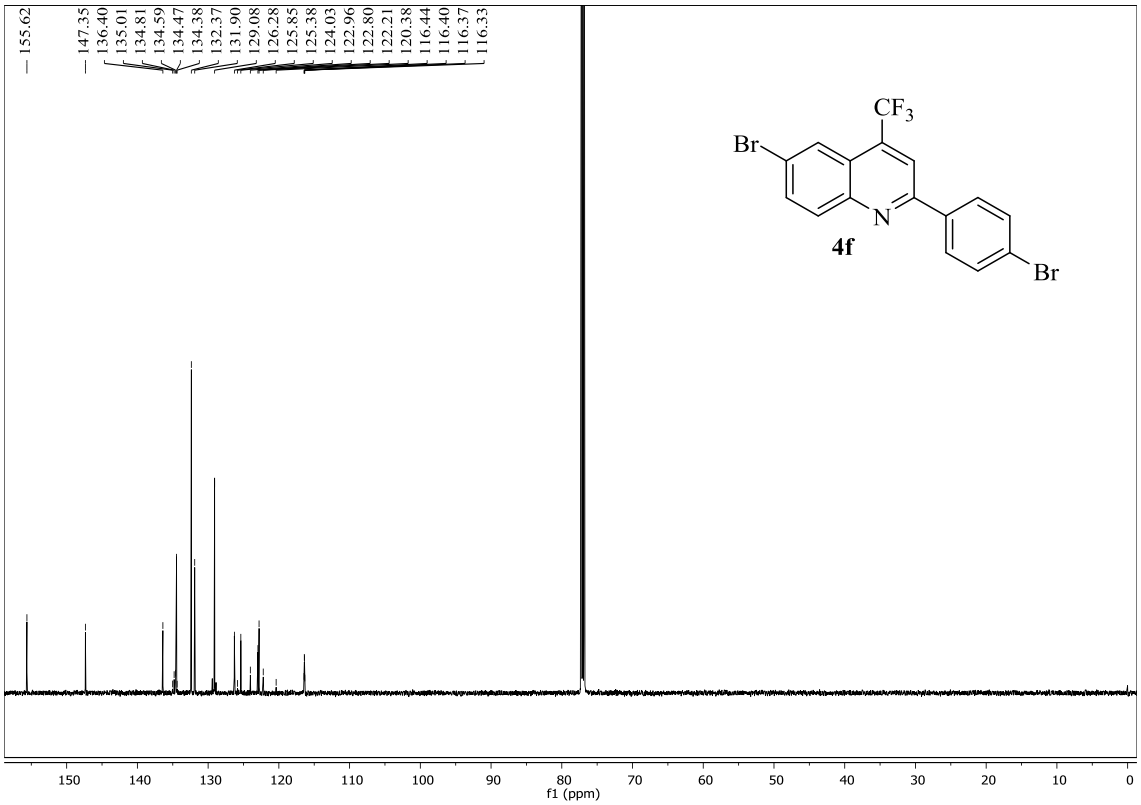
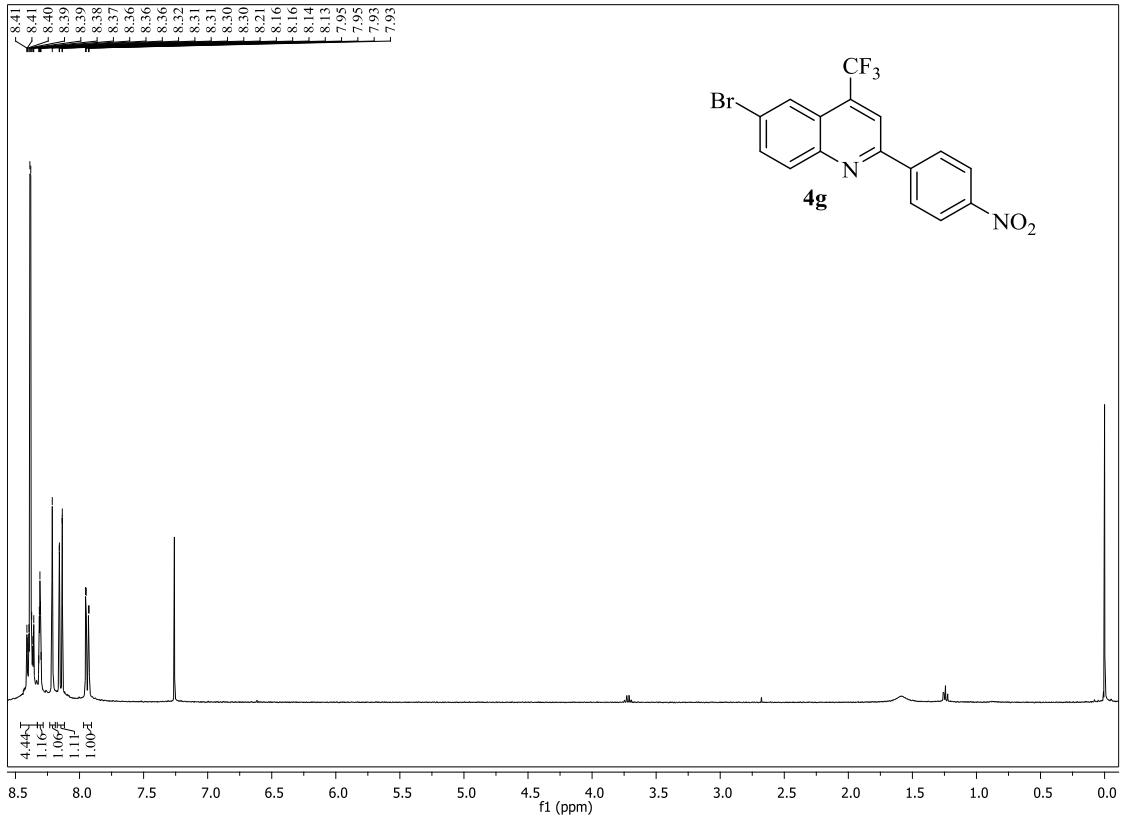


Figure 15. (a)^{1}H and (b)^{13}C NMR for compound **4f** in $CDCl_3$.

(a)



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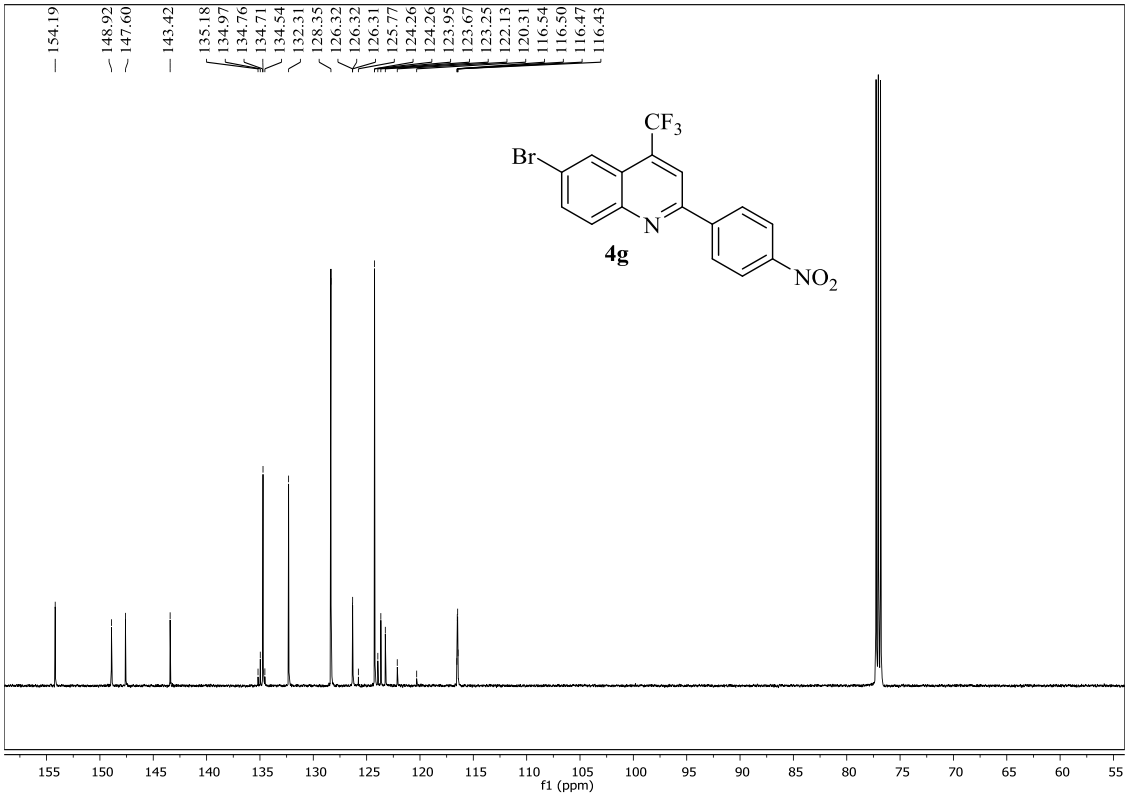
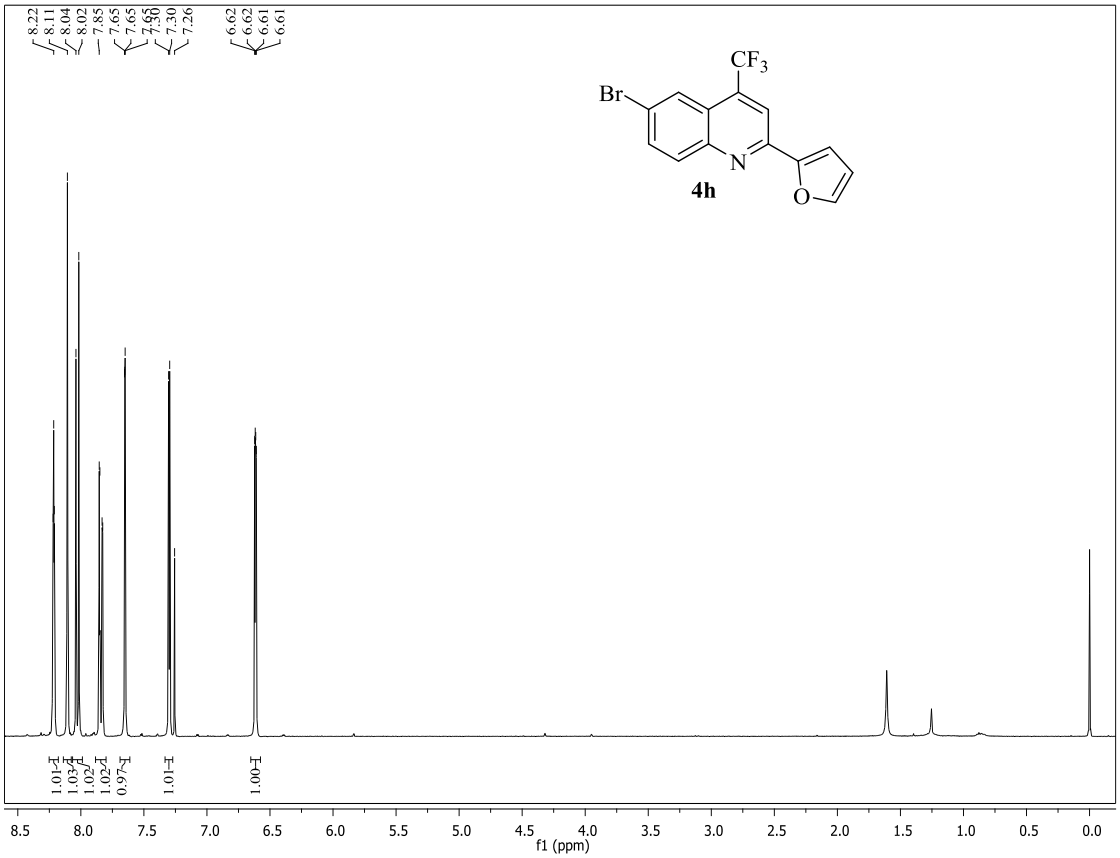


Figure 16. (a)^{1}H and (b)^{13}C NMR for compound **4g** in $CDCl_3$.

(a)



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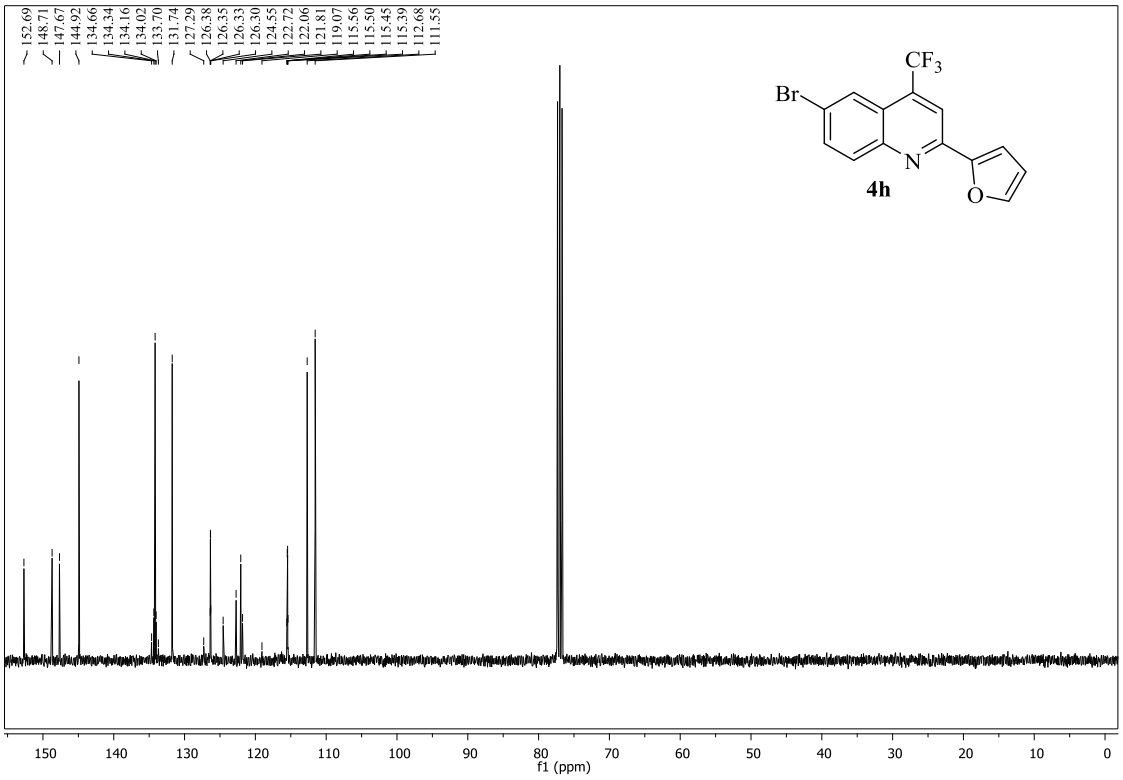
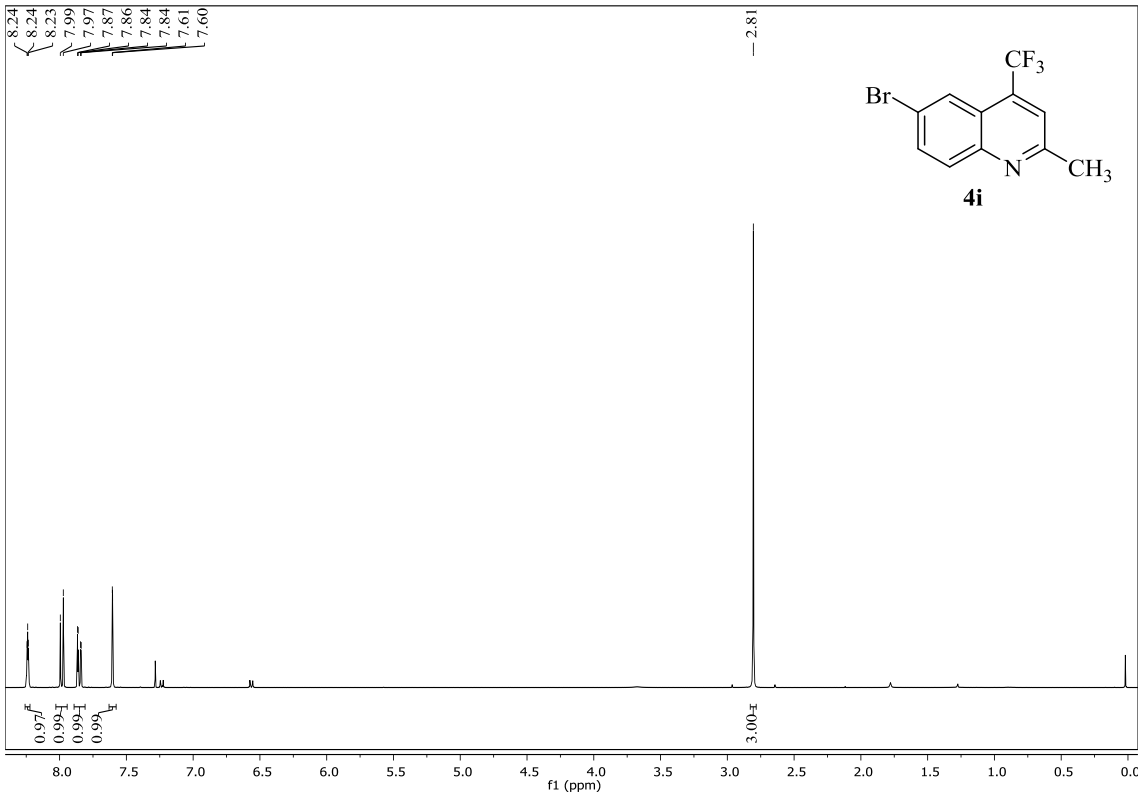


Figure 17. (a)^{1}H and (b)^{13}C NMR for compound **4h** in $CDCl_3$.

