Electronic Supplementary Material (ESI) for RSC Advances

The Supporting Information

Synthesis of 3,4-Dihydro-2*H*-1,4-Benzo[*b*]thiazine Derivatives *via* DABCO-Catalyzed One-Pot Three-Component Condensation Reactions

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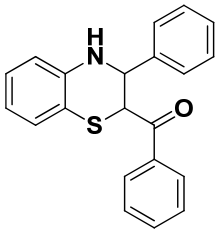
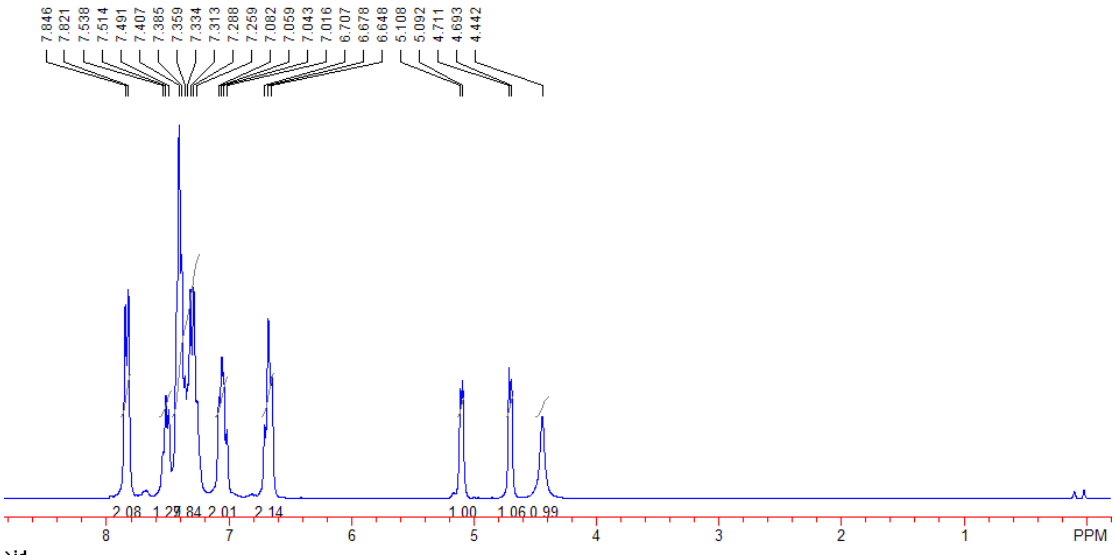
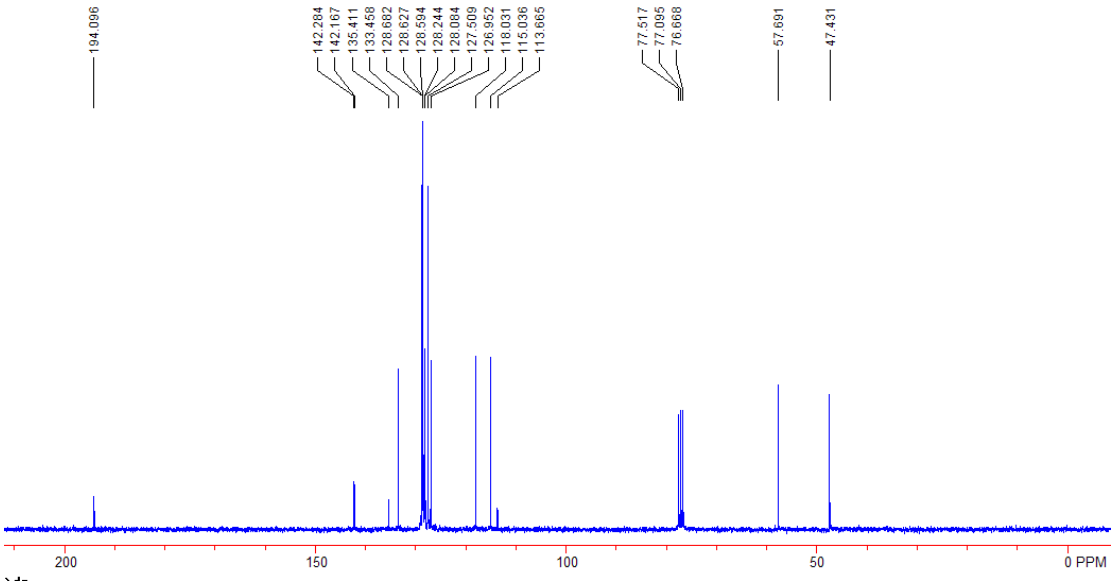
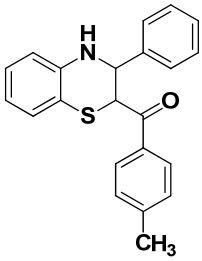
^{1}H and ^{13}C NMR spectra of 4aa

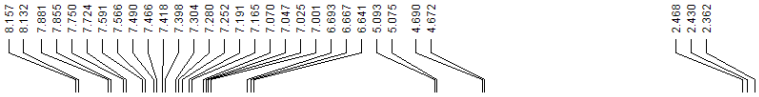


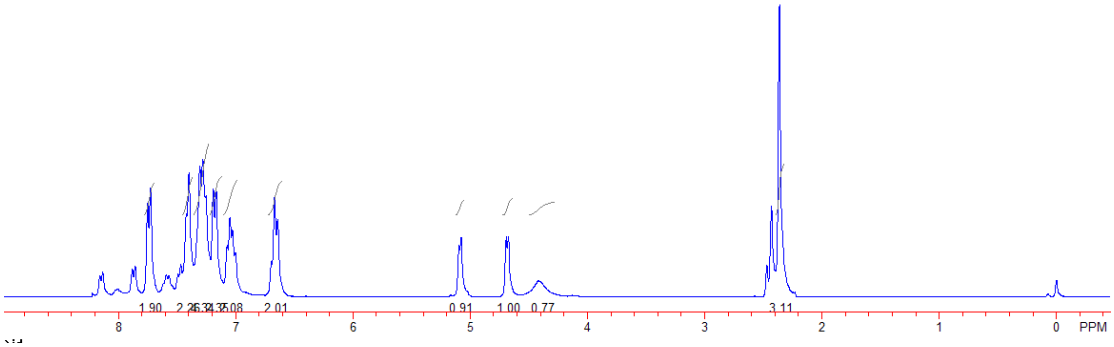


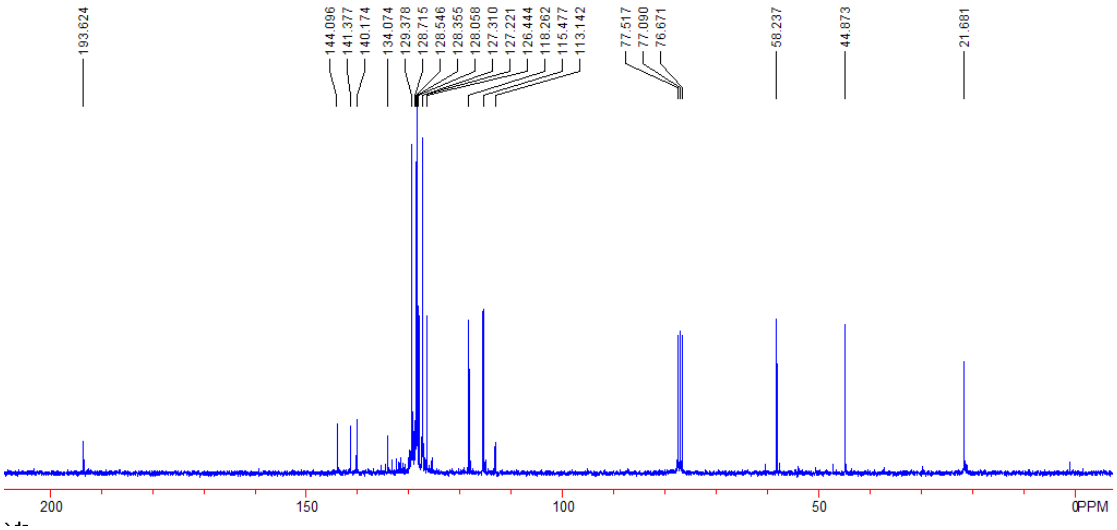


^{1}H and ^{13}C NMR spectra of 4ab









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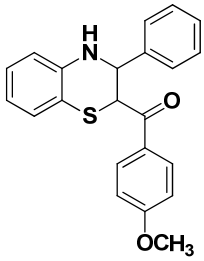