(a)



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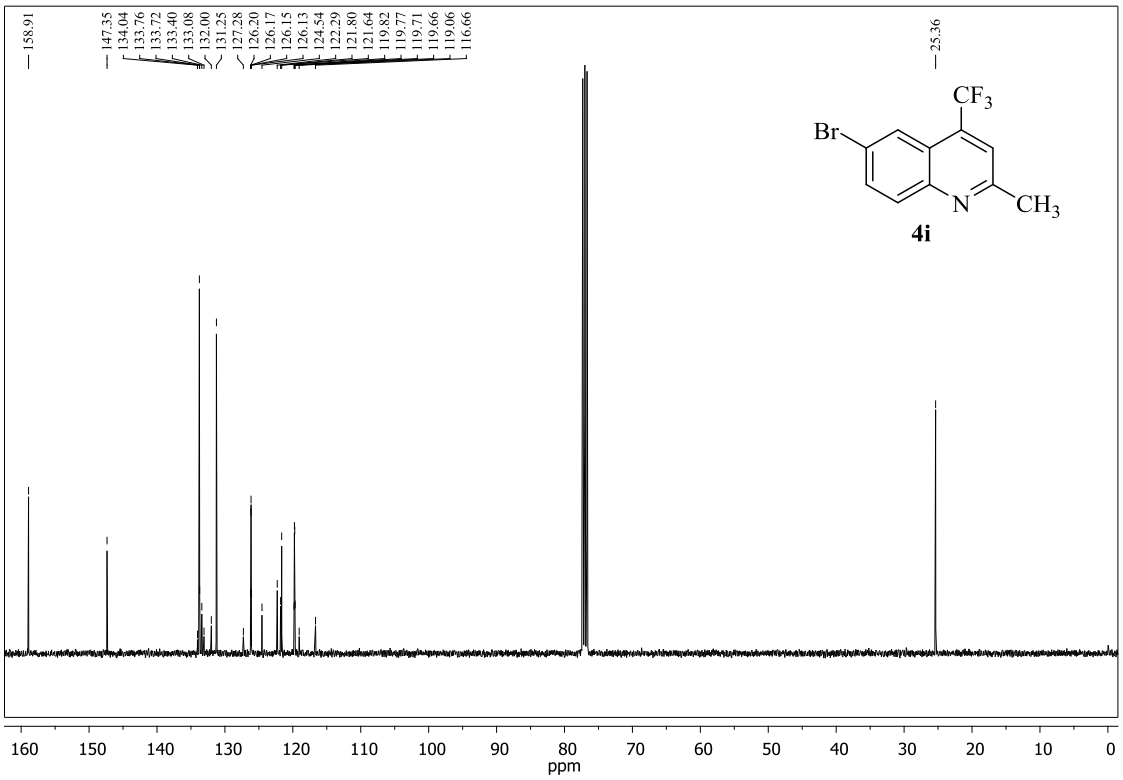


Figure 18. (a)^{1}H and (b)^{13}C NMR for compound **4i** in $CDCl_3$.

(a)

(b)

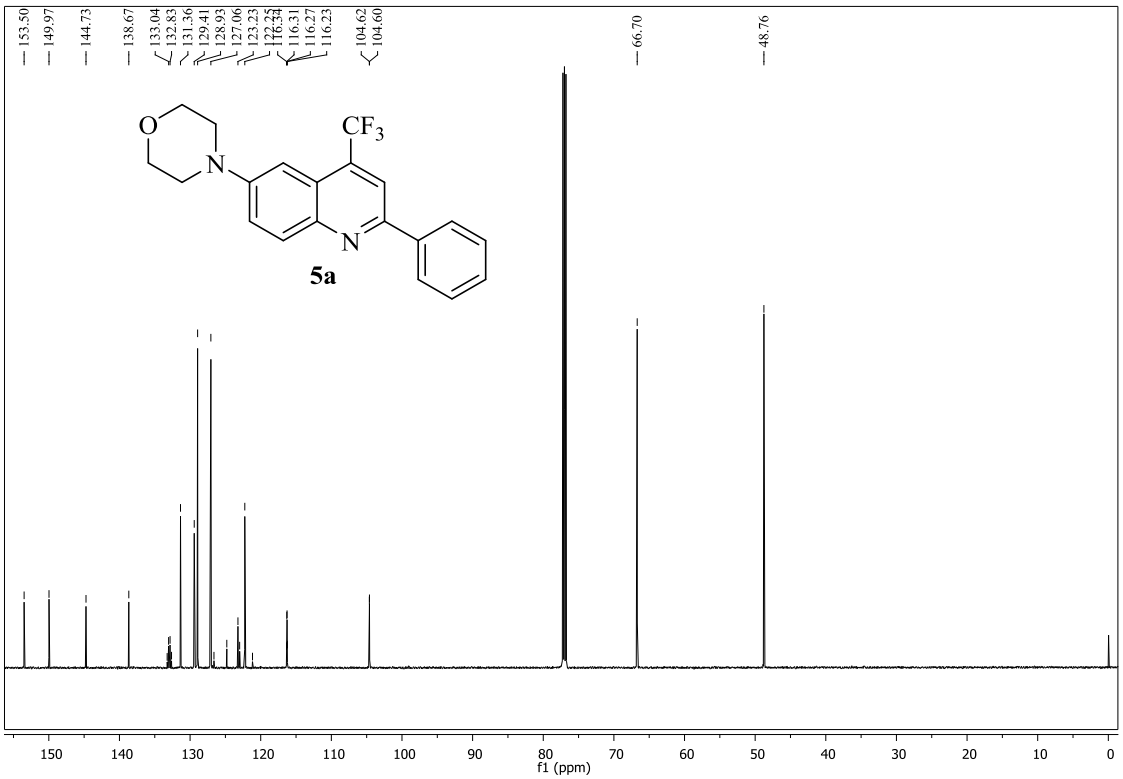
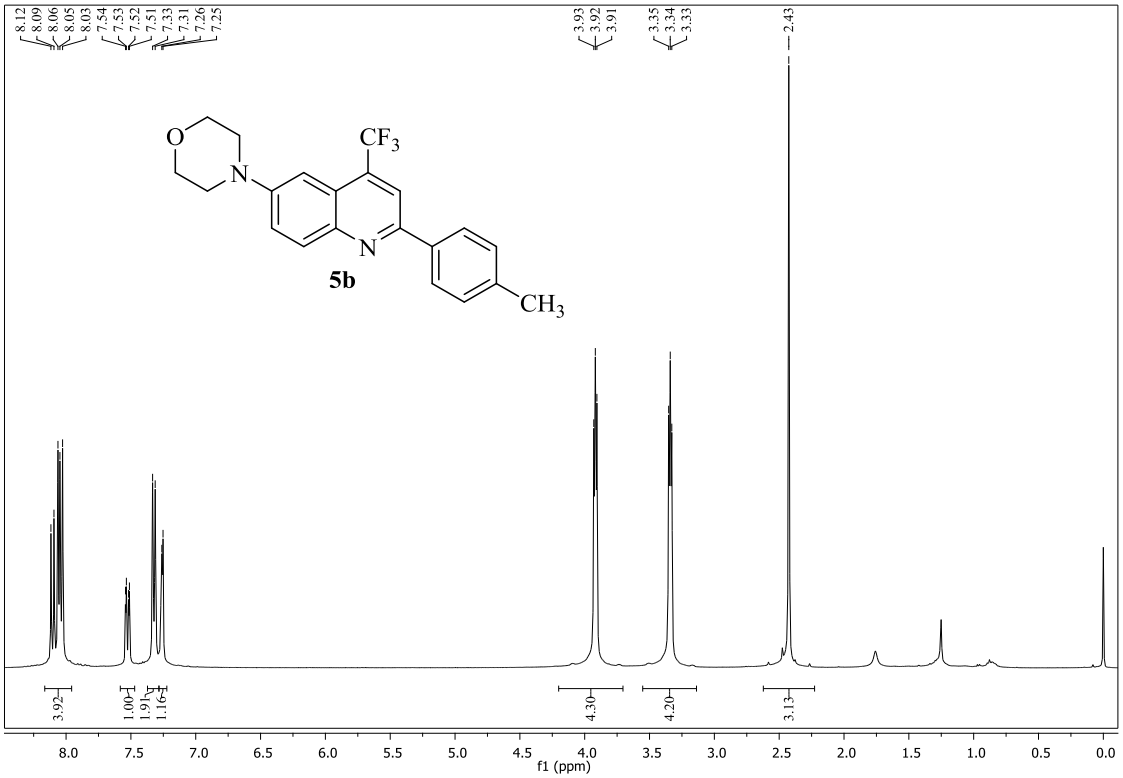


Figure 19.(a)^{1}H and (b)^{13}C NMR for compound **5a** in $CDCl_3$.

(a)



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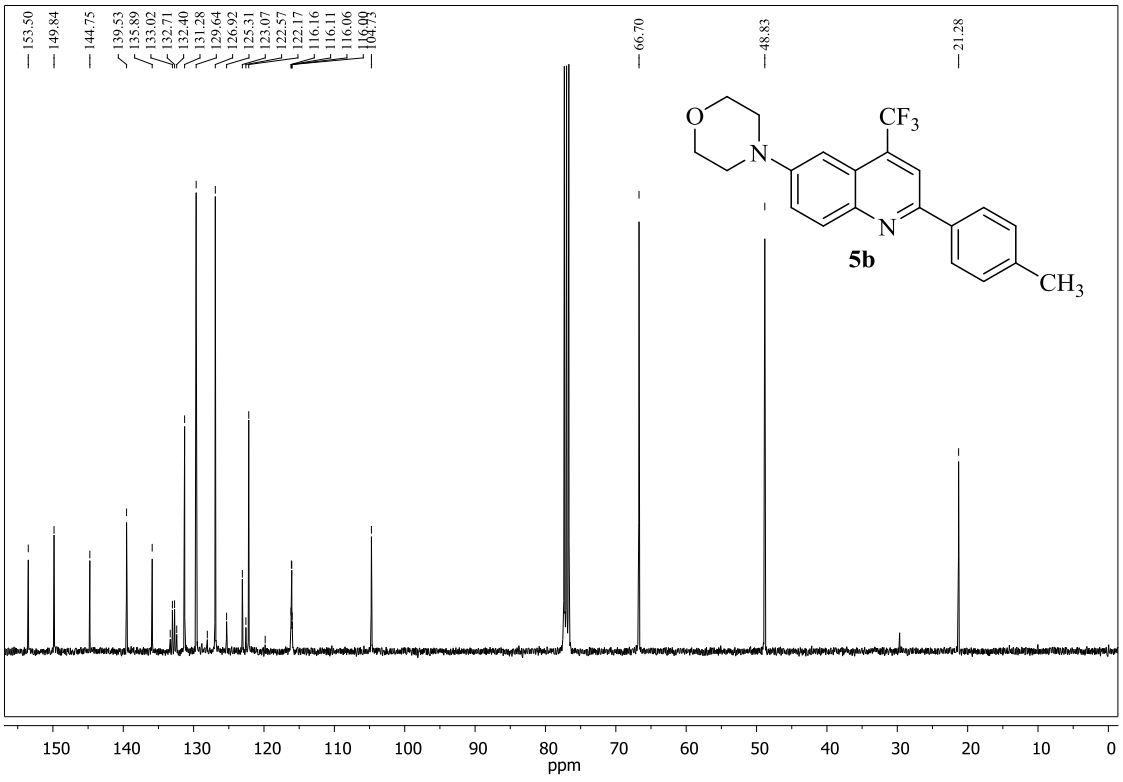
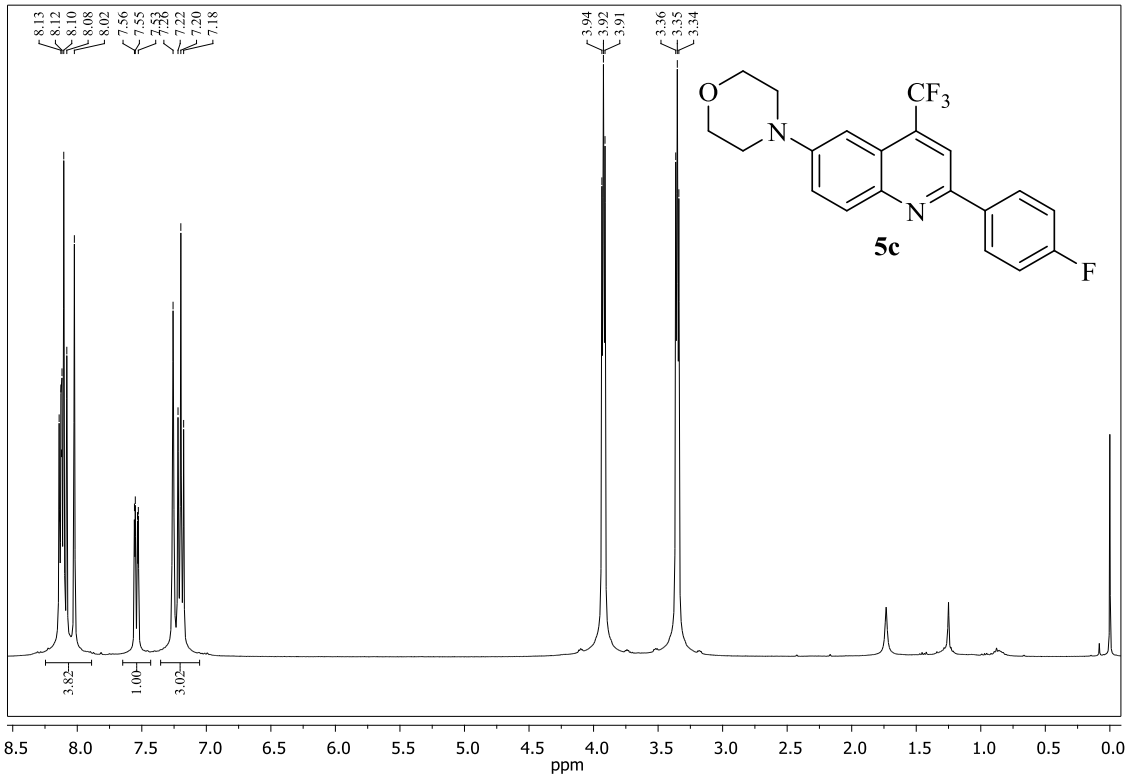


Figure 20. (a)^{1}H and (b)^{13}C NMR for compound **5b** in $CDCl_3$.