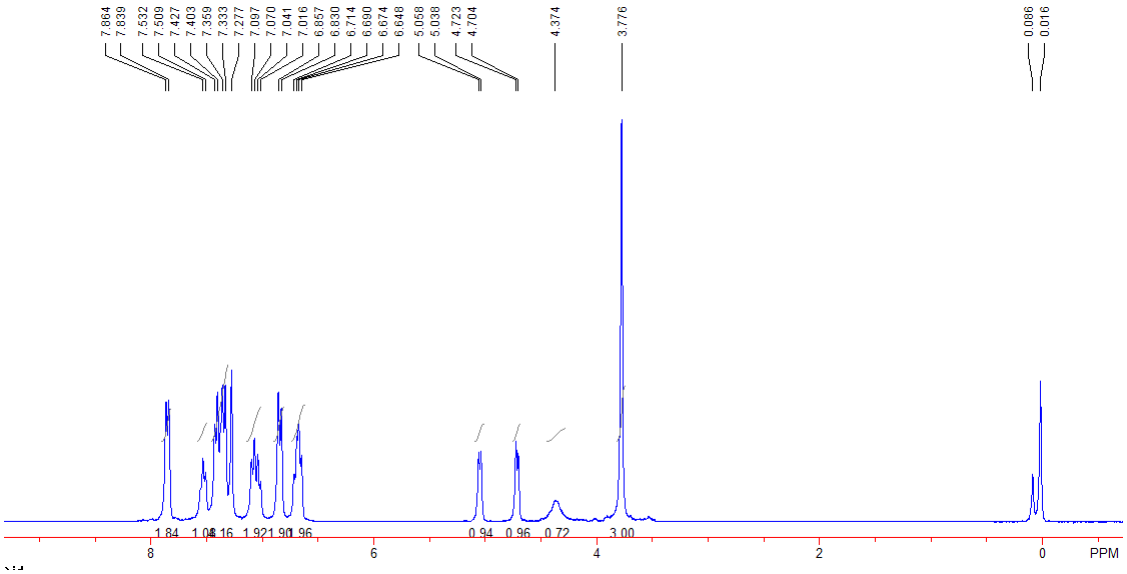

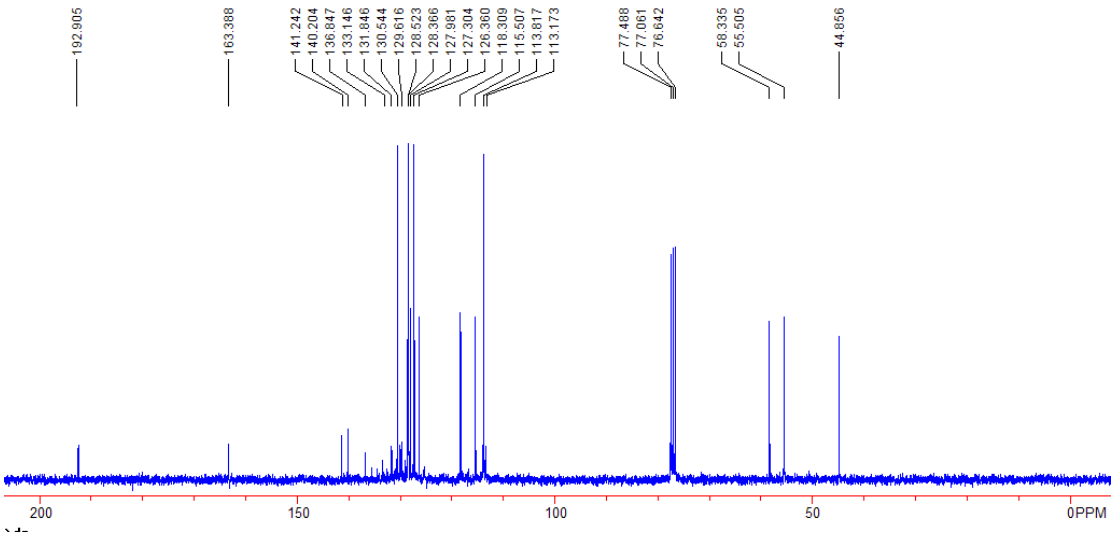

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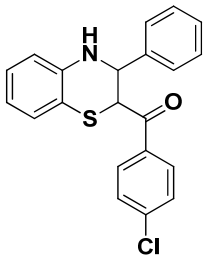

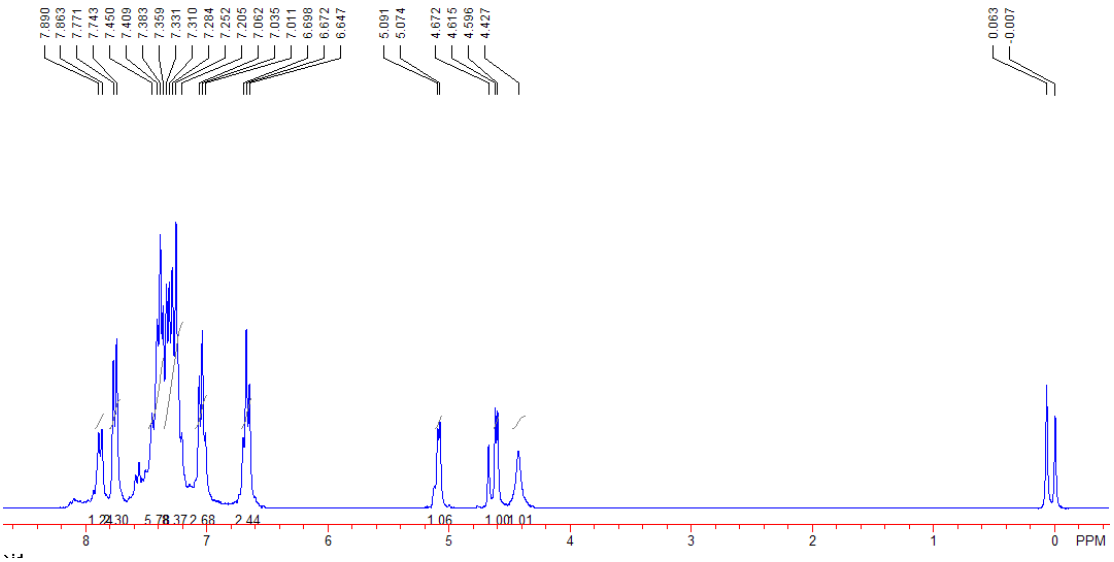

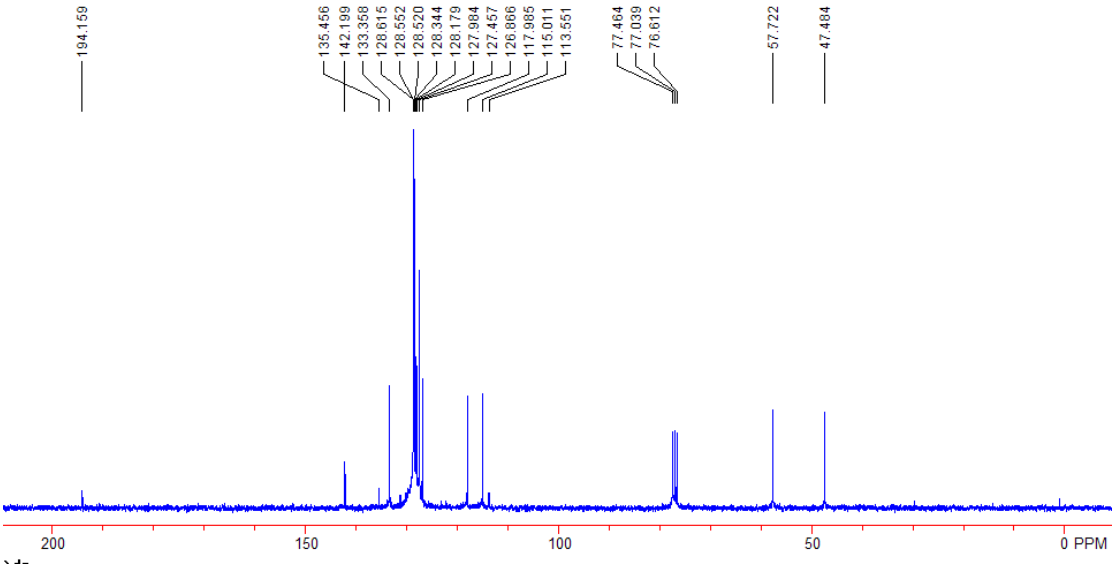

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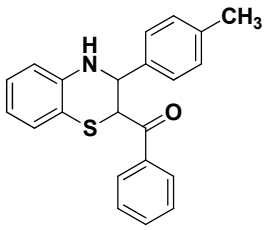
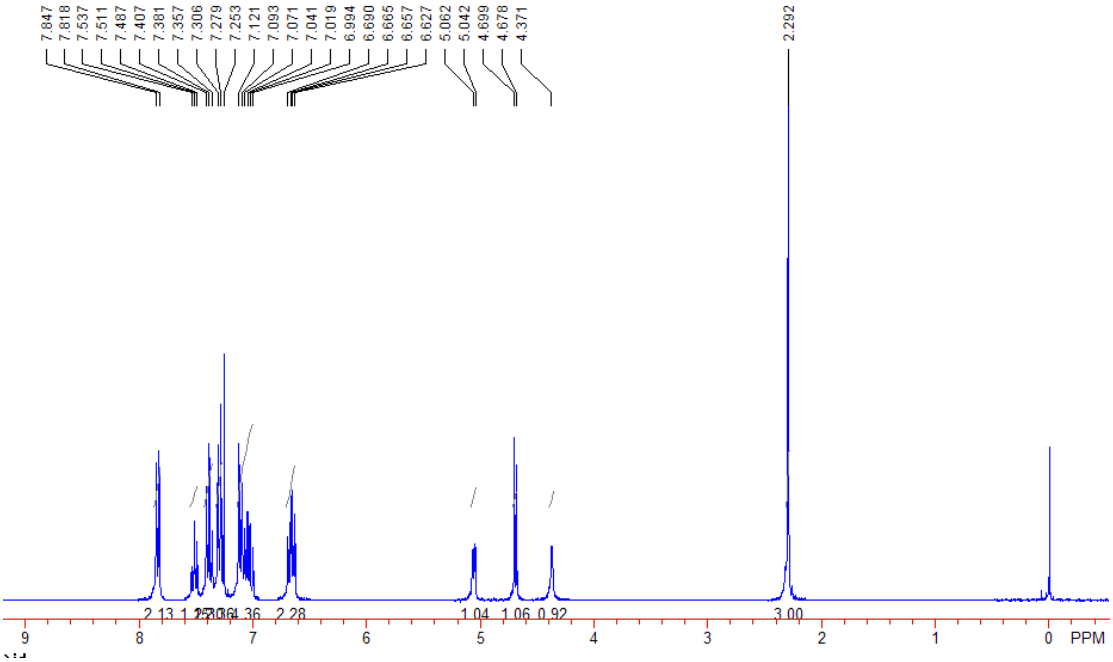
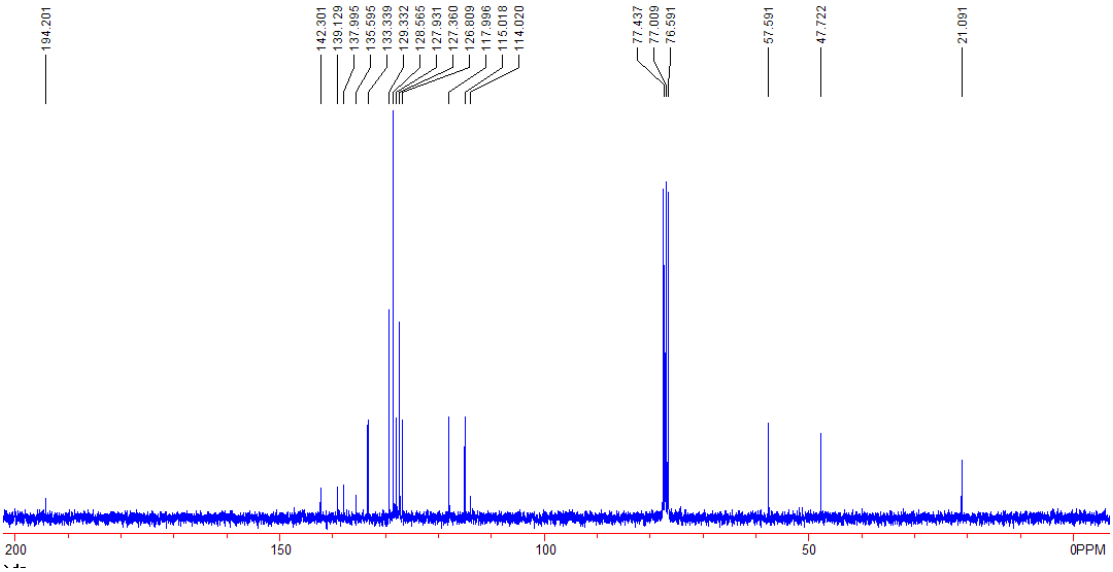
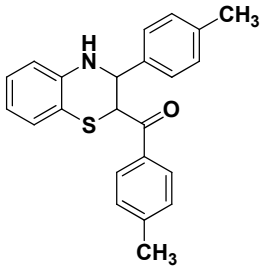
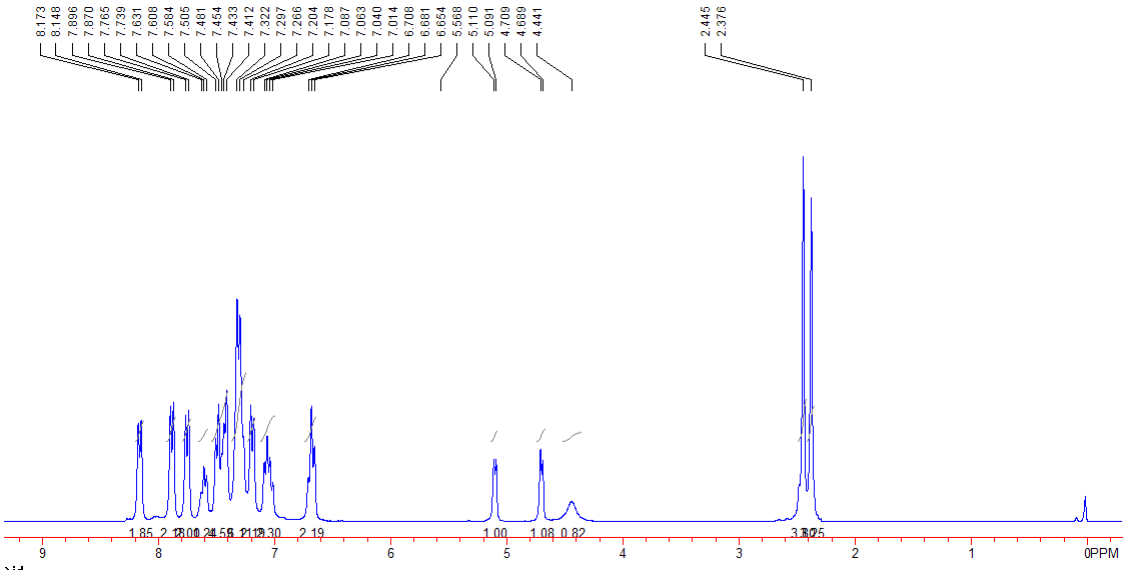


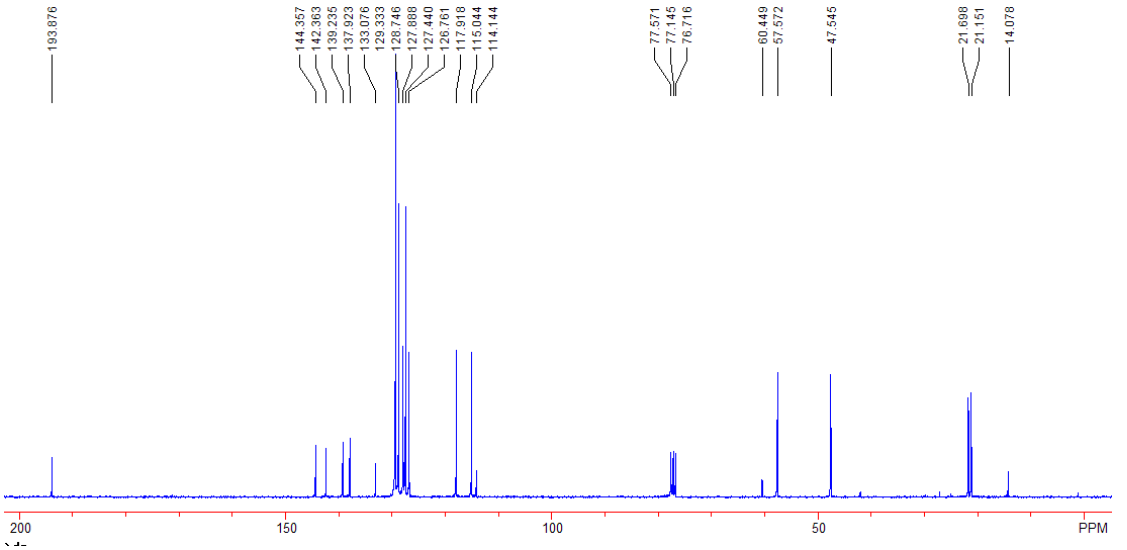




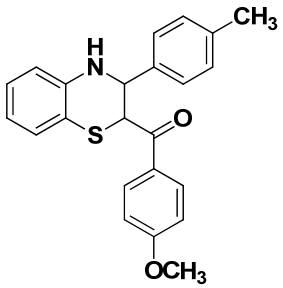
^{1}H and ^{13}C NMR spectra of 4bb

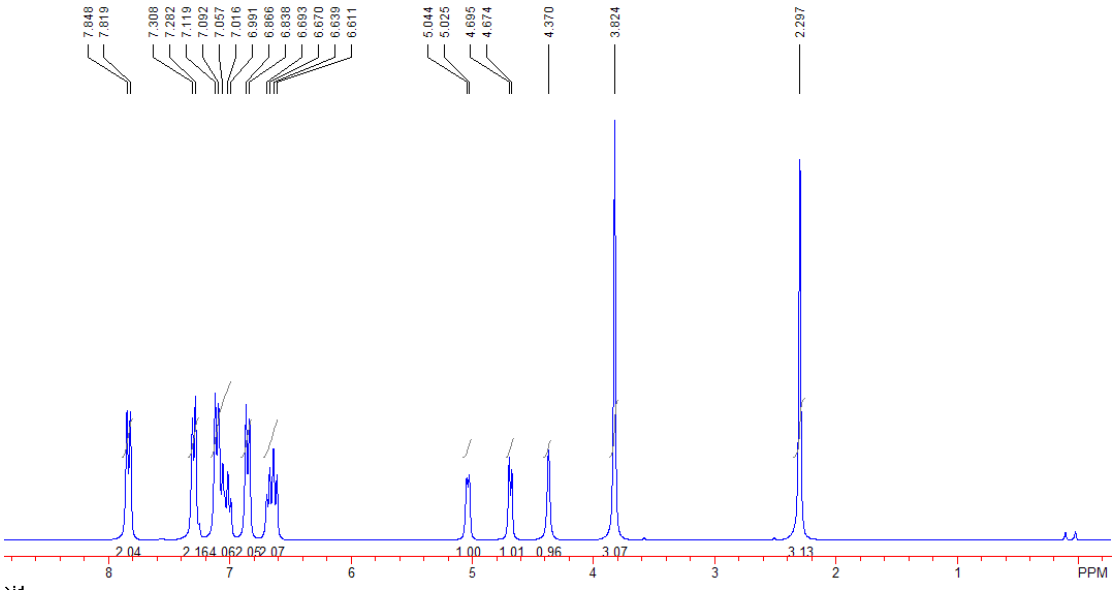


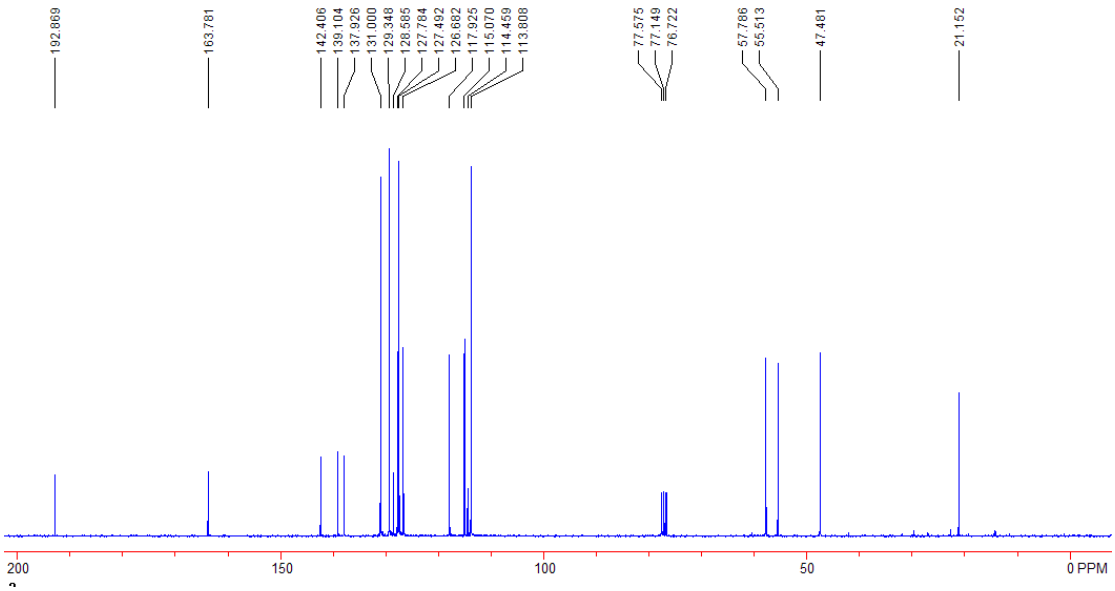




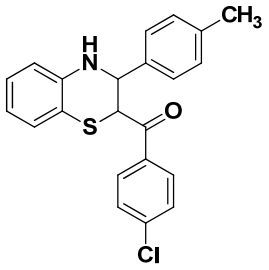
^{1}H and ^{13}C NMR spectra of 4bc

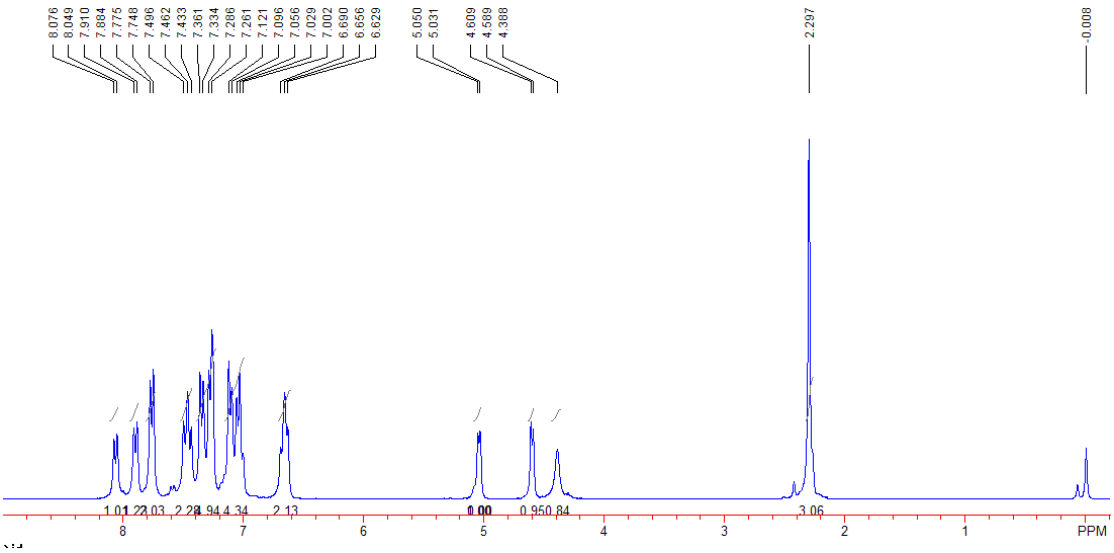


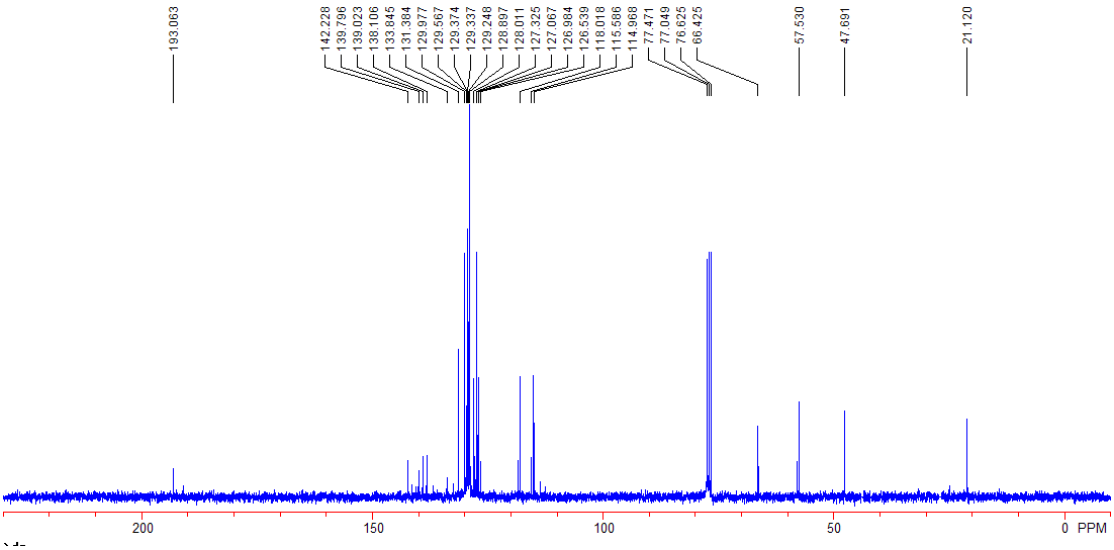




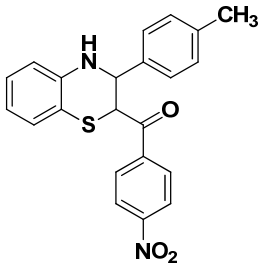