(a)



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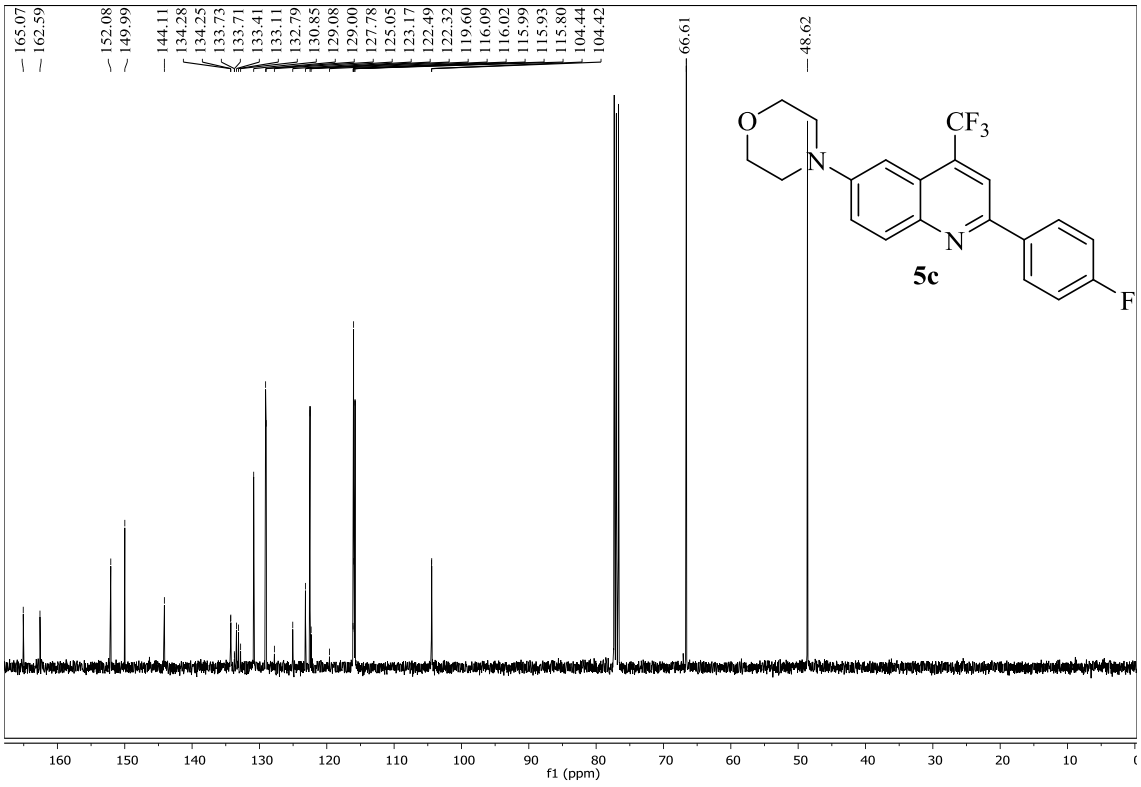
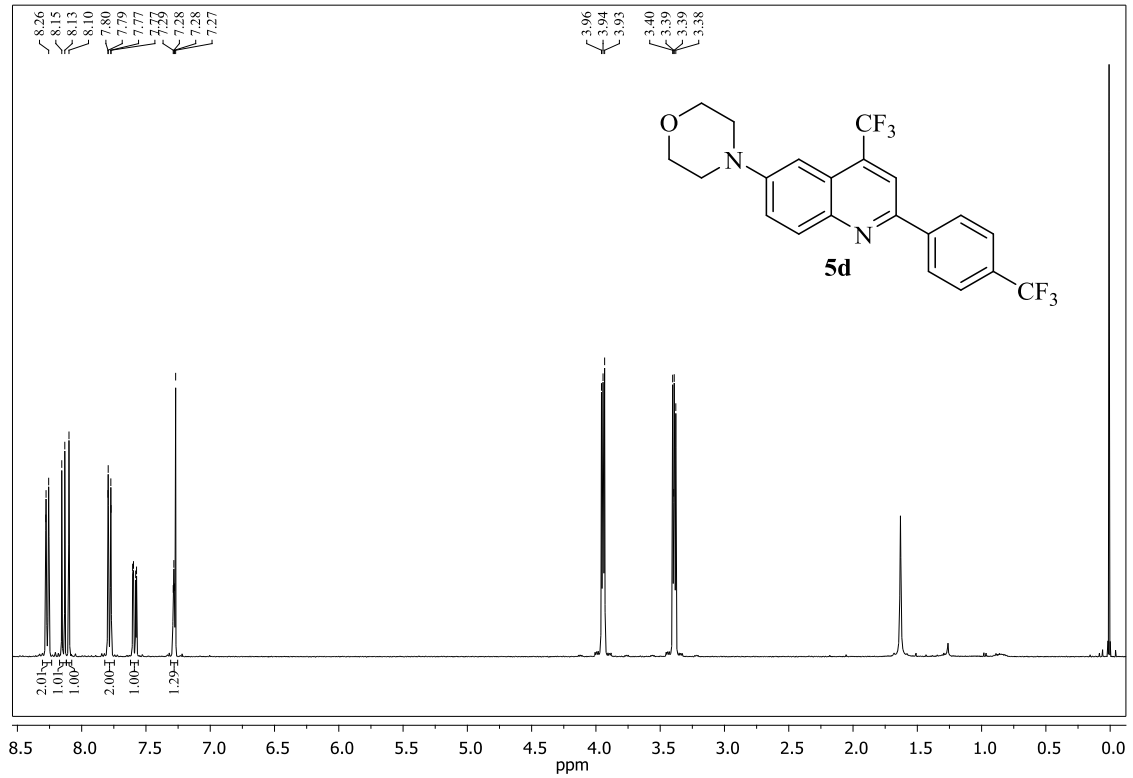


Figure 21. (a)^{1}H and (b)^{13}C NMR for compound **5c** in $CDCl_3$.

(a)



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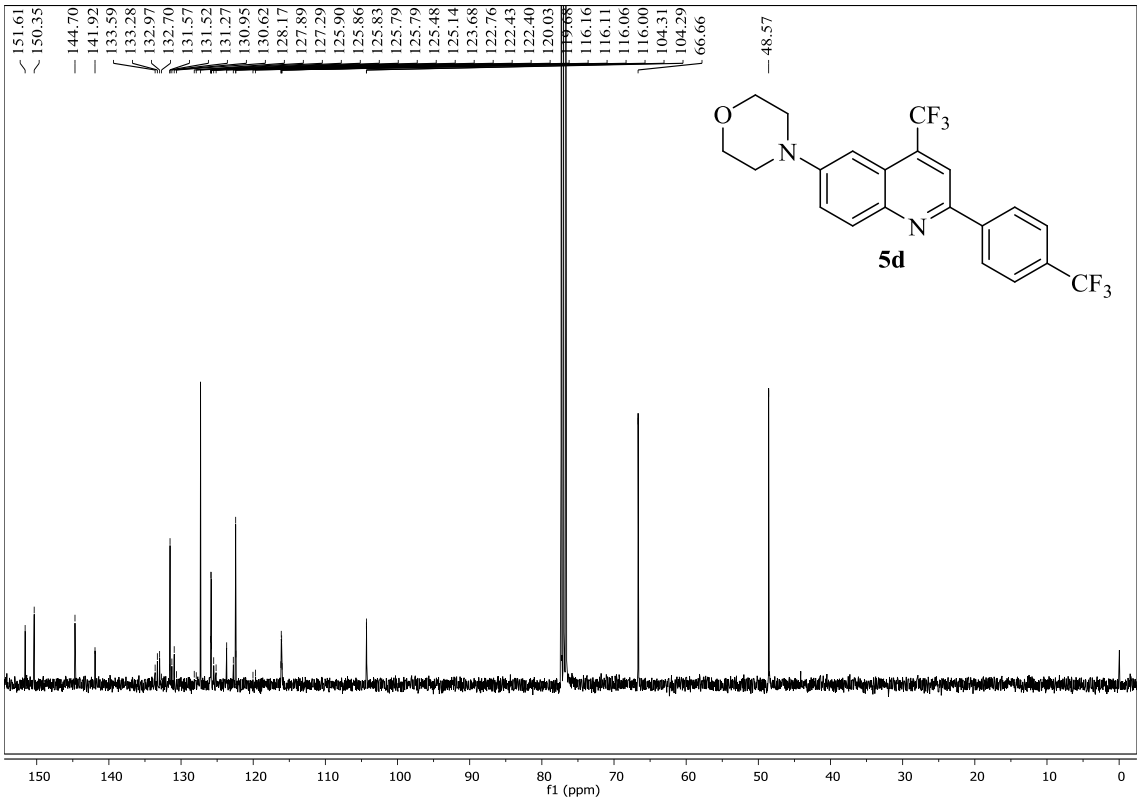
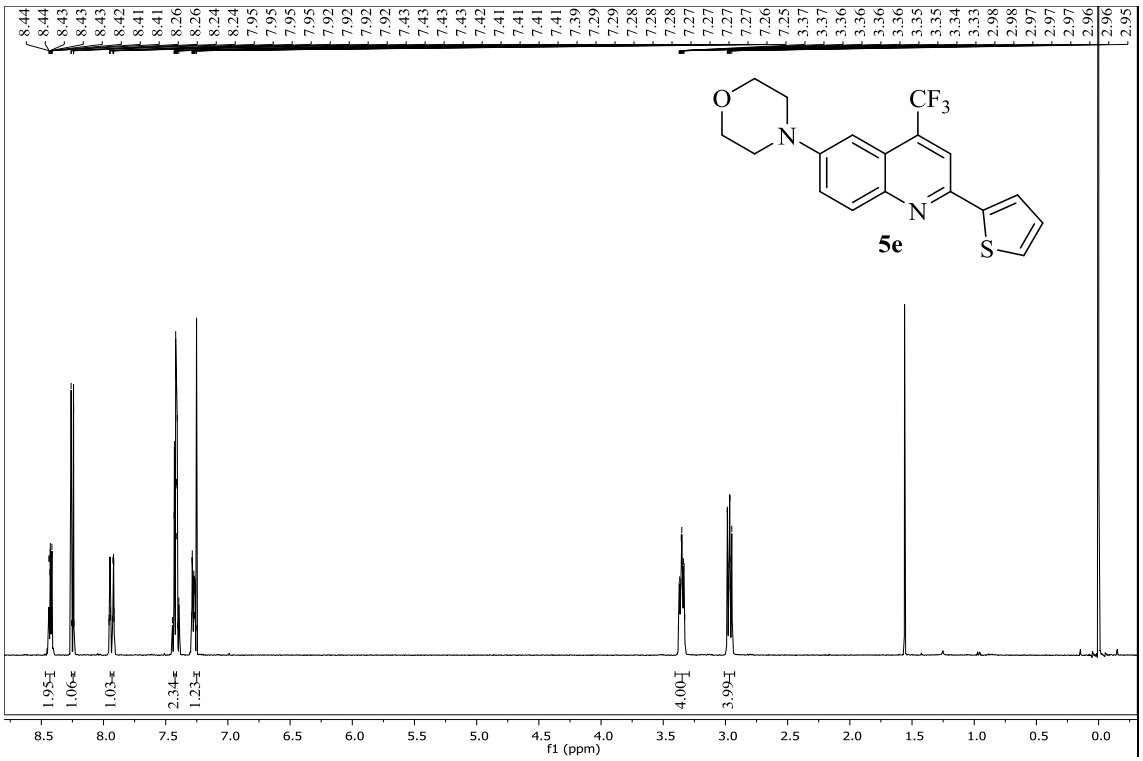


Figure 22. (a)^{1}H and (b)^{13}C NMR for compound **5d** in $CDCl_3$.

(a)



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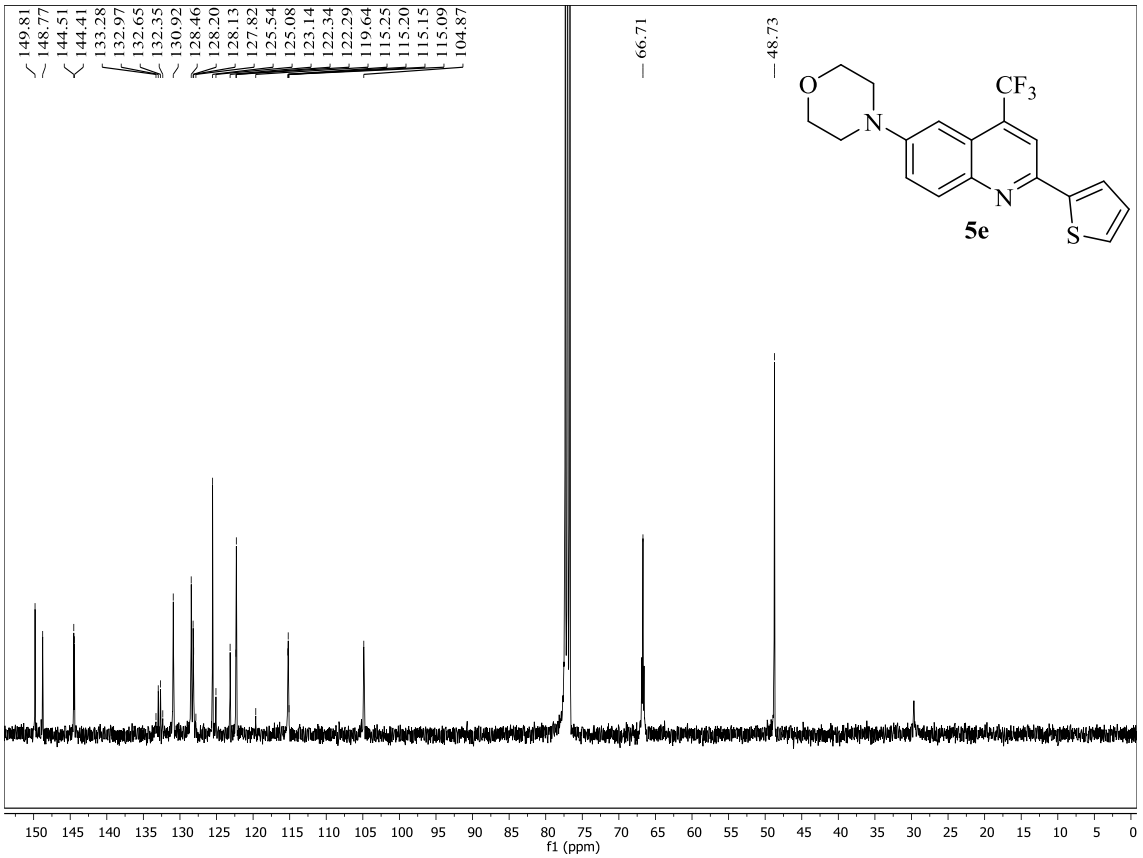
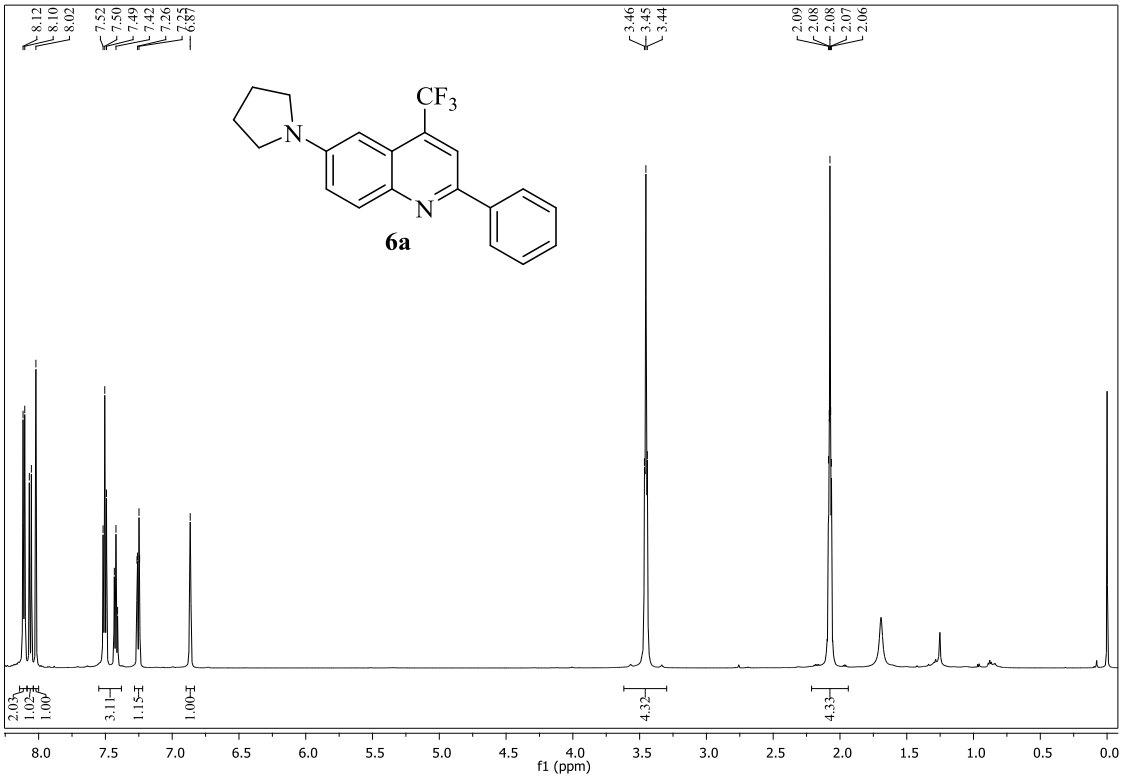


Figure 23. (a)^{1}H and (b)^{13}C NMR for compound **5e** in $CDCl_3$.