^{1}H and ^{13}C NMR spectra of 4bd

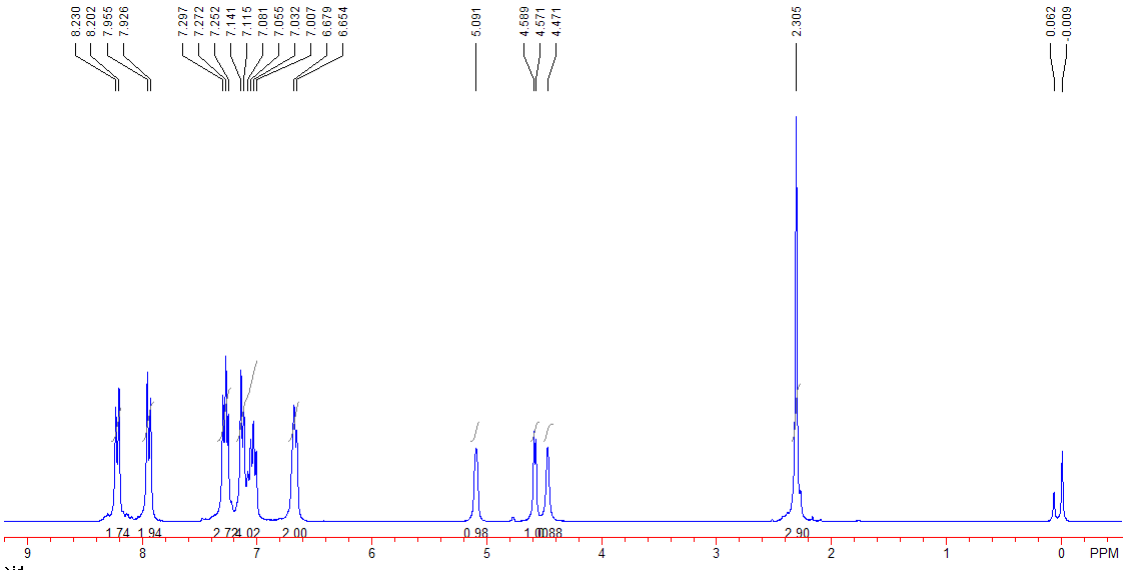


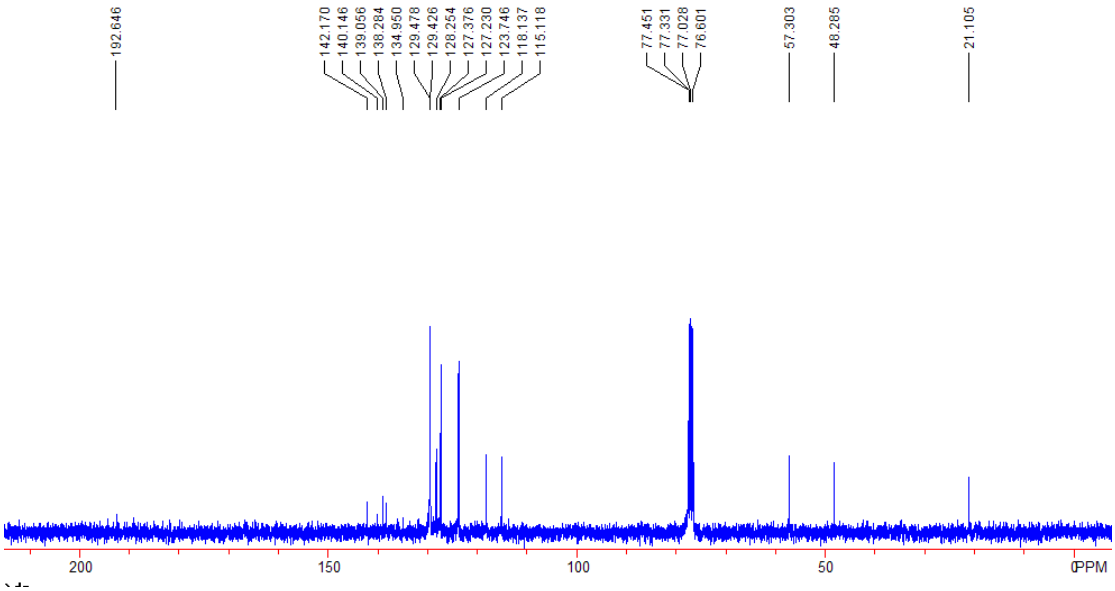




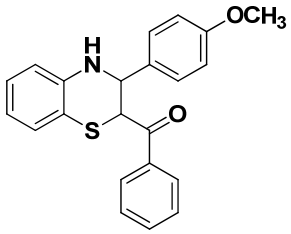
^{1}H and ^{13}C NMR spectra of 4be

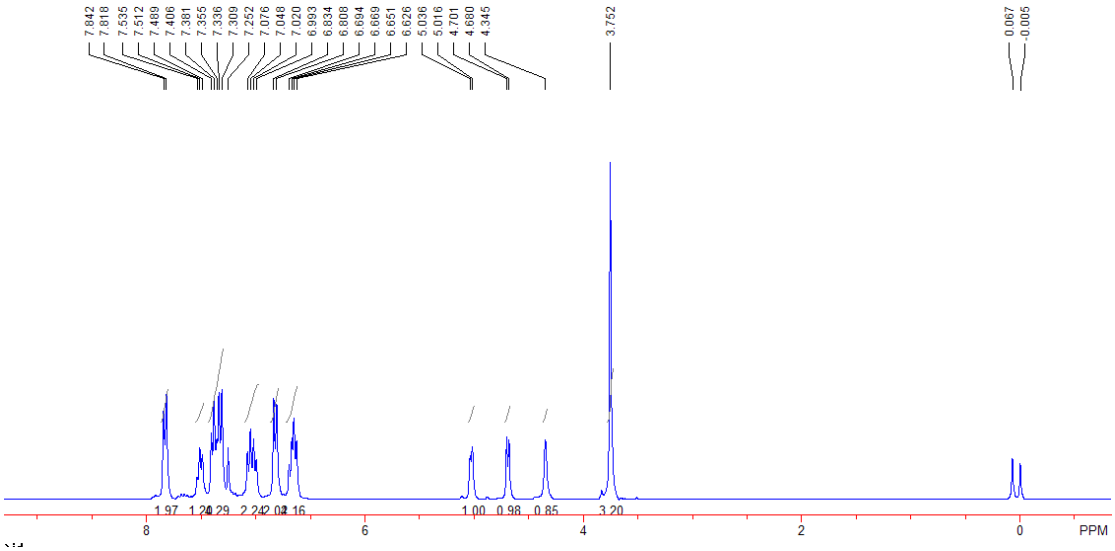


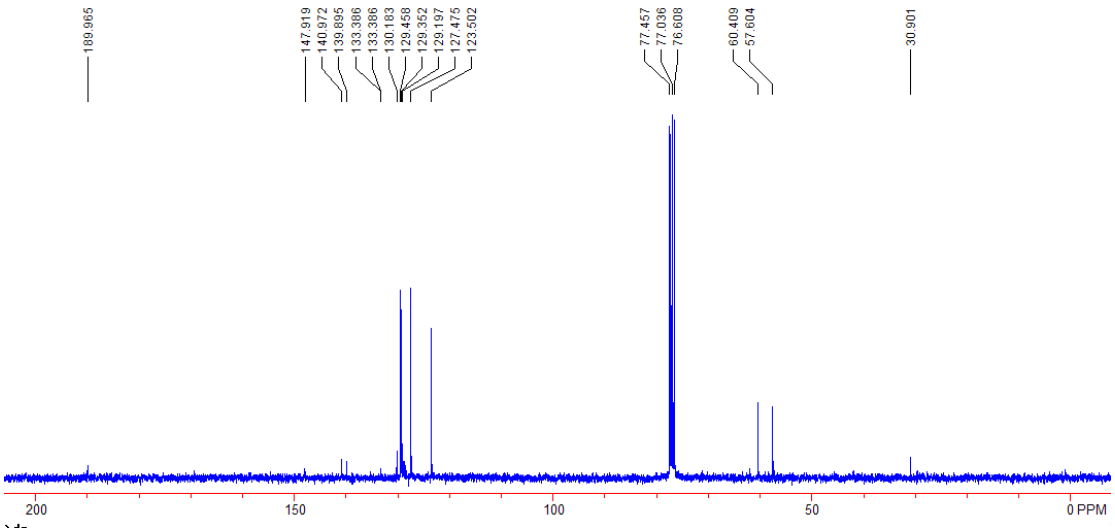




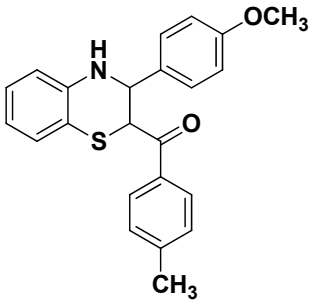
^{1}H and ^{13}C NMR spectra of 4ca

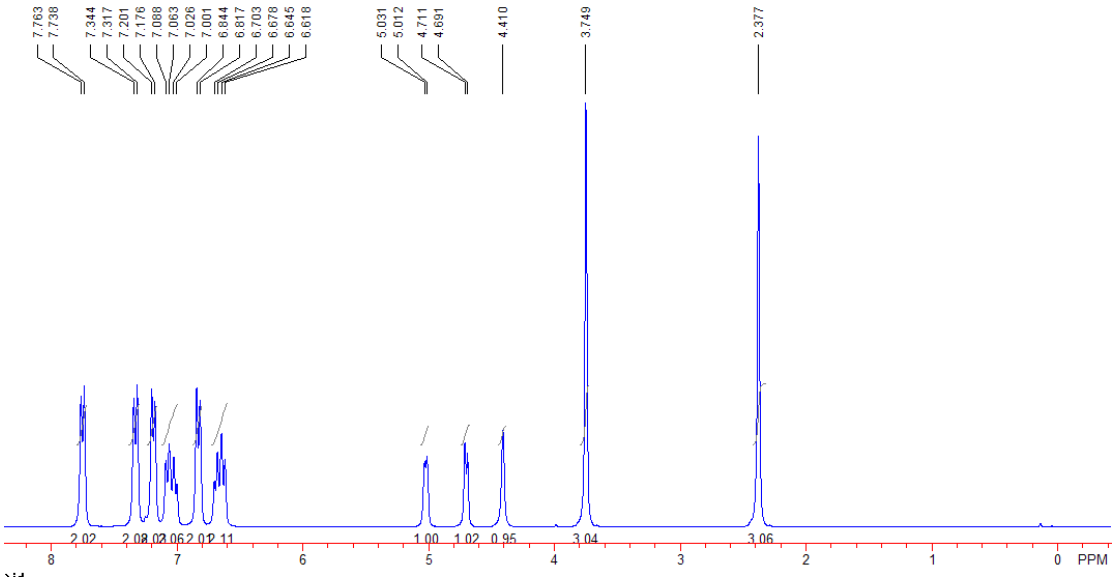


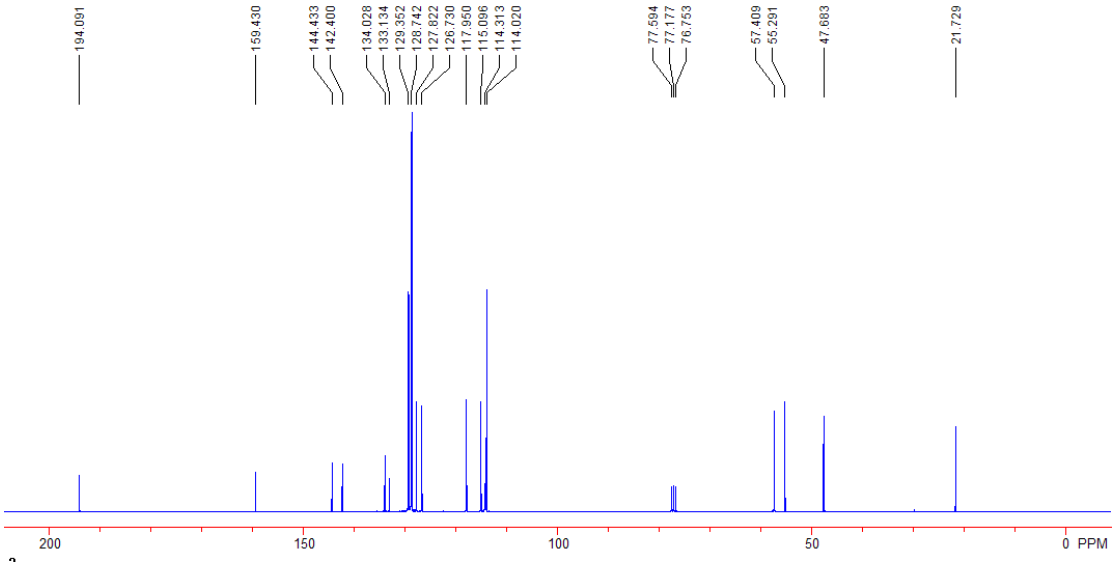




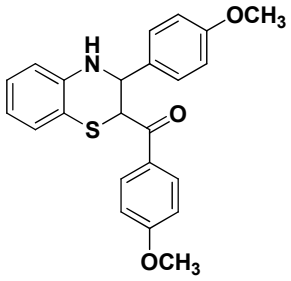
^{1}H and ^{13}C NMR spectra of 4cb

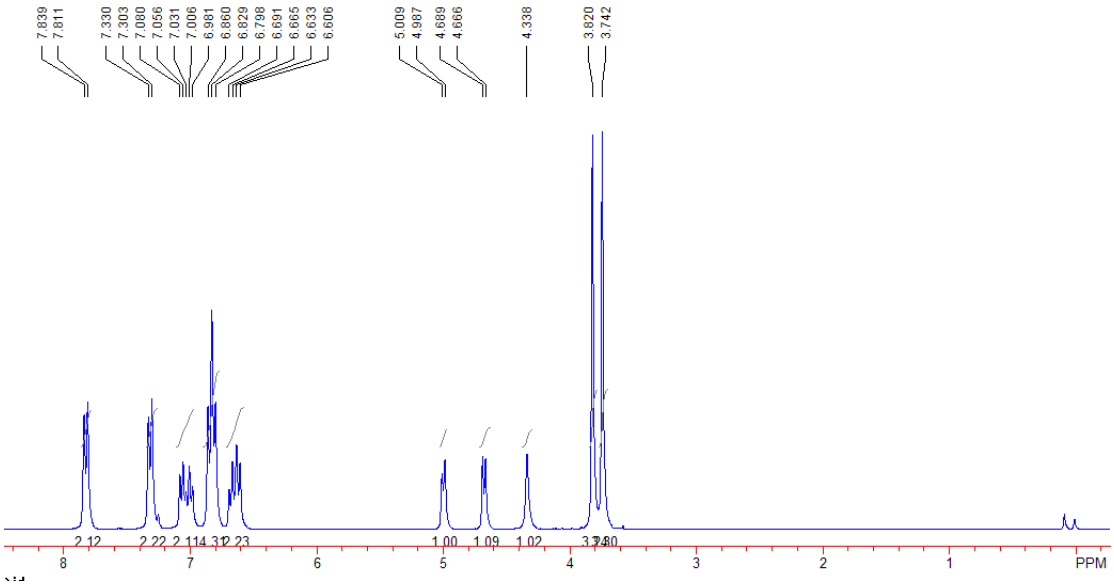


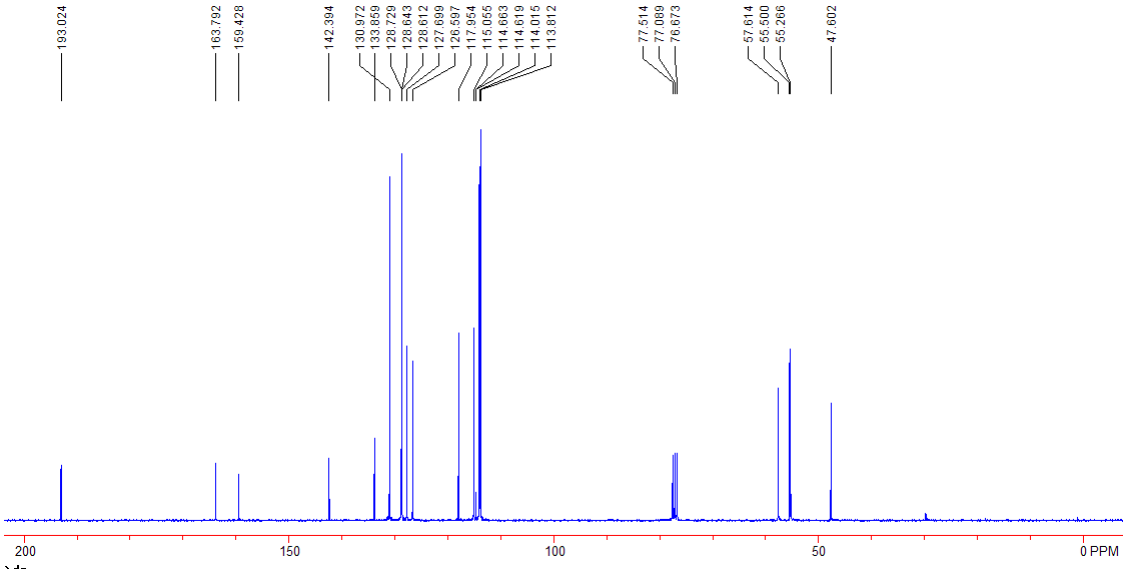




^{1}H and ^{13}C NMR spectra of 4cc







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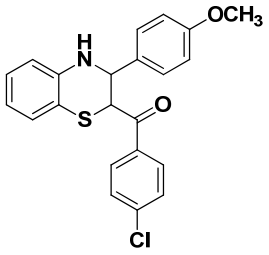
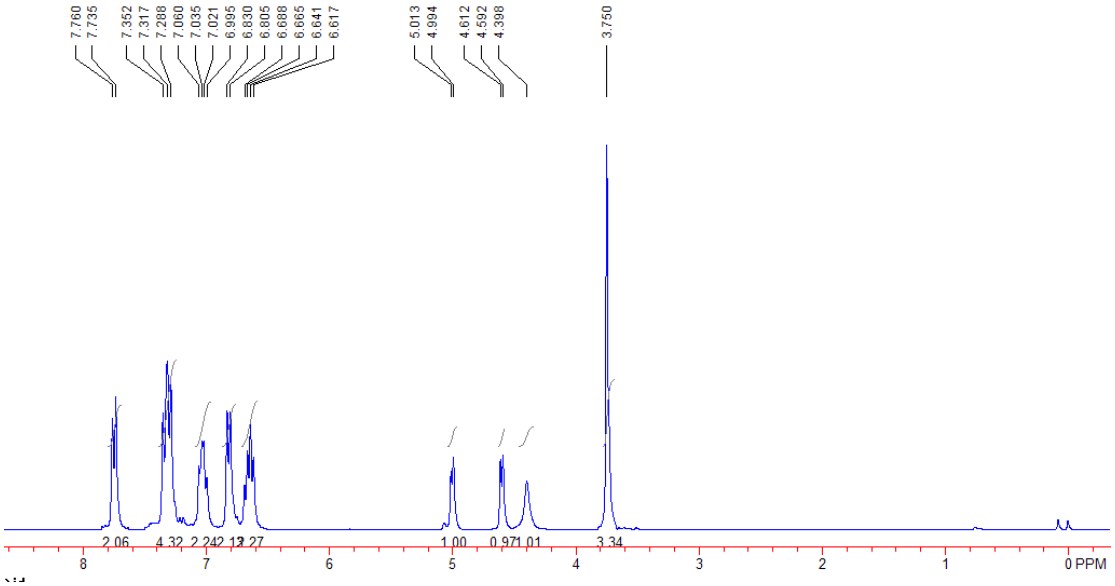
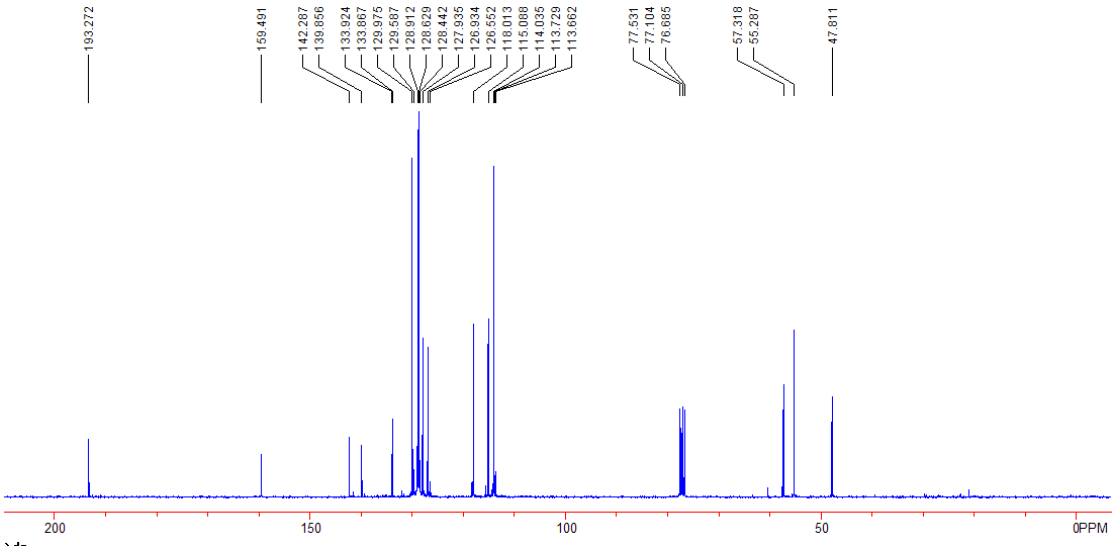