(a)



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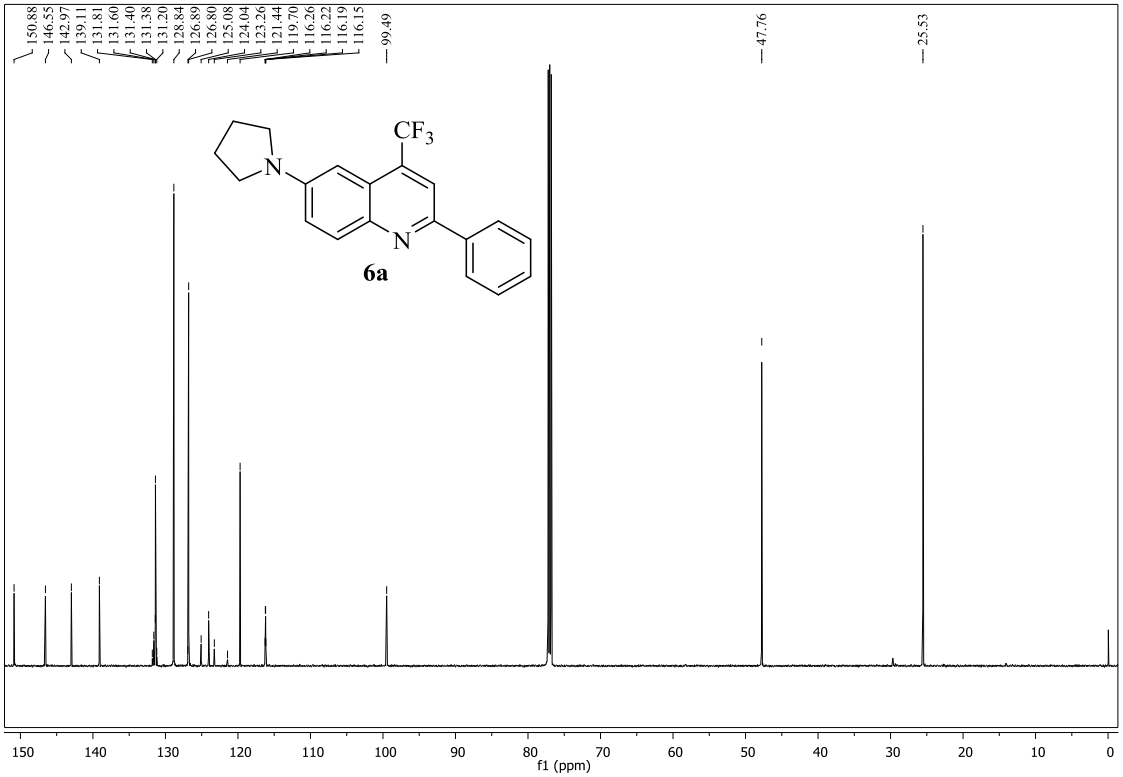


Figure 24. (a)^{1}H and (b)^{13}C NMR for compound **6a** in $CDCl_3$.

(a)

(b)

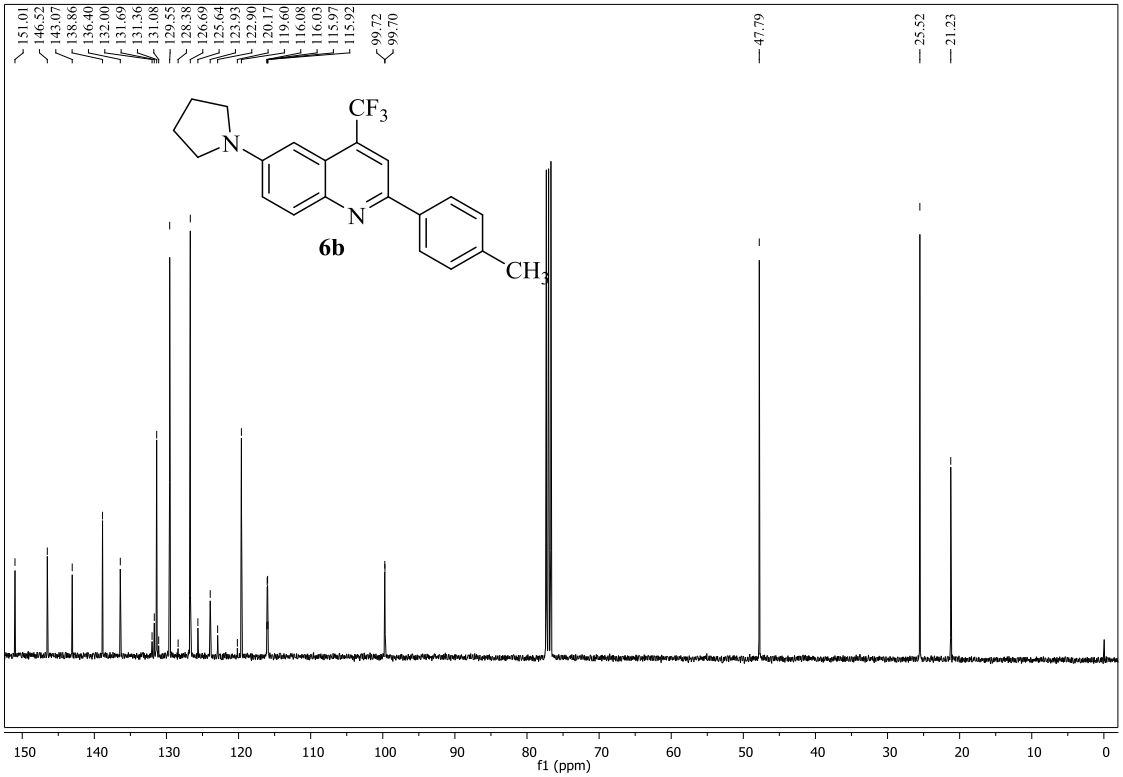
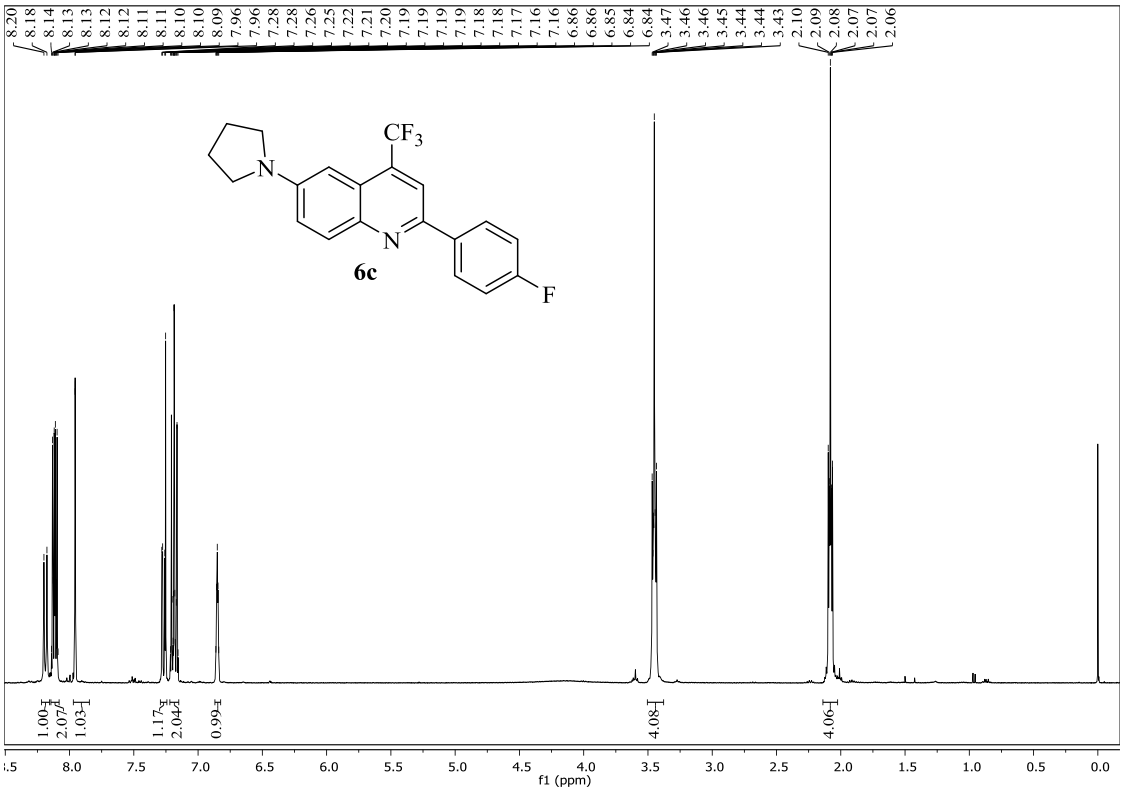


Figure 25. (a)^{1}H and (b)^{13}C NMR for compound **6b** in $CDCl_3$.

(a)



(b)

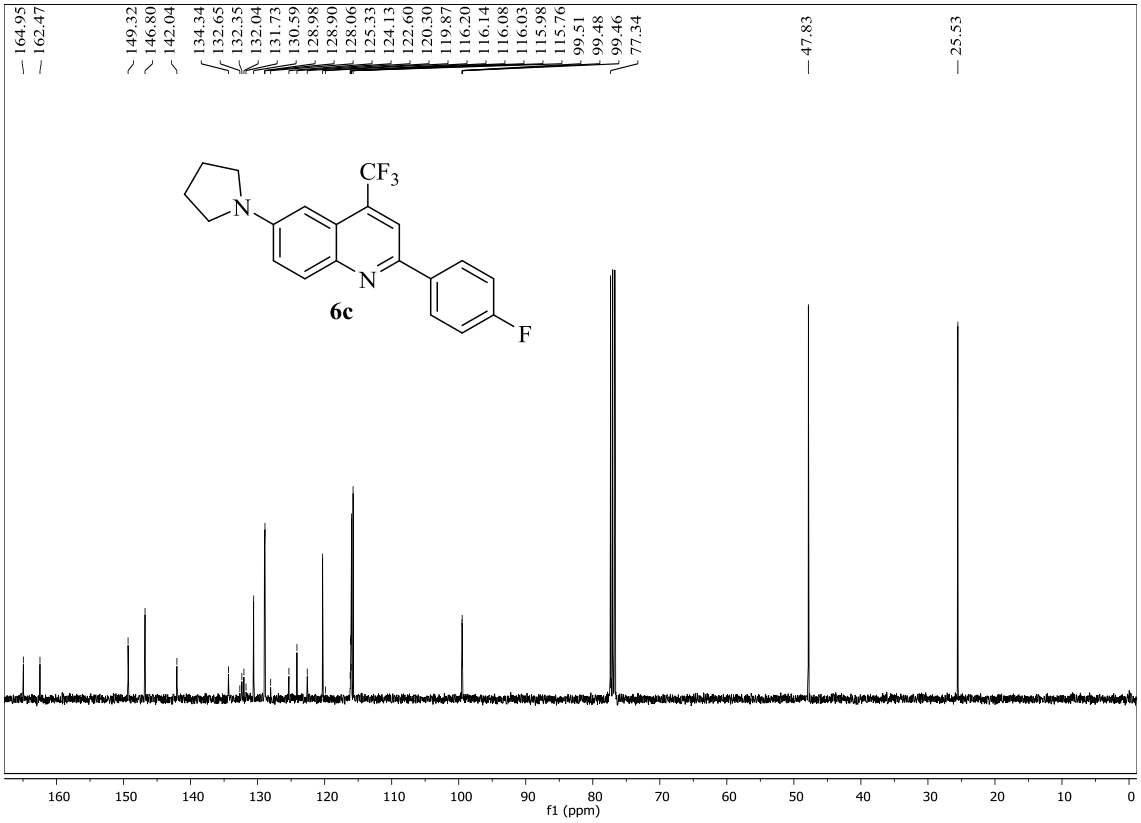
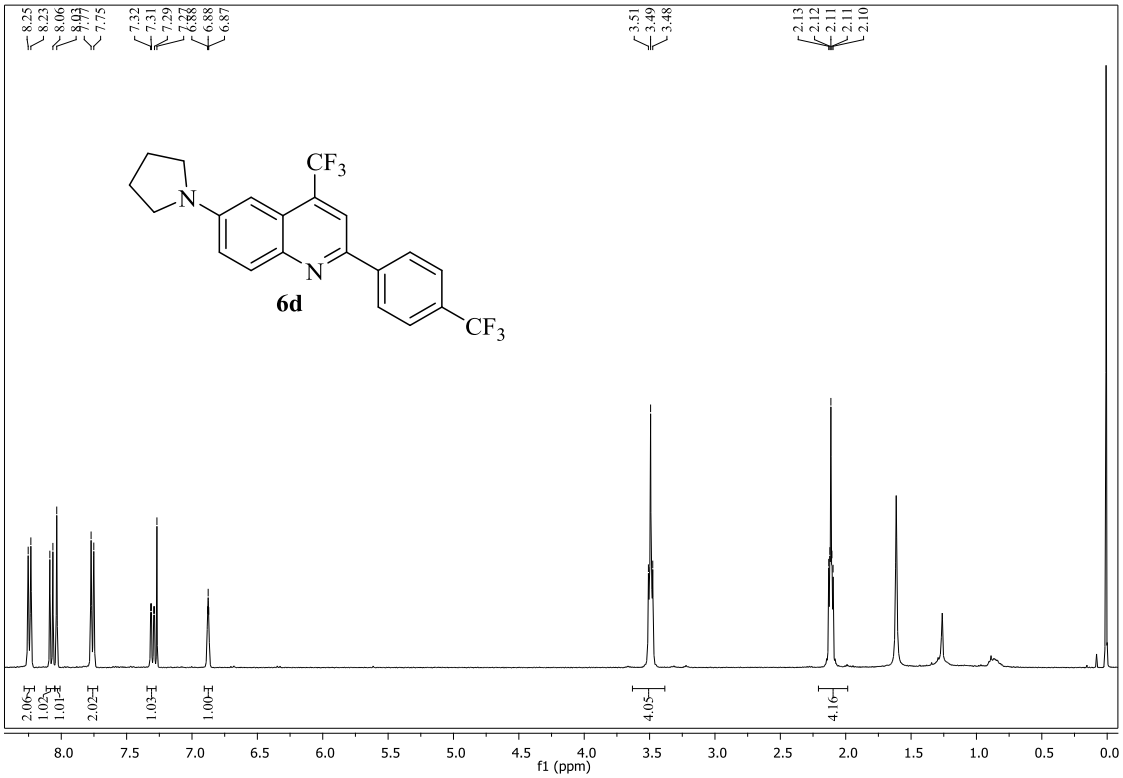


Figure 26. (a)^{1}H and (b)^{13}C NMR for compound **6c** in $CDCl_3$.

(a)



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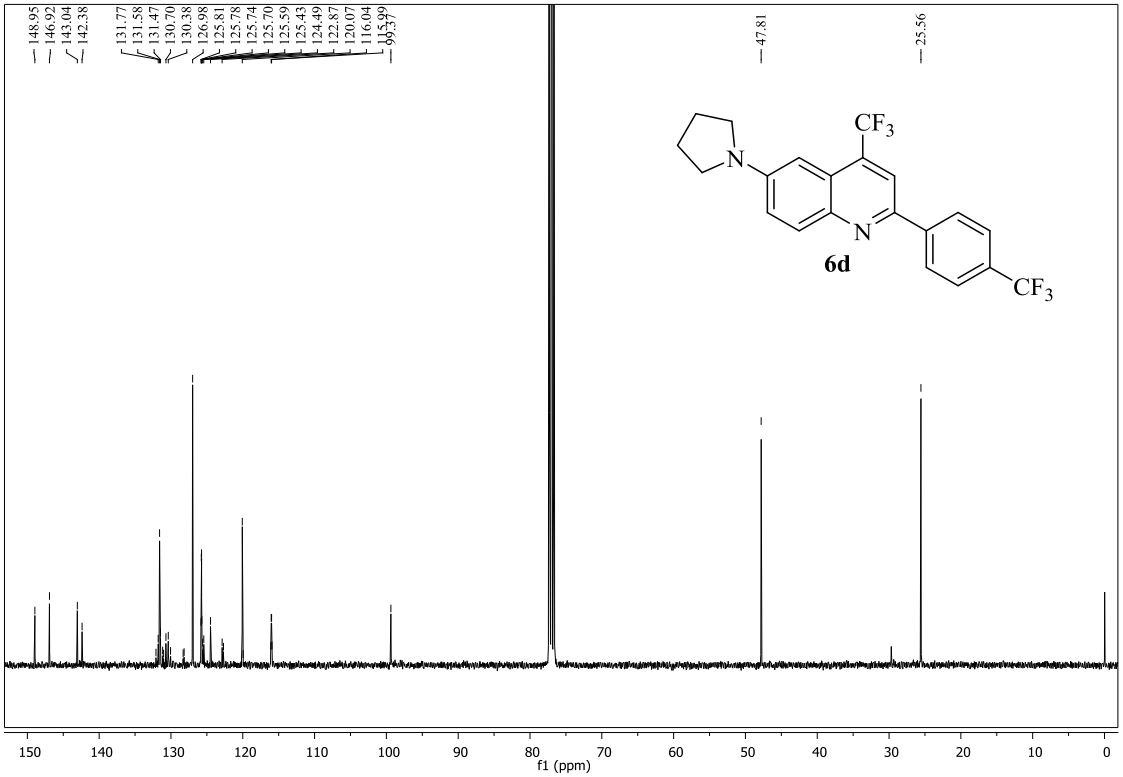
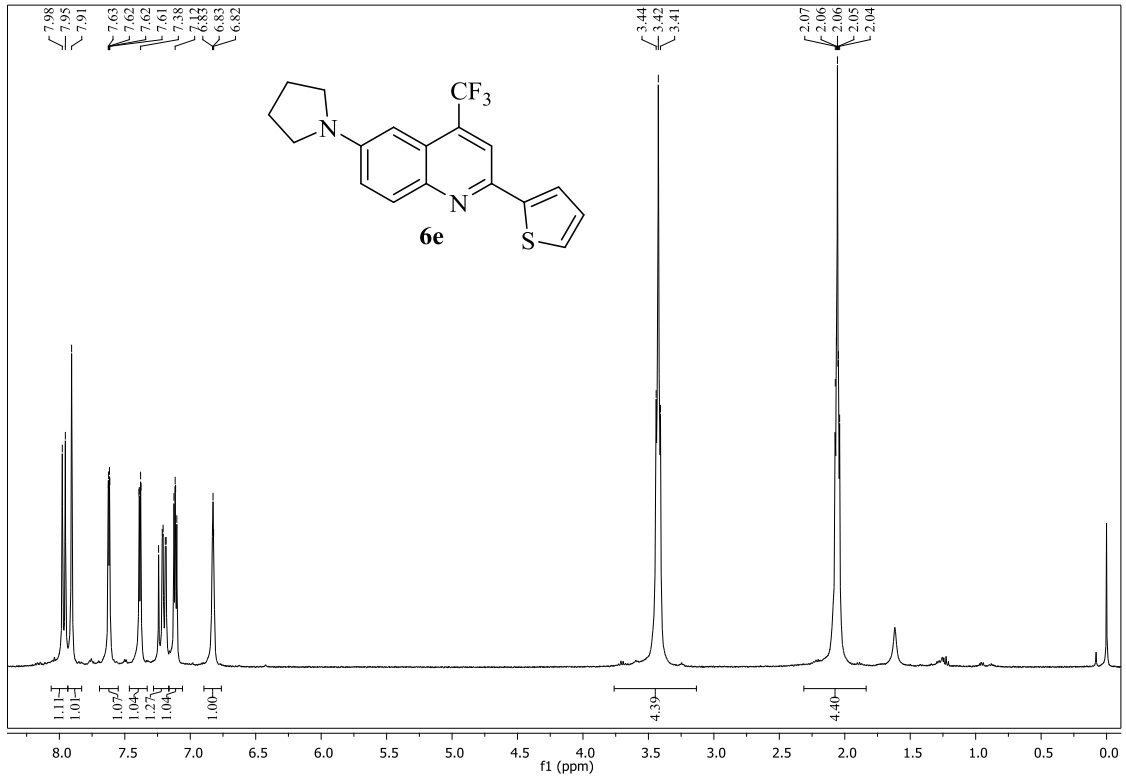


Figure 27. (a)^{1}H and (b)^{13}C NMR for compound **6d** in $CDCl_3$.

(a)



(b)

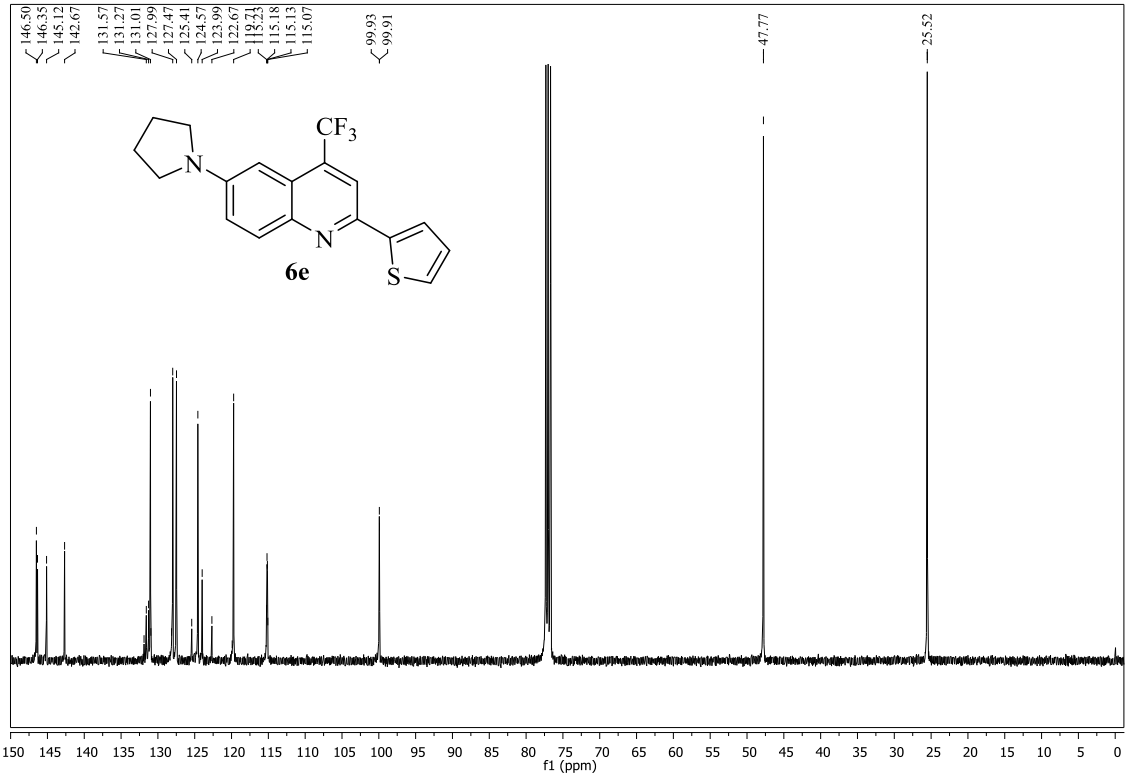
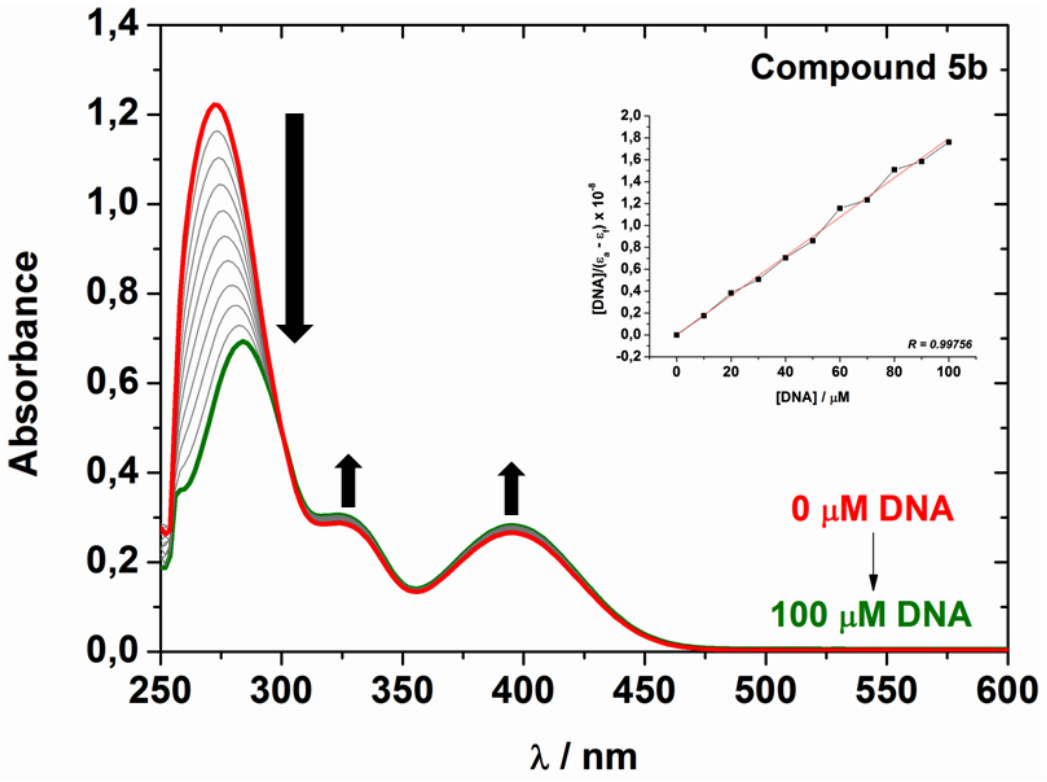


Figure 28.(a)^{1}H and (b)^{13}C NMR for compound **6e** in $CDCl_3$.

(a)



(b)

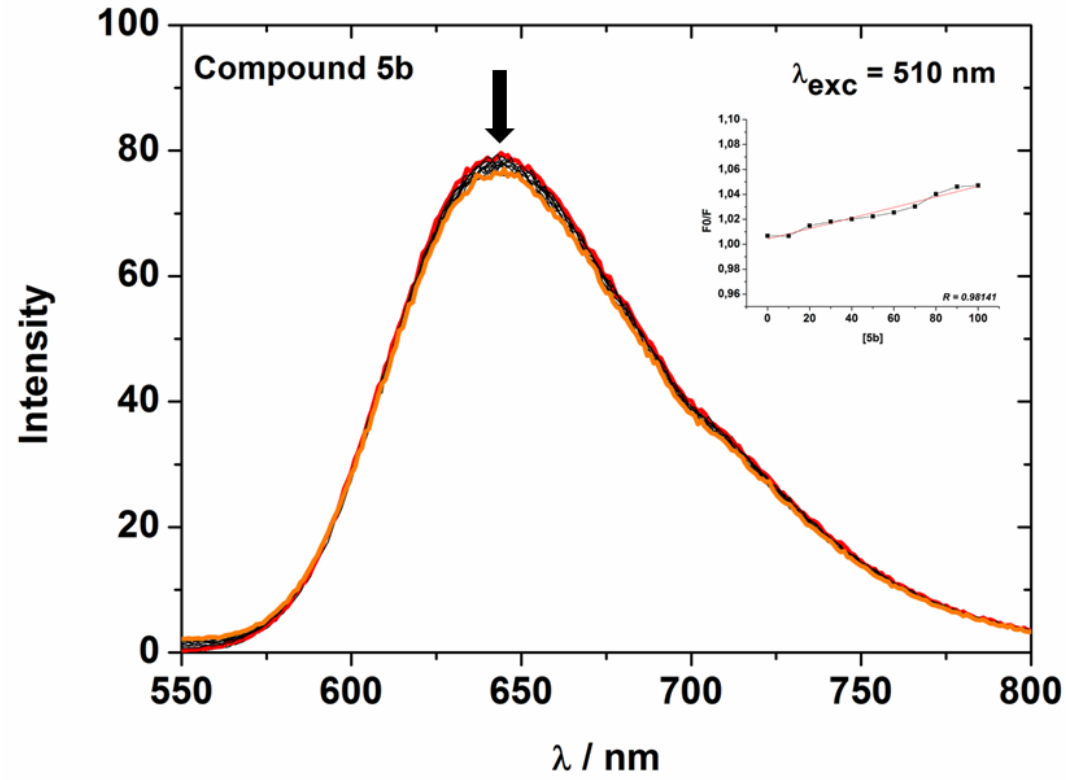
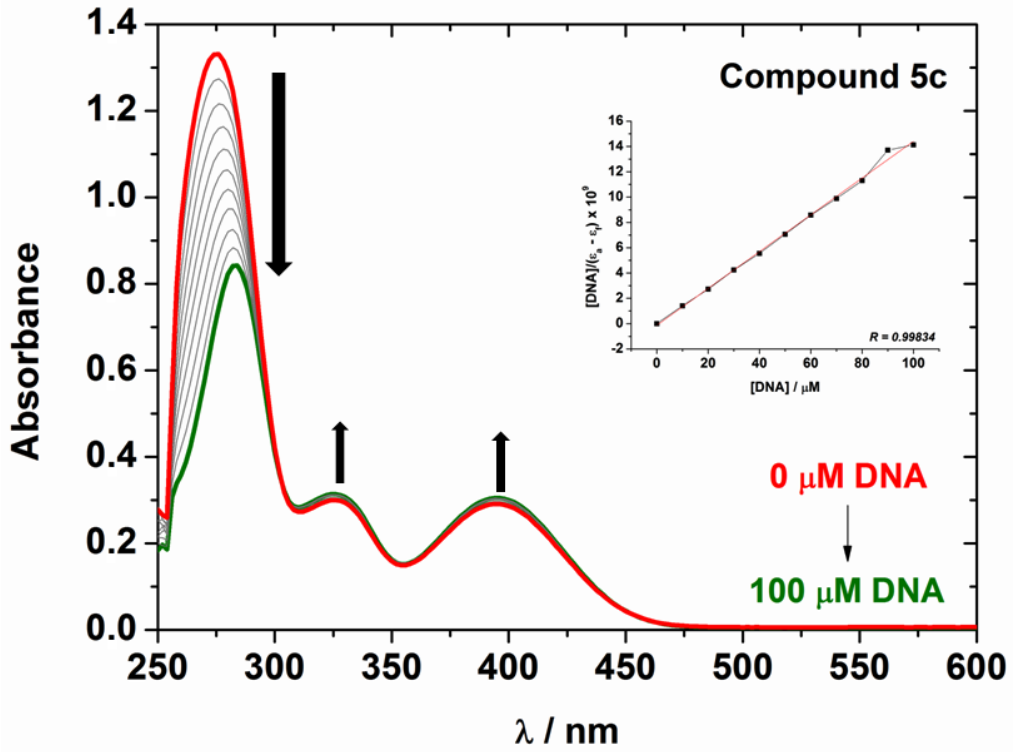


Figure 29. (a) UV-vis electronic absorption spectra and (b) Emission fluorescence spectra of EB-DNA for compound **5b.**

(a)



(b)