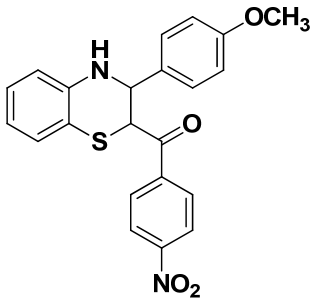
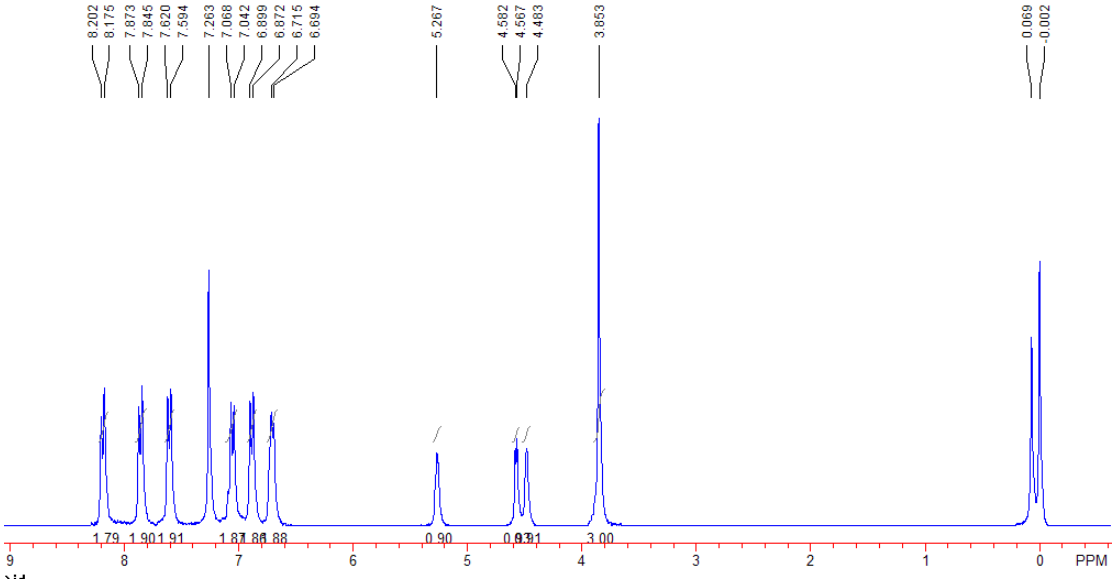


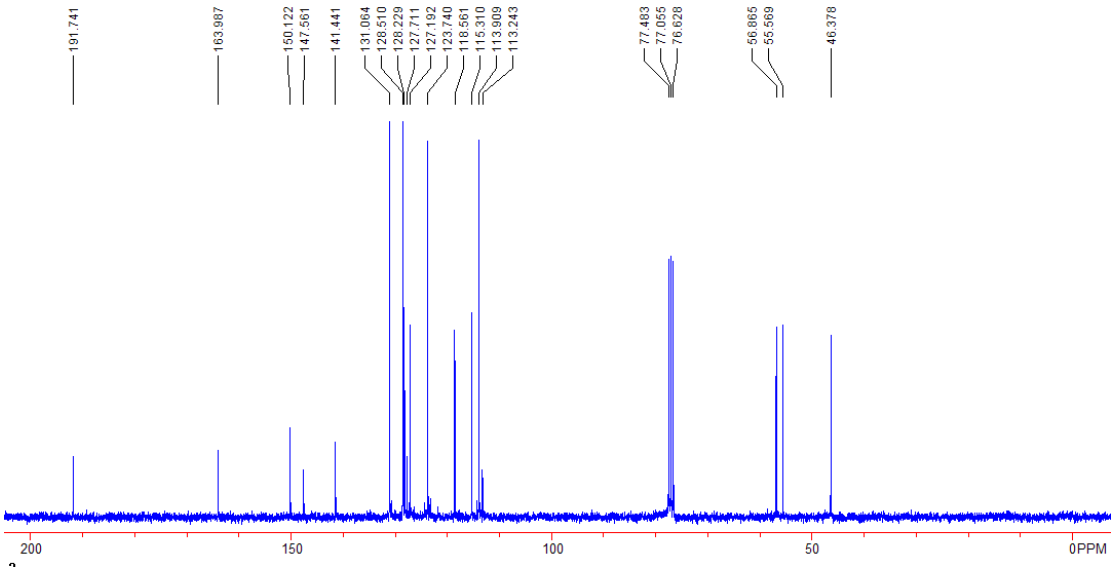




^{1}H and ^{13}C NMR spectra of 4ce







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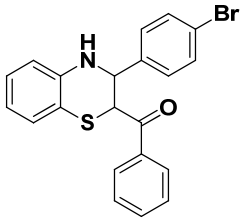

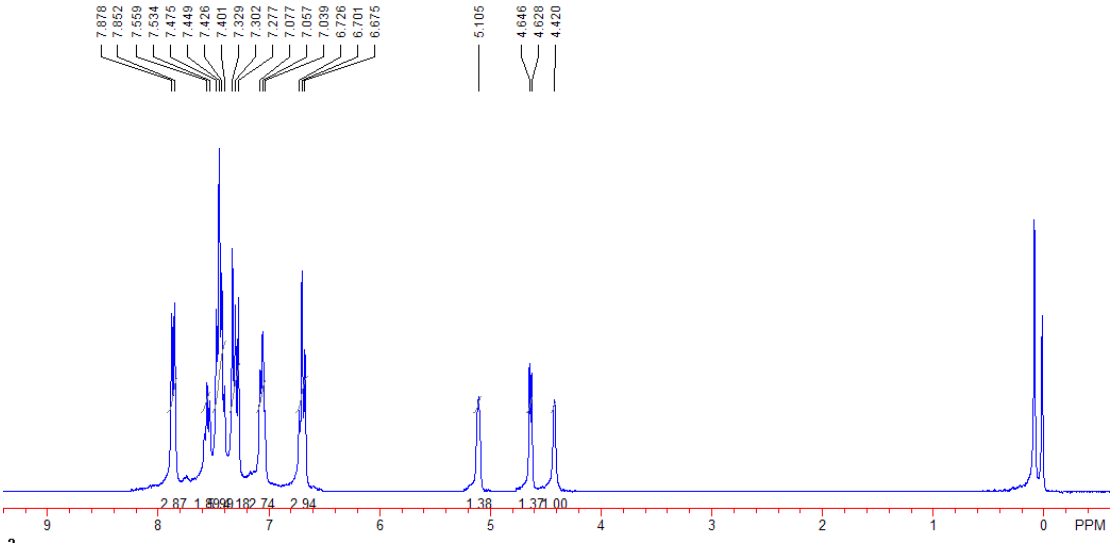

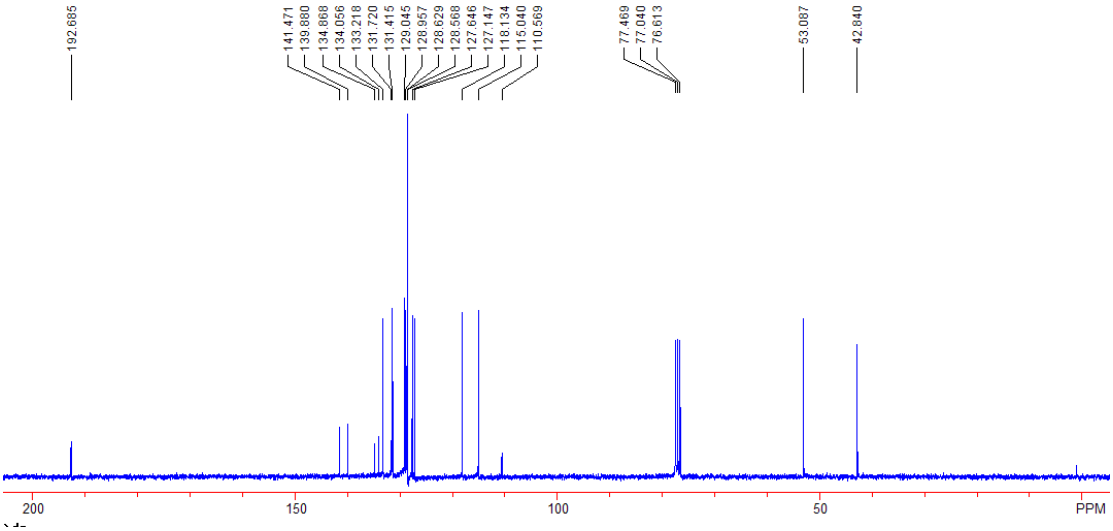

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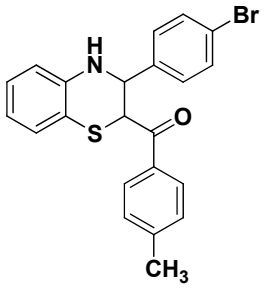