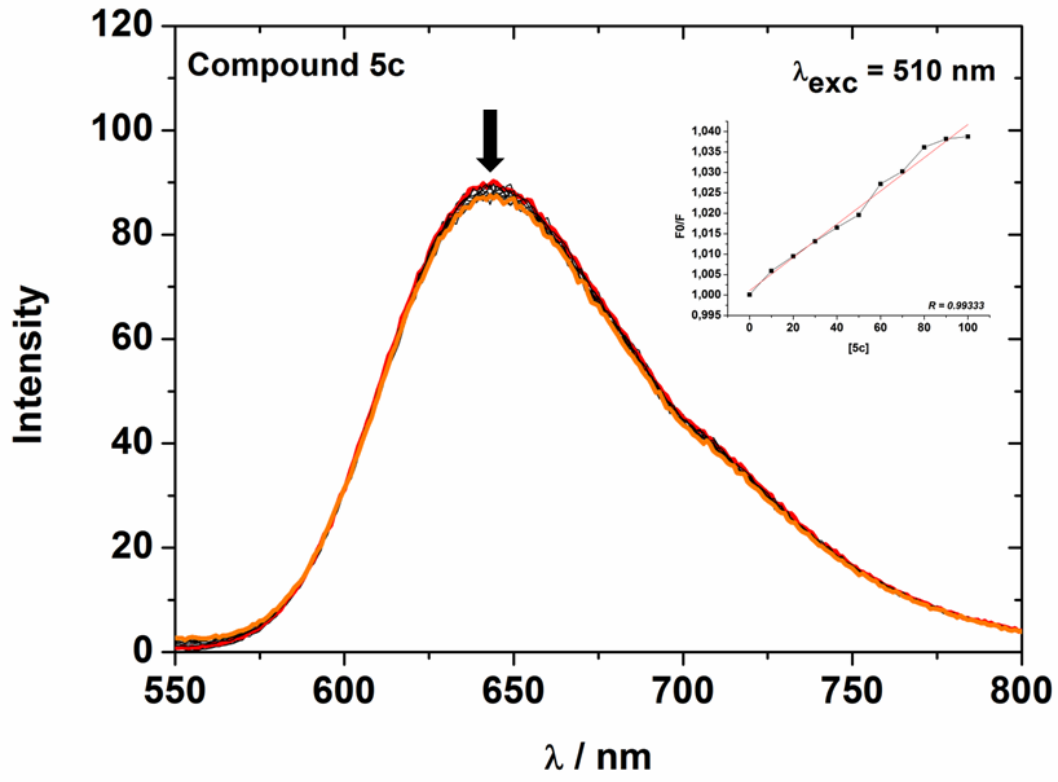
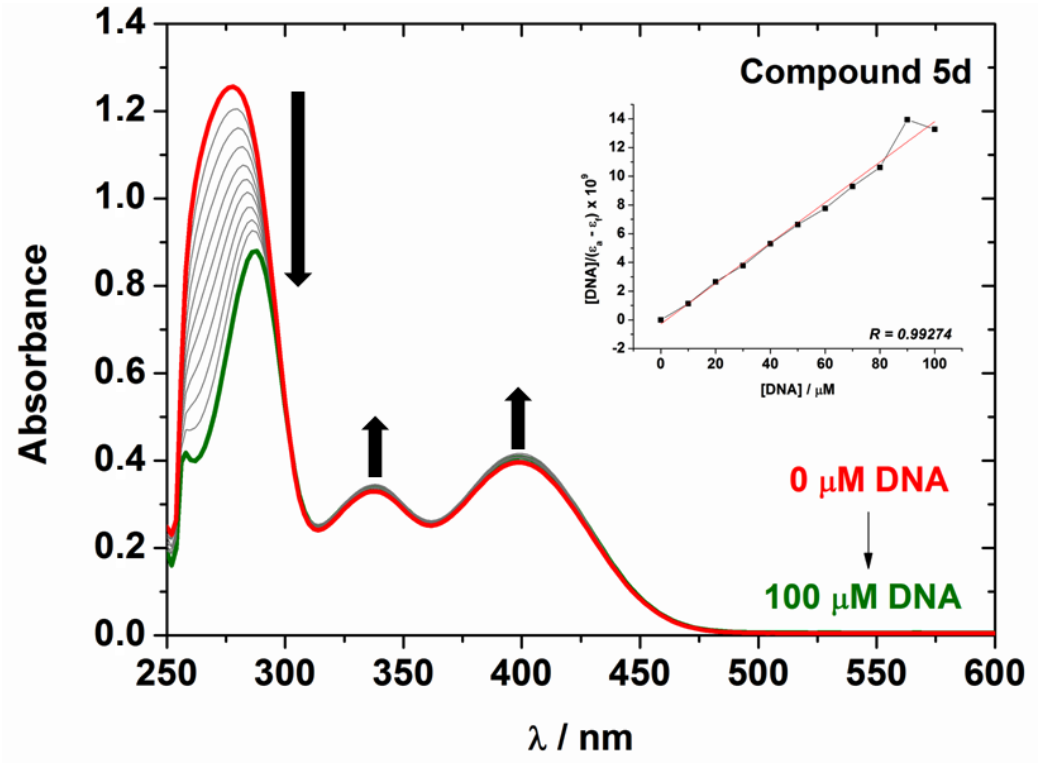


Figure 30. (a) UV-vis electronic absorption spectra and (b) Emission fluorescence spectra of EB-DNA for compound **5c.**

(a)



(b)

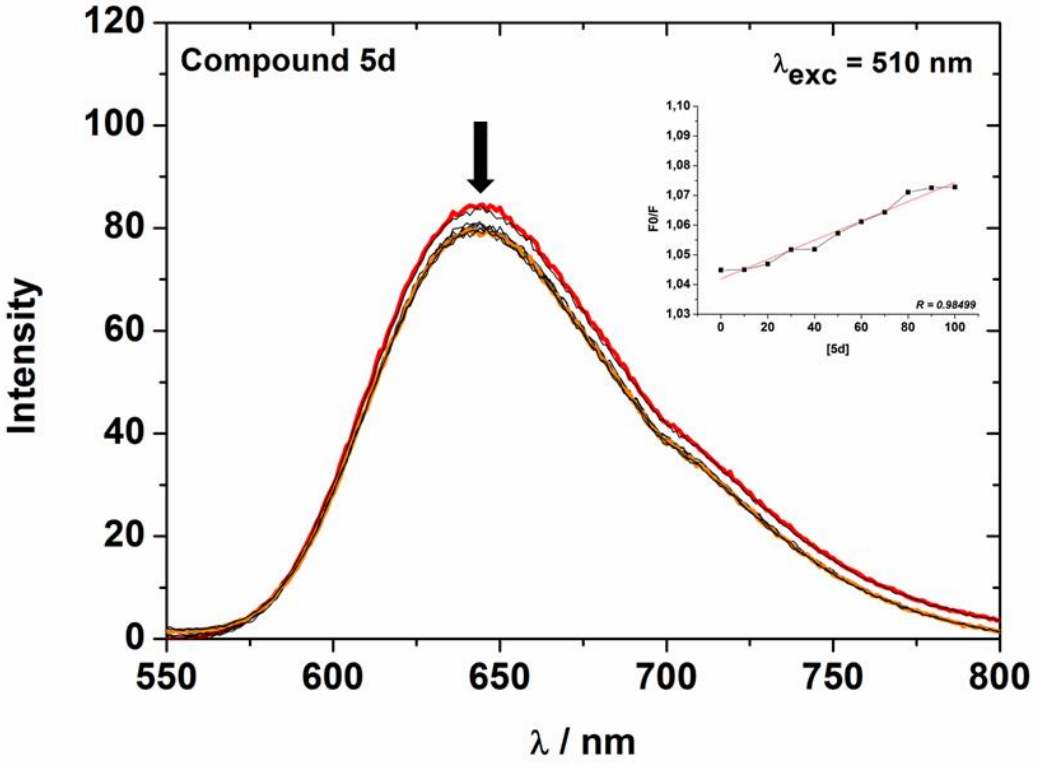
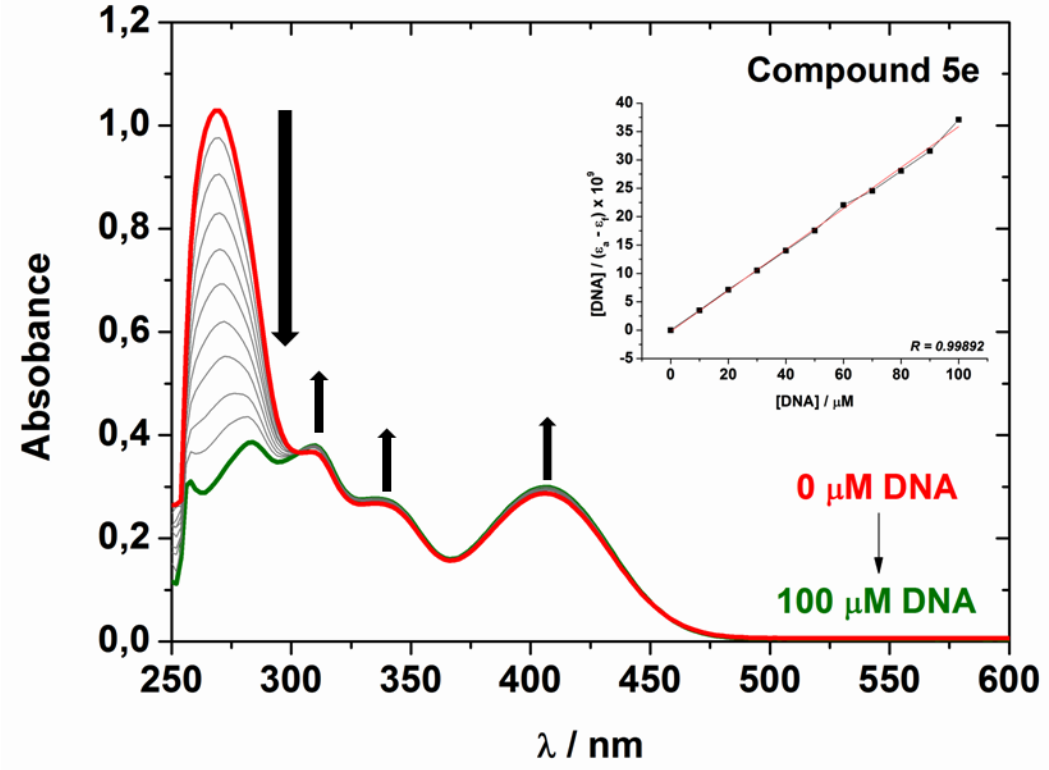


Figure 31. (a) UV-vis electronic absorption spectra and (b) Emission fluorescence spectra of EB-DNA for compound **5d.**

(a)



(b)

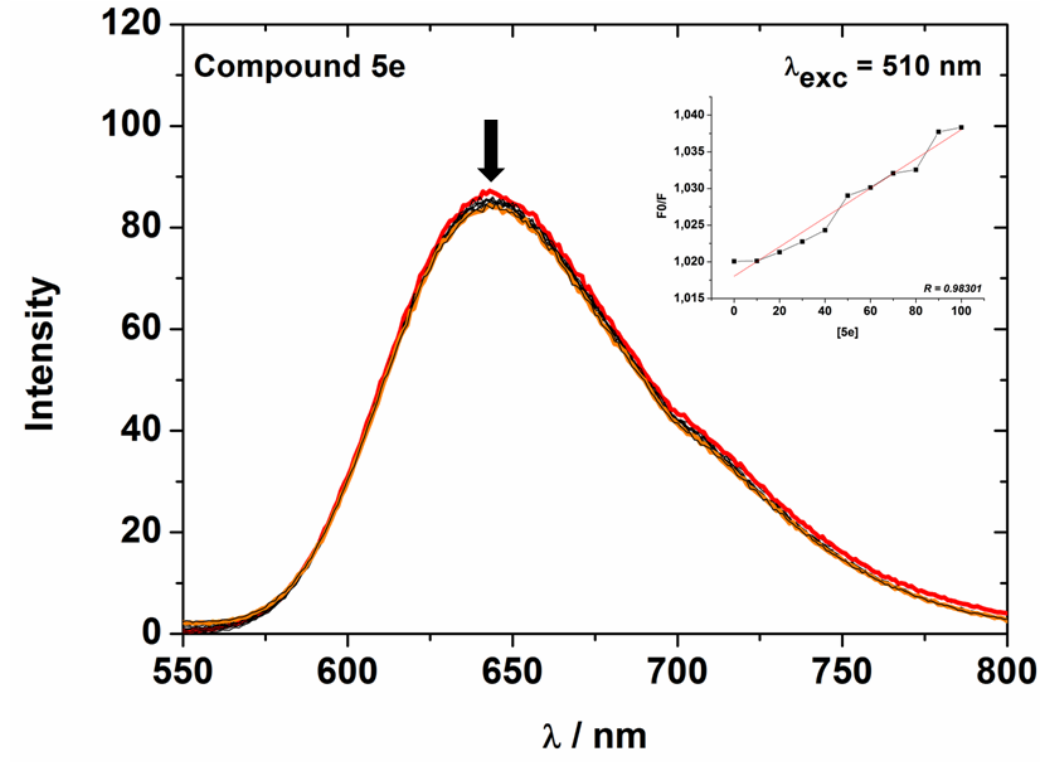
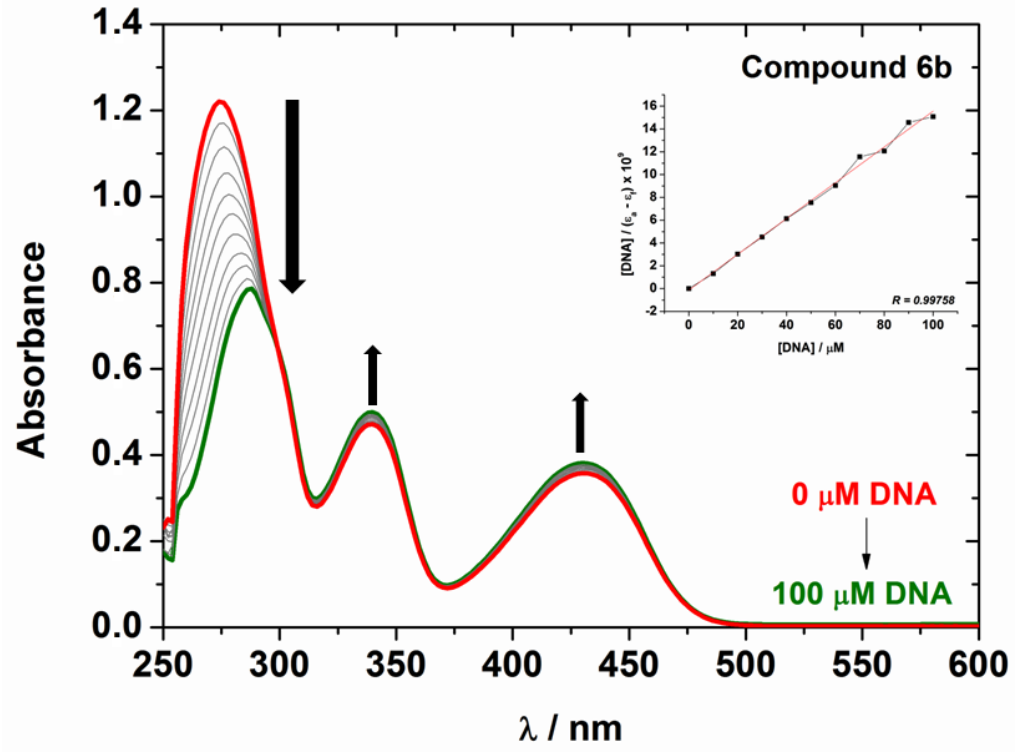


Figure 32. (a) UV-vis electronic absorption spectra and (b) Emission fluorescence spectra of EB-DNA for compound **5e.**

(a)



(b)

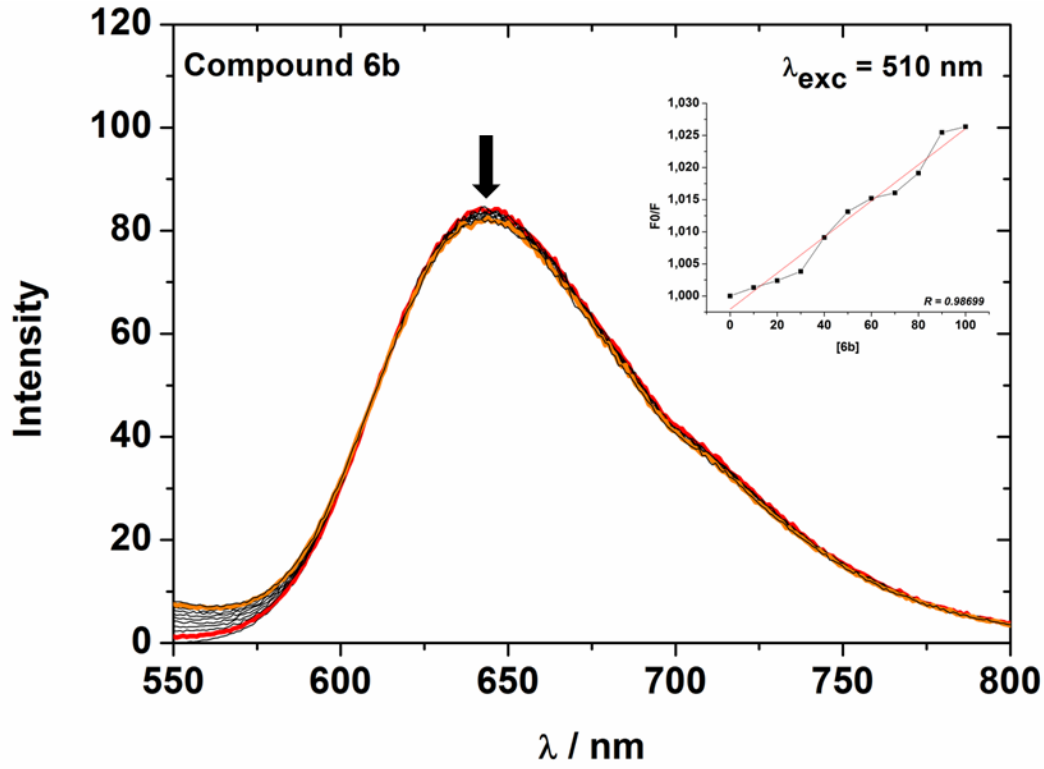
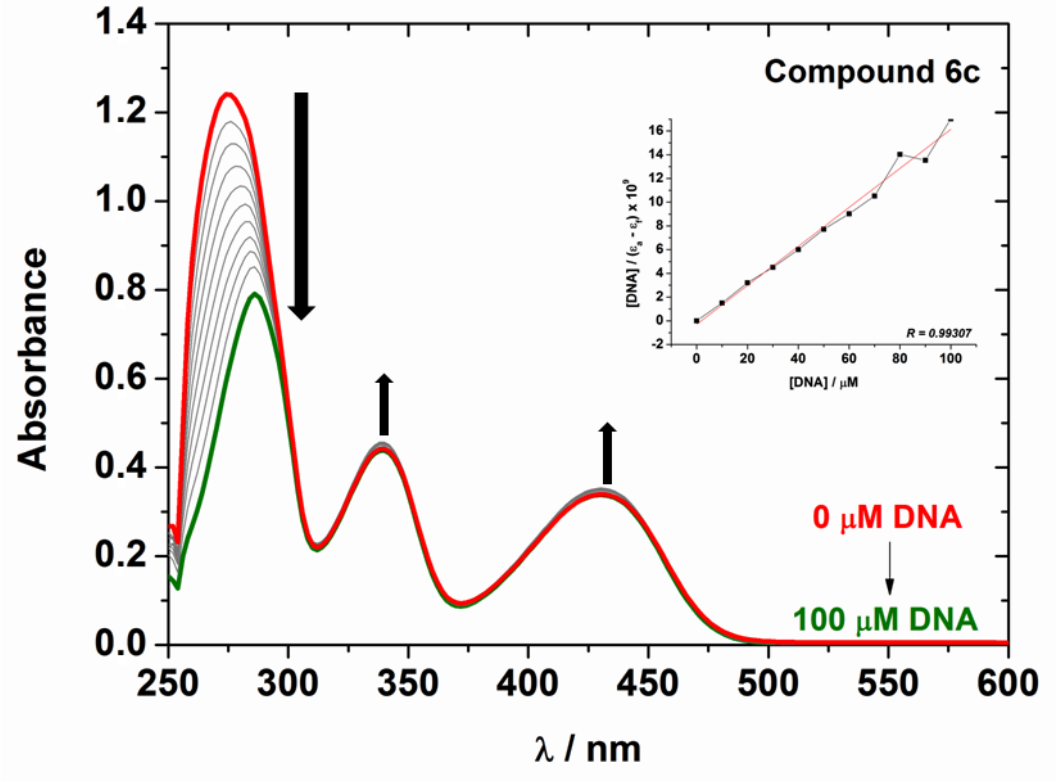