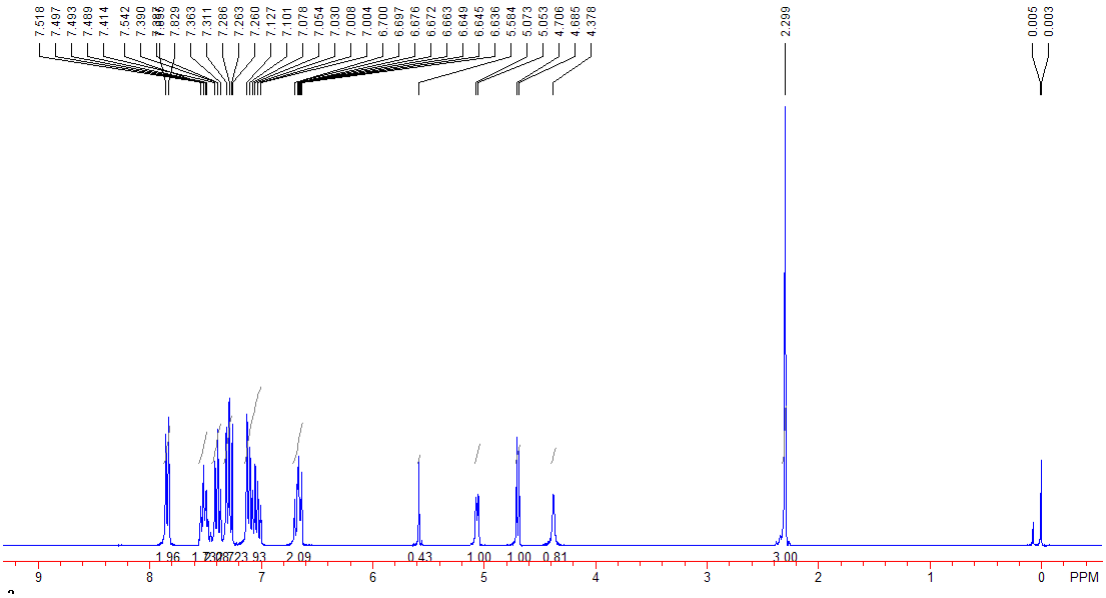

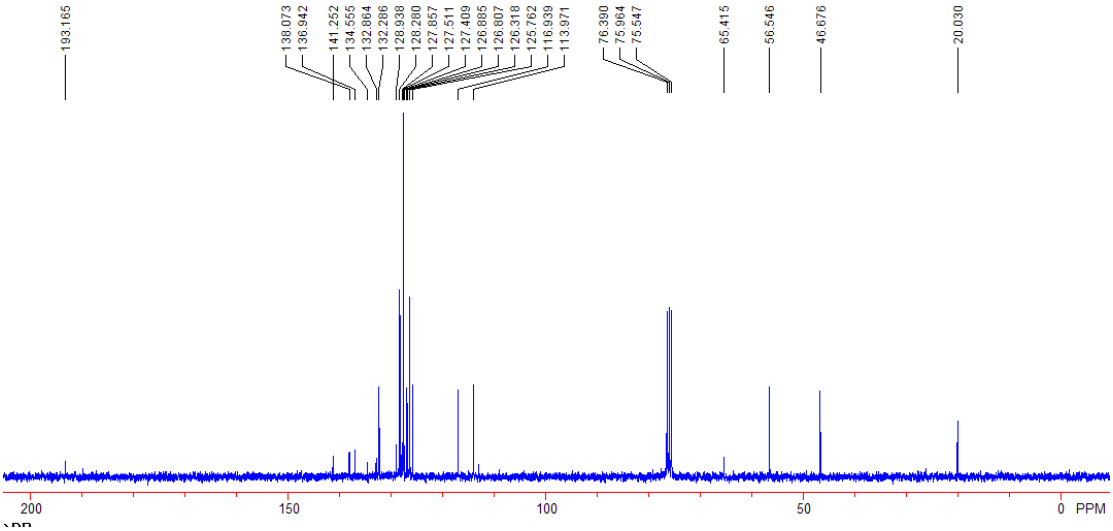

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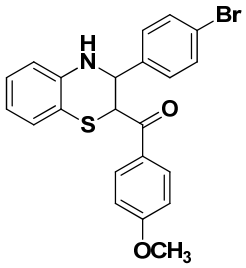

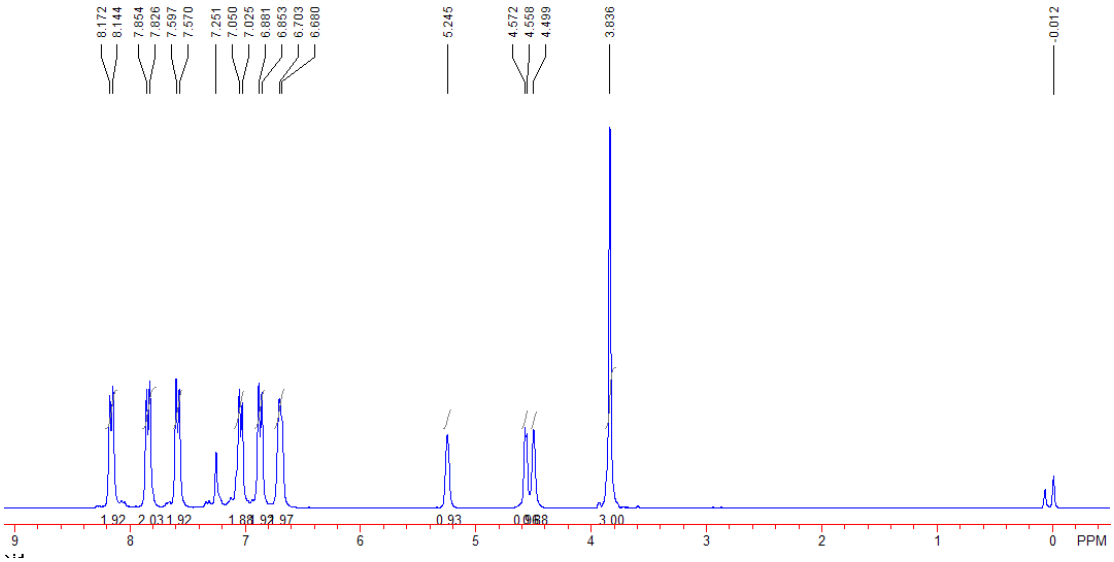

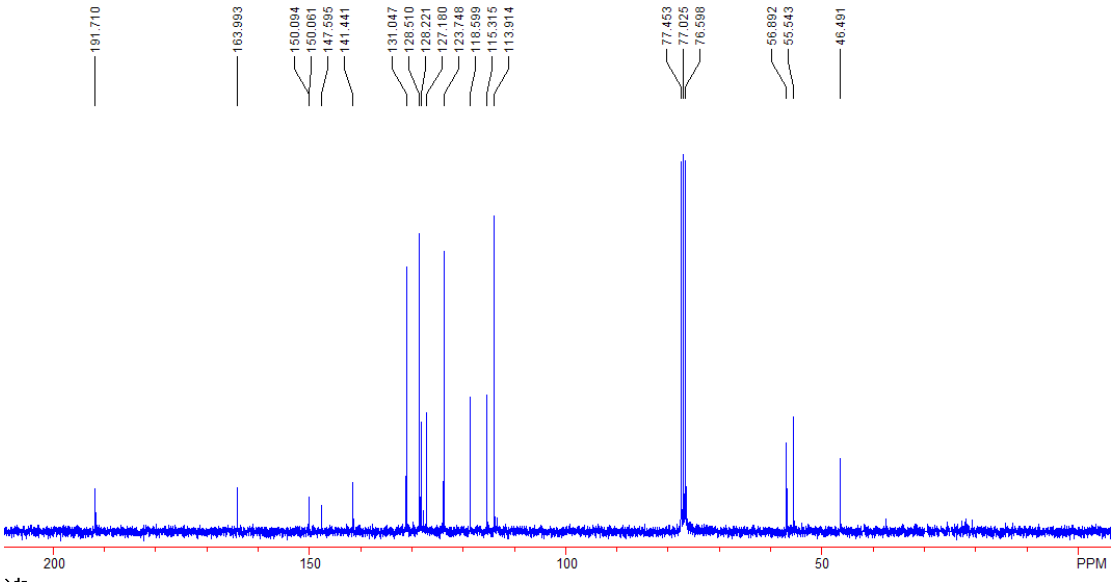

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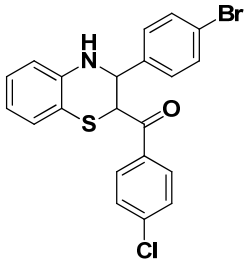
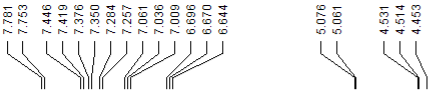
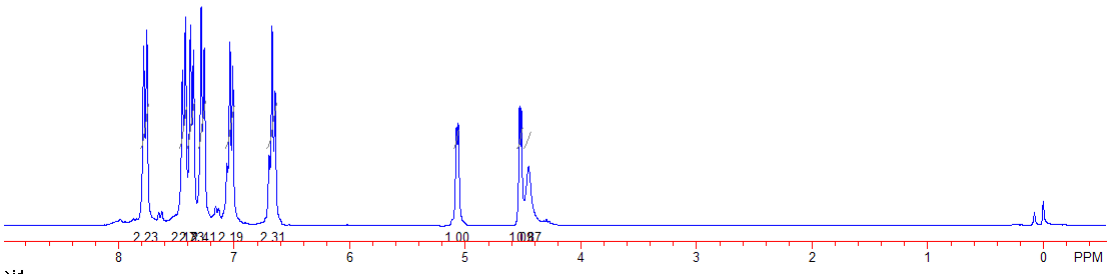
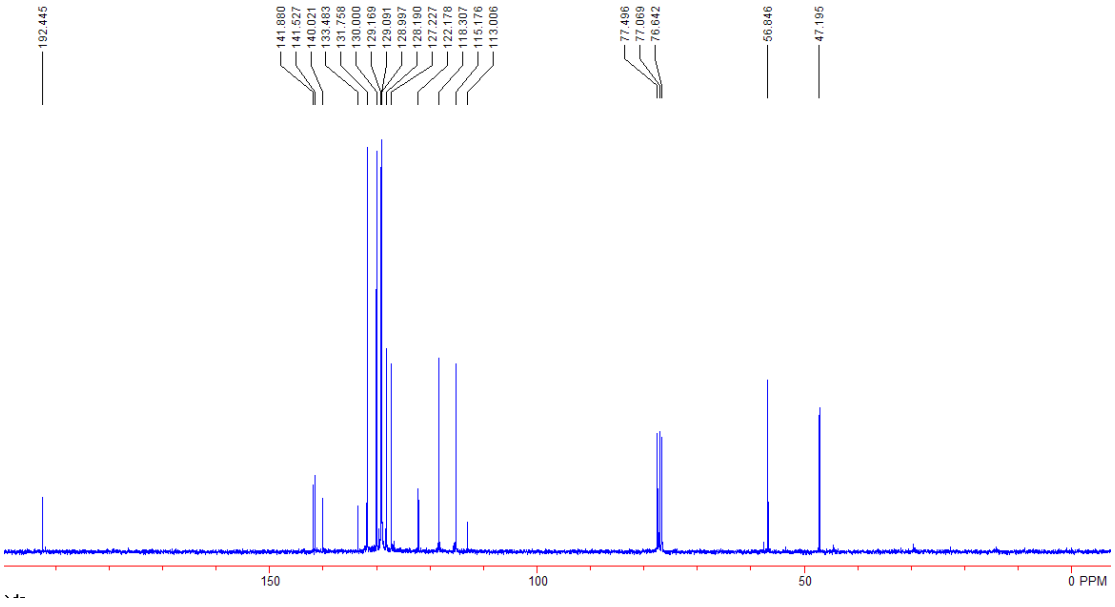
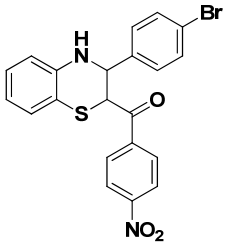