Figure 33. (a) UV-vis electronic absorption spectra and (b) Emission fluorescence spectra of EB-DNA for compound **6b.**

(a)



(b)

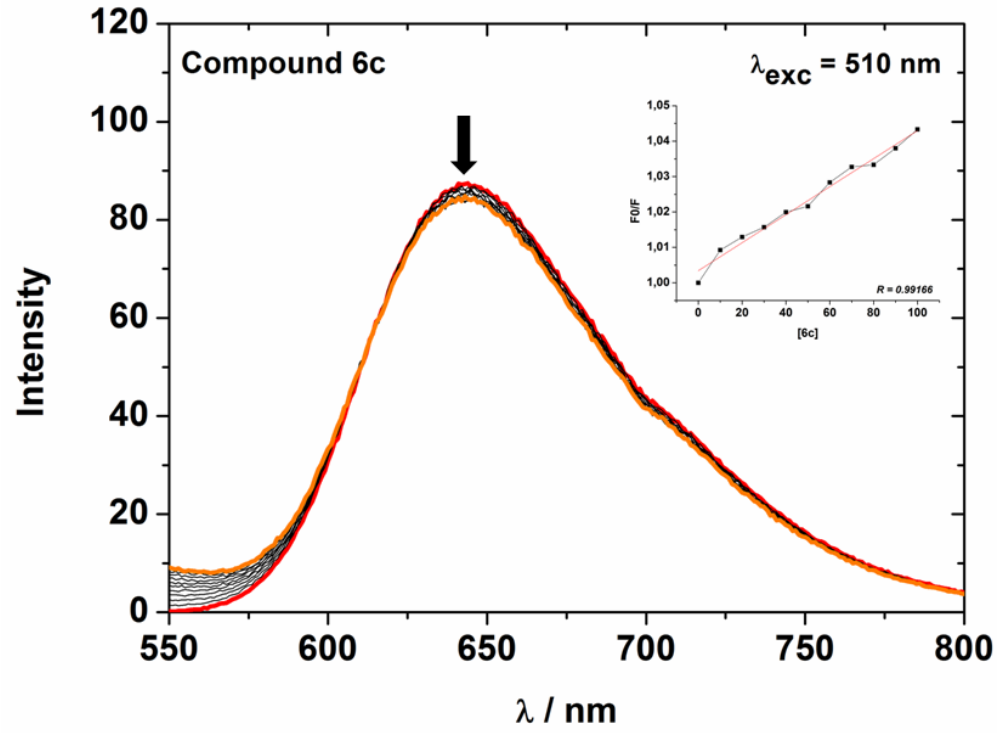
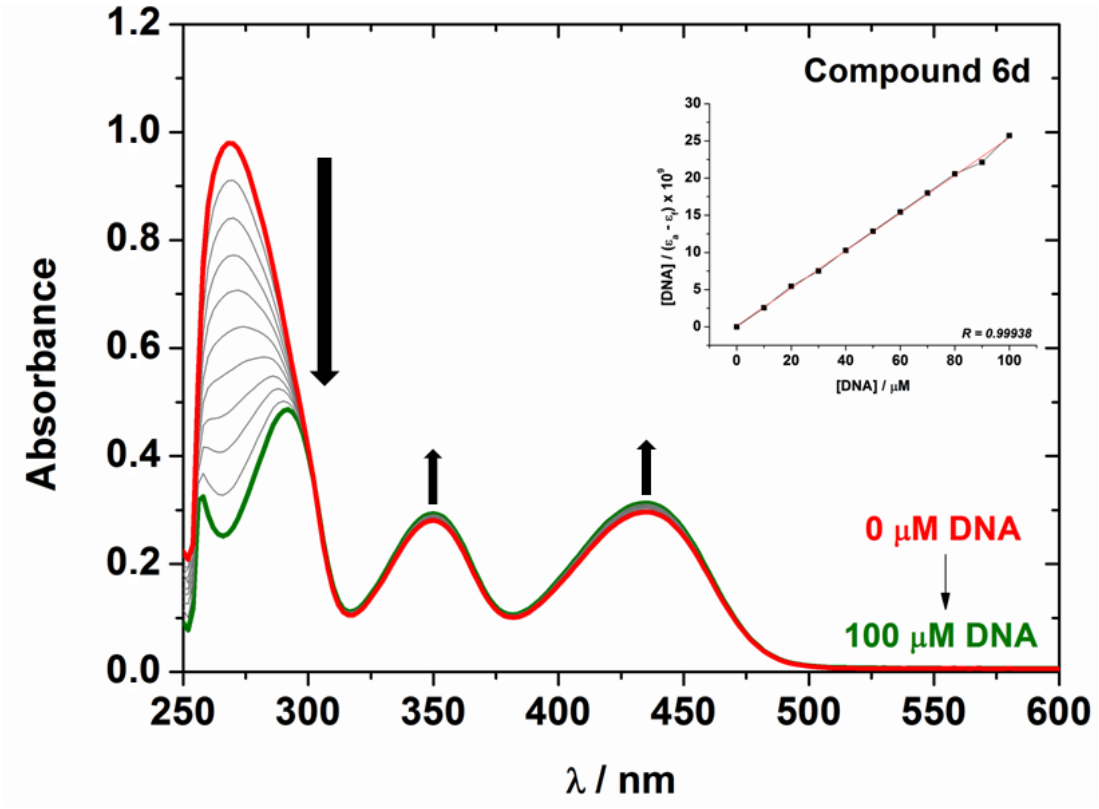


Figure 34. (a) UV-vis electronic absorption spectra and (b) Emission fluorescence spectra of EB-DNA for compound **6c.**

(a)



(b)

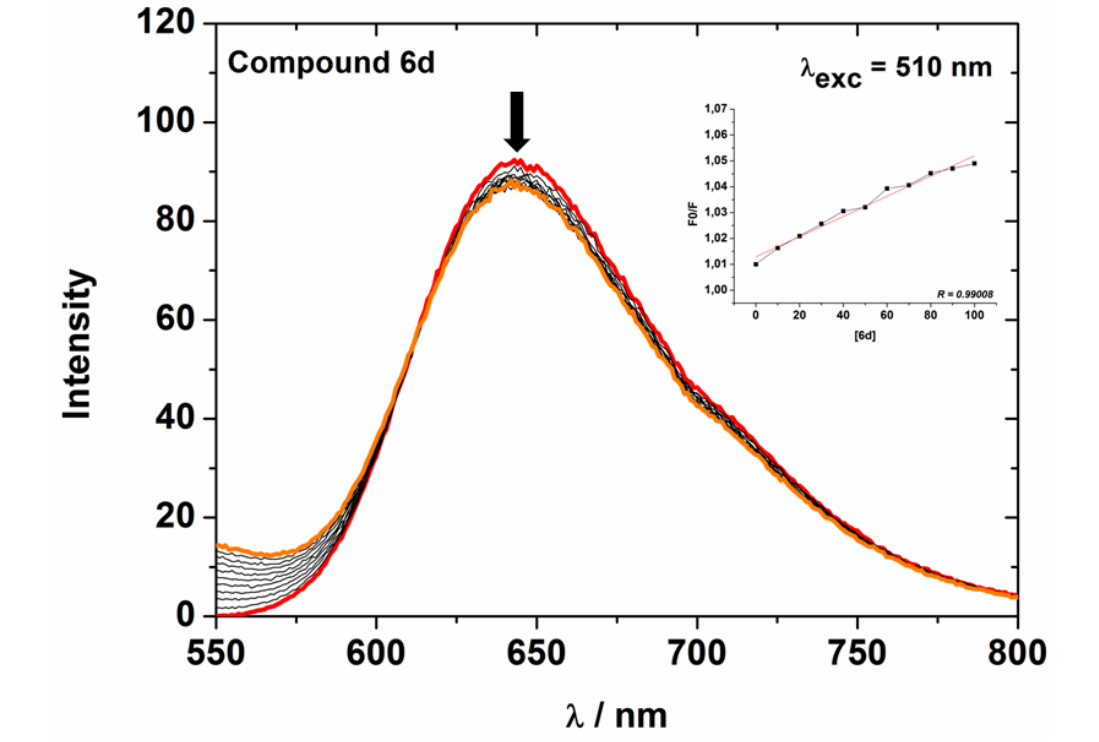
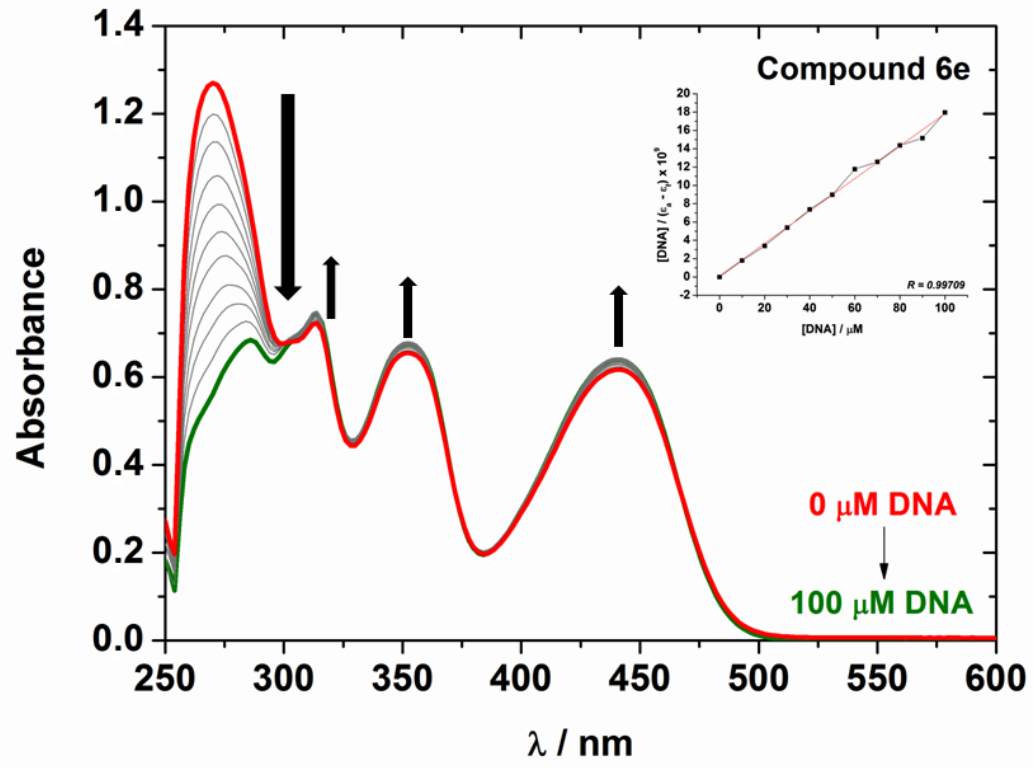


Figure 35. (a) UV-vis electronic absorption spectra and (b) Emission fluorescence spectra of EB-DNA for compound **6d.**

(a)



(b)

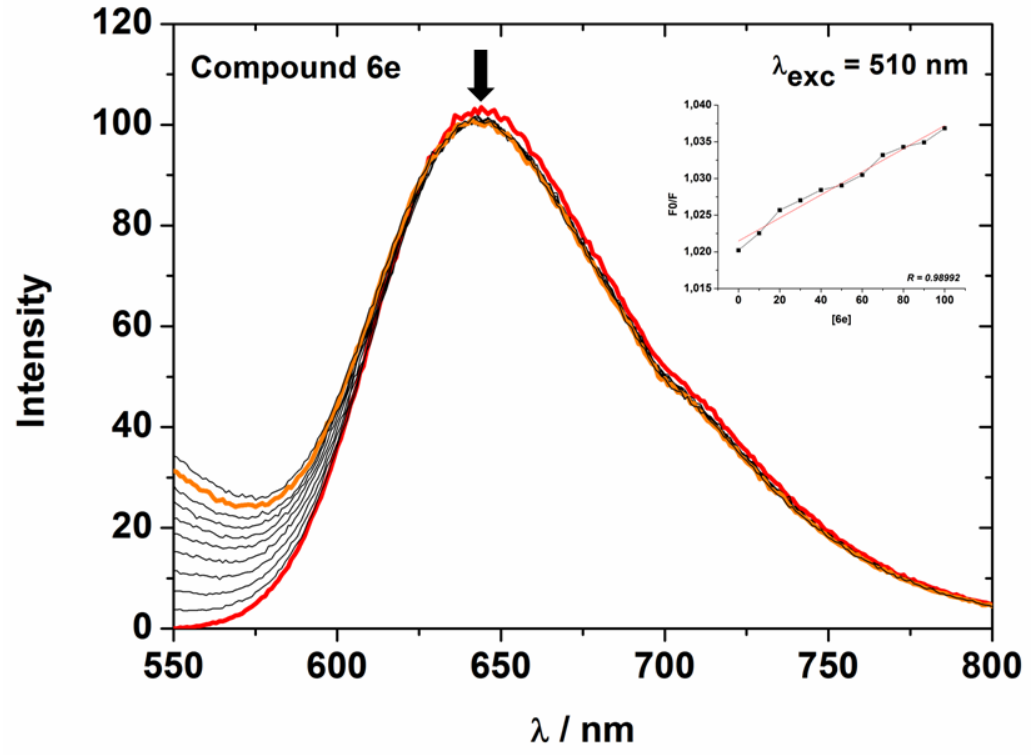


Figure 36. (a) UV-vis electronic absorption spectra and (b) Emission fluorescence spectra of EB-DNA for compound **6e.**

Crystallographic data of compound 6b.

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelx

```
Bond precision:  C-C = 0.0030 A          Wavelength=0.71073

Cell:              a=7.597(5)      b=10.743(5)      c=20.703(5)
                   alpha=90        beta=90          gamma=90
Temperature:       110 K

                Calculated                Reported
Volume          1689.7(14)                1689.7(14)
Space group     P 21 21 21                P 21 21 21
Hall group      P 2ac 2ab                 P 2ac 2ab
Moiety formula  C21 H19 F3 N2             C12 H19 F3 N2
Sum formula     C21 H19 F3 N2             C21 H19 F3 N2
Mr              356.38                    356.38
Dx,g cm-3       1.401                     1.401
Z               4                         4
Mu (mm-1)       0.106                     0.106
F000            744.0                     744.0
F000'           744.41
h,k,lmax        9,13,26                   9,13,26
Nref            3743[ 2156]               3738
Tmin,Tmax       0.983,0.994               0.724,0.746
Tmin'           0.983

Correction method= # Reported T Limits: Tmin=0.724 Tmax=0.746
AbsCorr = GAUSSIAN

Data completeness= 1.73/1.00      Theta(max)= 27.149

R(reflections)= 0.0355( 3385)     wR2(reflections)= 0.0883( 3738)

S = 1.058                 Npar= 235
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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

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ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as gaussian
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
            C21 H19 F3 N2
```

Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C21 H19 F3 N2
           Atom count from _chemical_formula_moiety:C12 H19 F3 N2
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT153_ALERT_1_G The s.u.'s on the Cell Axes   are Equal ..(Note)      0.005 Ang.
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C27 Check
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   4 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_ABSTY02_shelx
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_PLAT790_shelx
;
PROBLEM: Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
RESPONSE: ...
;
# end Validation Reply Form
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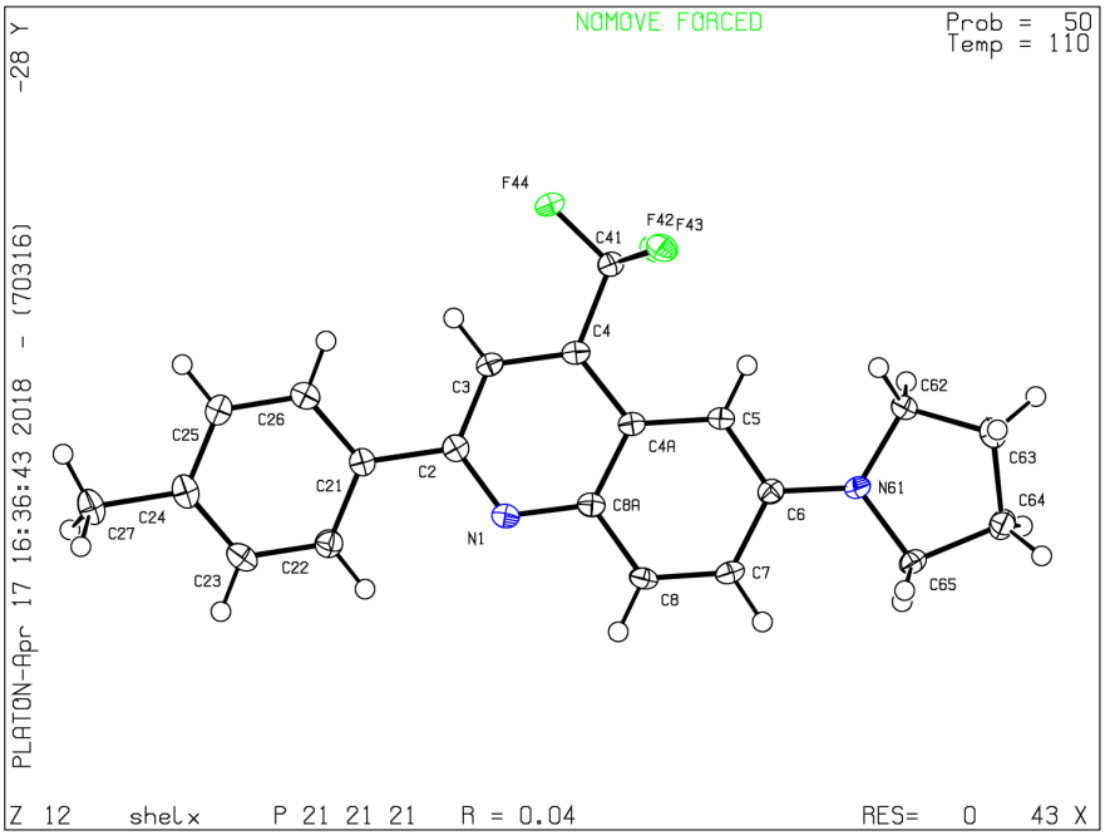
NOMOVE FORCED
Prob = 50
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-28 Y
PLATON-Apr 17 16:36:43 2018 - (70316)
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F43
C41
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C3
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C4A
C62
C63
C64
C65
N61
C6
C8A
N1
C2
C21
C25
C26
C24
C27
C22
C23
C7
C8
Z 12 shelx P 21 21 21 R = 0.04 RES= 0 43 X

Table 1. Crystal data and structure refinement for 6-fluoro-7-(phenylethynyl)-4-(trifluoromethyl)-2-(4-(trifluoromethyl)phenyl)quinoline (**6b**)

Empirical Formula	$C_{21}H_{19}F_3N_2$
Fromula Weight	356.38
Temperature	110 K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P 21 21 21
Unit cell dimensions	a = 7.597(5) A alpha = 90.000 deg. b = 10.743(5) A beta = 90.000 deg. c = 20.703(5) A gamma = 90.000 deg.
Volume	1689.7(14) A^3
z, calculated density	4, 1.401 Mg/m^3
Absorption coeficiente	0.106 mm^{-1}
F(000)	744
Crystal size	0.157 x 0.134 x 0.055 mm
Theta range for data collection	2.73 to 27.15 deg.
Limiting indices	-9<=h<=9, -13<=k<=13, -26<=l<=26
Reflections collected/unique	57067 / 3738 [R(int) = 0.0428]
Completeness to theta = 27.15	99.8 %
Absorption correction	Gaussian
Max. and min. transmission	0.7455 and 0.7241
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3738 / 0 / 235
Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R1 = 0.0355, wR2 = 0.0850
R índices (all data)	R1 = 0.0424, wR2 = 0.0883
Absolute structure parameter	0.7(6)
Extinction coeficiente	None
Largest diff. peak and hole	0.264 and -0.248 $e.A^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6b**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
F(43)	13422(1)	-2806(1)	741(1)	28(1)
F(42)	14655(1)	-1596(1)	43(1)	26(1)
F(44)	16215(1)	-2919(1)	569(1)	27(1)
N(1)	15916(2)	602(1)	2101(1)	16(1)
N(61)	9679(2)	1086(1)	718(1)	18(1)
C(21)	18669(2)	-368(1)	2382(1)	16(1)
C(6)	11225(2)	935(2)	1043(1)	15(1)
C(5)	12359(2)	-49(2)	909(1)	15(1)
C(2)	17029(2)	-321(2)	1990(1)	16(1)
C(3)	16682(2)	-1237(2)	1513(1)	16(1)
C(65)	8478(2)	2128(2)	820(1)	18(1)
C(26)	20087(2)	-1128(2)	2212(1)	18(1)
C(4A)	13946(2)	-191(1)	1253(1)	14(1)
C(62)	9153(2)	296(2)	178(1)	18(1)
C(8A)	14408(2)	668(2)	1747(1)	15(1)
C(7)	11697(2)	1797(2)	1540(1)	17(1)
C(8)	13226(2)	1661(2)	1876(1)	17(1)
C(24)	21810(2)	-380(2)	3112(1)	20(1)
C(25)	21618(2)	-1140(2)	2572(1)	19(1)
C(41)	14870(2)	-2114(2)	631(1)	19(1)
C(22)	18842(2)	372(2)	2936(1)	20(1)
C(4)	15182(2)	-1170(1)	1149(1)	15(1)
C(23)	20384(2)	352(2)	3291(1)	22(1)
C(27)	23521(2)	-357(2)	3482(1)	25(1)
C(64)	6946(2)	1856(2)	362(1)	22(1)
C(63)	7755(2)	1056(2)	-170(1)	24(1)

Table 3. Bond lengths [A] and angles [º] for **6b**.

F(43)-C(41)	1.347(2)
F(42)-C(41)	1.3476(19)
F(44)-C(41)	1.344(2)
N(1)-C(2)	1.323(2)
N(1)-C(8A)	1.361(2)
N(61)-C(6)	1.364(2)
N(61)-C(62)	1.458(2)
N(61)-C(65)	1.459(2)
C(21)-C(26)	1.396(2)
C(21)-C(22)	1.402(2)
C(21)-C(2)	1.487(2)
C(6)-C(5)	1.391(2)
C(6)-C(7)	1.429(2)
C(5)-C(4A)	1.409(2)
C(2)-C(3)	1.420(2)
C(3)-C(4)	1.368(2)
C(65)-C(64)	1.530(2)
C(26)-C(25)	1.381(2)
C(4A)-C(8A)	1.423(2)
C(4A)-C(4)	1.425(2)
C(62)-C(63)	1.522(2)
C(8A)-C(8)	1.419(2)
C(7)-C(8)	1.362(3)
C(24)-C(23)	1.389(3)
C(24)-C(25)	1.392(2)
C(24)-C(27)	1.509(2)
C(41)-C(4)	1.496(2)
C(22)-C(23)	1.383(2)
C(64)-C(63)	1.526(2)
C(2)-N(1)-C(8A)	118.89(14)
C(6)-N(61)-C(62)	123.01(13)

Table 3. Bond lengths [A] and angles [º] for **6b** (continued).

C(6)-N(61)-C(65)	123.87(14)
C(62)-N(61)-C(65)	112.77(13)
C(26)-C(21)-C(22)	117.68(15)
C(26)-C(21)-C(2)	121.96(14)
C(22)-C(21)-C(2)	120.35(15)
N(61)-C(6)-C(5)	121.65(15)
N(61)-C(6)-C(7)	119.63(15)
C(5)-C(6)-C(7)	118.72(15)
C(6)-C(5)-C(4A)	120.78(15)
N(1)-C(2)-C(3)	121.46(15)
N(1)-C(2)-C(21)	117.80(14)
C(3)-C(2)-C(21)	120.74(14)
C(4)-C(3)-C(2)	120.07(15)
N(61)-C(65)-C(64)	103.78(13)
C(25)-C(26)-C(21)	121.33(15)
C(5)-C(4A)-C(8A)	120.28(14)
C(5)-C(4A)-C(4)	124.61(14)
C(8A)-C(4A)-C(4)	115.11(14)
N(61)-C(62)-C(63)	103.97(13)
N(1)-C(8A)-C(8)	118.09(15)
N(1)-C(8A)-C(4A)	124.12(15)
C(8)-C(8A)-C(4A)	117.79(15)
C(8)-C(7)-C(6)	120.76(15)
C(7)-C(8)-C(8A)	121.68(15)
C(23)-C(24)-C(25)	117.70(16)
C(23)-C(24)-C(27)	121.78(16)
C(25)-C(24)-C(27)	120.51(16)
C(26)-C(25)-C(24)	121.02(16)
F(44)-C(41)-F(43)	106.35(13)
F(44)-C(41)-F(42)	105.79(13)
F(43)-C(41)-F(42)	106.33(13)

Table 3. Bond lengths [A] and angles [º] for **6b** (continued).

F(44)-C(41)-C(4)	112.61(14)
F(43)-C(41)-C(4)	112.47(13)
F(42)-C(41)-C(4)	112.75(13)
C(23)-C(22)-C(21)	120.39(16)
C(3)-C(4)-C(4A)	120.33(14)
C(3)-C(4)-C(41)	119.39(14)
C(4A)-C(4)-C(41)	120.26(14)
C(22)-C(23)-C(24)	121.81(16)
C(63)-C(64)-C(65)	104.45(14)
C(62)-C(63)-C(64)	103.93(14)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **6b.**

	U11	U22	U33	U23	U13	U12
F(43)	25(1)	21(1)	37(1)	-9(1)	0(1)	-6(1)
F(42)	31(1)	31(1)	16(1)	-6(1)	-2(1)	5(1)
F(44)	24(1)	23(1)	34(1)	-12(1)	-5(1)	9(1)
N(1)	18(1)	15(1)	14(1)	0(1)	2(1)	-2(1)
N(61)	18(1)	18(1)	18(1)	-4(1)	0(1)	5(1)
C(21)	16(1)	15(1)	15(1)	4(1)	1(1)	-3(1)
C(6)	16(1)	17(1)	13(1)	1(1)	3(1)	1(1)
C(5)	17(1)	14(1)	15(1)	-2(1)	2(1)	-1(1)
C(2)	17(1)	15(1)	15(1)	3(1)	2(1)	-2(1)
C(3)	17(1)	14(1)	18(1)	-1(1)	2(1)	1(1)
C(65)	18(1)	17(1)	19(1)	-2(1)	2(1)	4(1)
C(26)	21(1)	18(1)	16(1)	1(1)	2(1)	-3(1)
C(4A)	17(1)	13(1)	12(1)	2(1)	4(1)	-1(1)
C(62)	18(1)	18(1)	17(1)	-3(1)	-1(1)	0(1)
C(8A)	19(1)	15(1)	12(1)	1(1)	3(1)	-1(1)
C(7)	20(1)	14(1)	18(1)	-1(1)	4(1)	4(1)
C(8)	23(1)	15(1)	14(1)	-3(1)	0(1)	0(1)
C(24)	20(1)	20(1)	18(1)	8(1)	-2(1)	-6(1)
C(25)	17(1)	19(1)	21(1)	4(1)	1(1)	0(1)
C(41)	17(1)	18(1)	21(1)	-4(1)	-1(1)	2(1)
C(22)	20(1)	19(1)	20(1)	1(1)	0(1)	0(1)
C(4)	18(1)	13(1)	15(1)	0(1)	4(1)	-1(1)
C(23)	27(1)	20(1)	17(1)	-1(1)	-2(1)	-5(1)
C(27)	23(1)	28(1)	25(1)	2(1)	-6(1)	-6(1)
C(64)	18(1)	22(1)	26(1)	1(1)	-1(1)	2(1)
C(63)	21(1)	26(1)	24(1)	-3(1)	-5(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x10^3) for **6b.**

	x	y	z	U(eq)
H(5)	12066	-618	588	18
H(3)	17476	-1883	1447	20
H(65A)	9039	2913	713	22
H(65B)	8080	2158	1265	22
H(26)	19998	-1636	1850	22
H(62A)	8673	-487	332	21
H(62B)	10144	125	-103	21
H(7)	10951	2459	1635	21
H(8)	13503	2233	2197	21
H(25)	22535	-1664	2451	23
H(22)	17915	879	3065	24
H(23)	20468	842	3660	26
H(27A)	24340	-923	3286	38
H(27B)	23311	-603	3921	38
H(27C)	24000	470	3474	38
H(64A)	6015	1409	583	26
H(64B)	6468	2621	185	26
H(63A)	6876	519	-365	28
H(63B)	8278	1571	-504	28

Table 6. Torsion angles [°] for **6b**.

C8A N1 C2 C21	-179.8(1)
C8A N1 C2 C3	0.0(2)
C2 N1 C8A C4A	0.8(2)
C2 N1 C8A C8	-179.7(1)
C65 N61 C6 C5	177.4(1)
C65 N61 C6 C7	-3.2(2)
C62 N61 C6 C5	4.6(2)
C62 N61 C6 C7	-176.1(1)
C6 N61 C65 C64	178.5(1)
C62 N61 C65 C64	-8.0(2)
C6 N61 C62 C63	160.6(1)
C6 N61 C62 C63	160.6(1)
C65 N61 C62 C63	-12.9(2)
C26 C21 C2 N1	165.9(1)
C26 C21 C2 C3	-13.9(2)
C22 C21 C2 N1	-13.4(2)
C22 C21 C2 C3	166.8(2)
C2 C21 C26 C25	-178.5(1)
C22 C21 C26 C25	0.9(2)
C2 C21 C22 C23	178.4(1)
C26 C21 C22 C23	-0.9(2)
N61 C6 C5 C4A	179.7(1)
C7 C6 C5 C4A	0.3(2)

Table 6. Torsion angles [°] for **6b** (continued).

N61 C6 C7 C8	-179.4(1)
C5 C6 C7 C8	-0.0(2)
C6 C5 C4A C8A	-0.4(2)
C6 C5 C4A C4	-179.9(1)
N1 C2 C3 C4	-0.9(2)
C21 C2 C3 C4	178.9(1)
C2 C3 C4 C4A	0.9(2)
C2 C3 C4 C41	-177.6(1)
N61 C65 C64 C63	25.6(2)
C21 C26 C25 C24	0.9(2)
C5 C4A C8A N1	179.7(1)
C5 C4A C8A C8	0.2(2)
C4 C4A C8A N1	-0.8(2)
C4 C4A C8A C8	179.7(1)
C5 C4A C4 C3	179.4(2)
C5 C4A C4 C41	-2.1(2)
C8A C4A C4 C3	-0.1(2)
C8A C4A C4 C41	178.4(1)
N61 C62 C63 C64	28.5(2)
N1 C8A C8 C7	-179.5(1)
N1 C8A C8 H8	0.5
C4A C8A C8 C7	0.0(2)
C4A C8A C8 H8	-180.0
C6 C7 C8 C8A	-0.1(2)

Table 6. Torsion angles [°] for **6b** (continued).

C23 C24 C25 C26	-2.5(2)
C27 C24 C25 C26	177.1(2)
C25 C24 C23 C22	2.5(2)
C27 C24 C23 C22	-177.1(2)
F43 C41 C4 C3	-117.5(2)
F43 C41 C4 C4A	64.0(2)
F42 C41 C4 C3	122.3(2)
F42 C41 C4 C4A	-56.2(2)
F44 C41 C4 C3	2.7(2)
F44 C41 C4 C4A	-175.8(1)
C21 C22 C23 C24	-0.8(3)
C65 C64 C63 C62	-33.7(2)