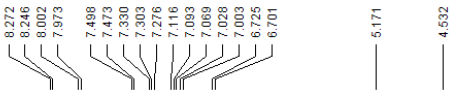


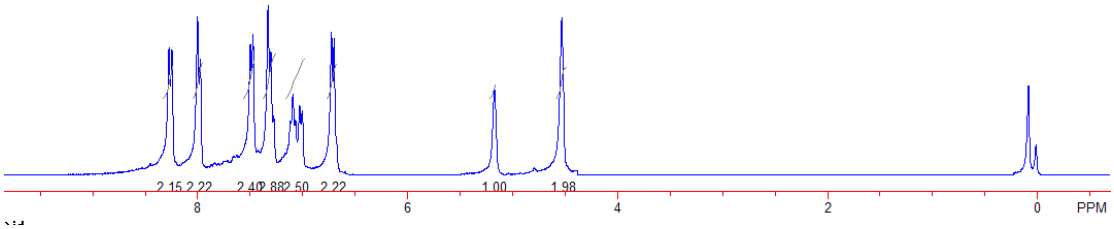


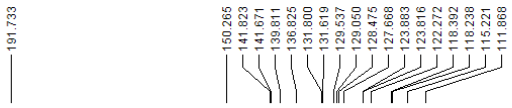


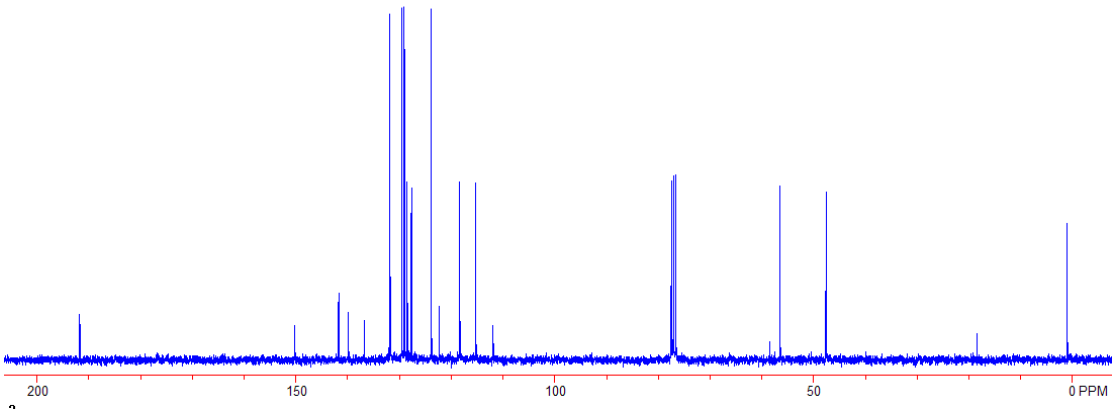
^{1}H and ^{13}C NMR spectra of 4de



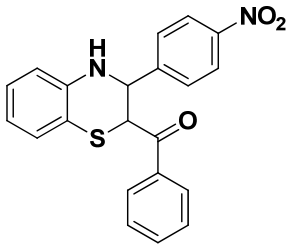


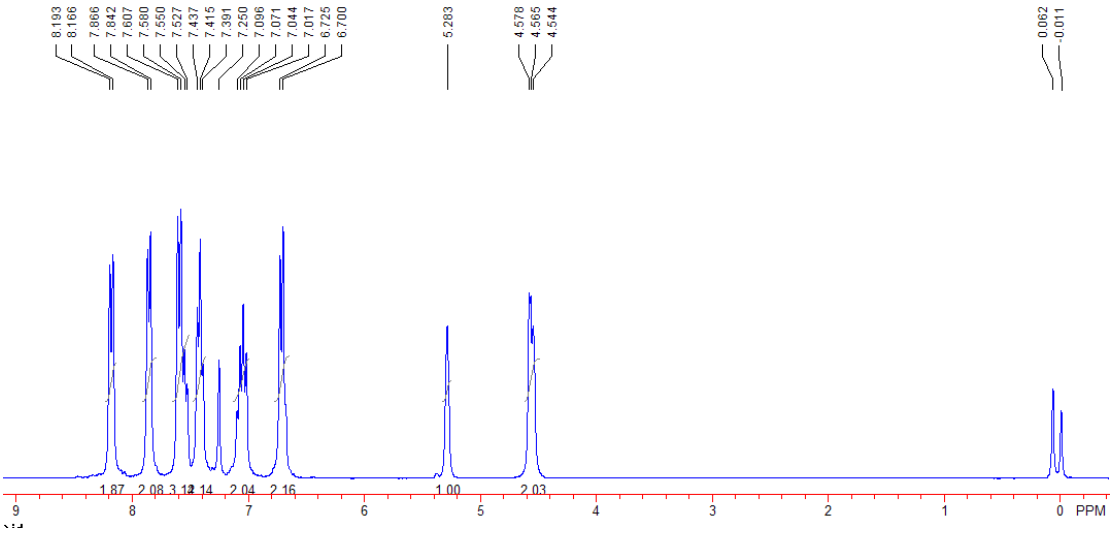


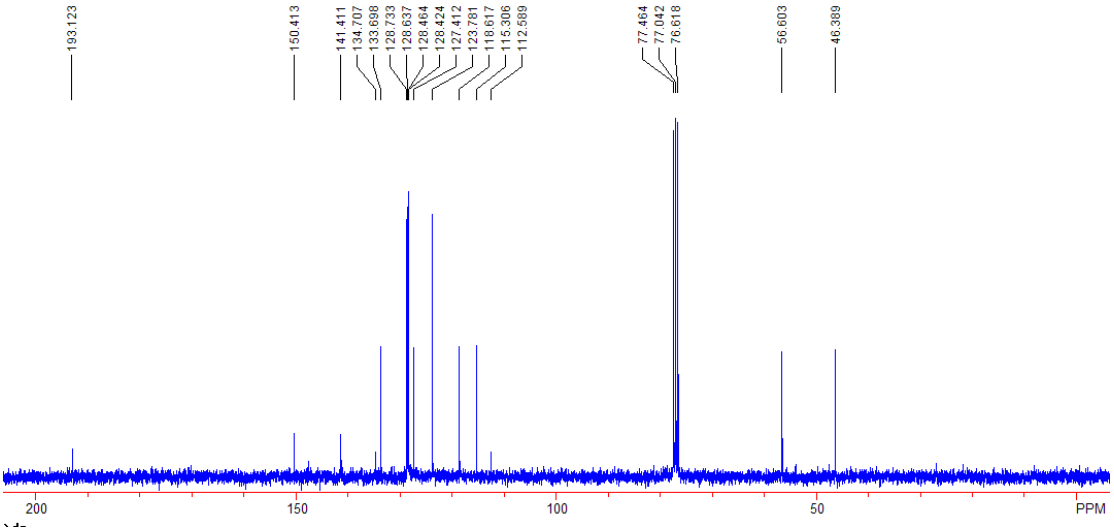




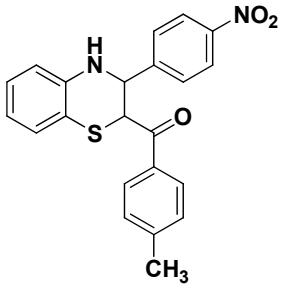
^{1}H and ^{13}C NMR spectra of 4ea

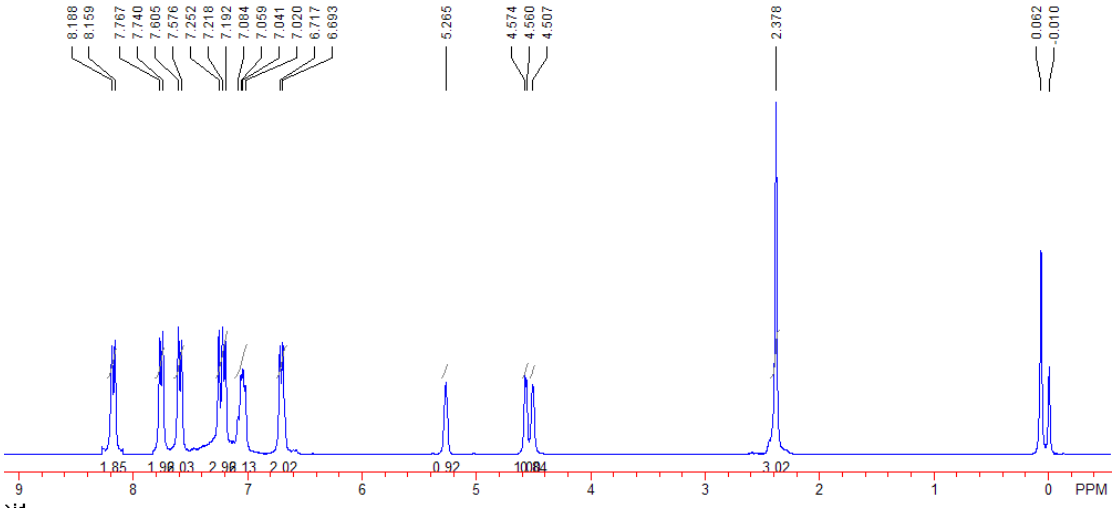


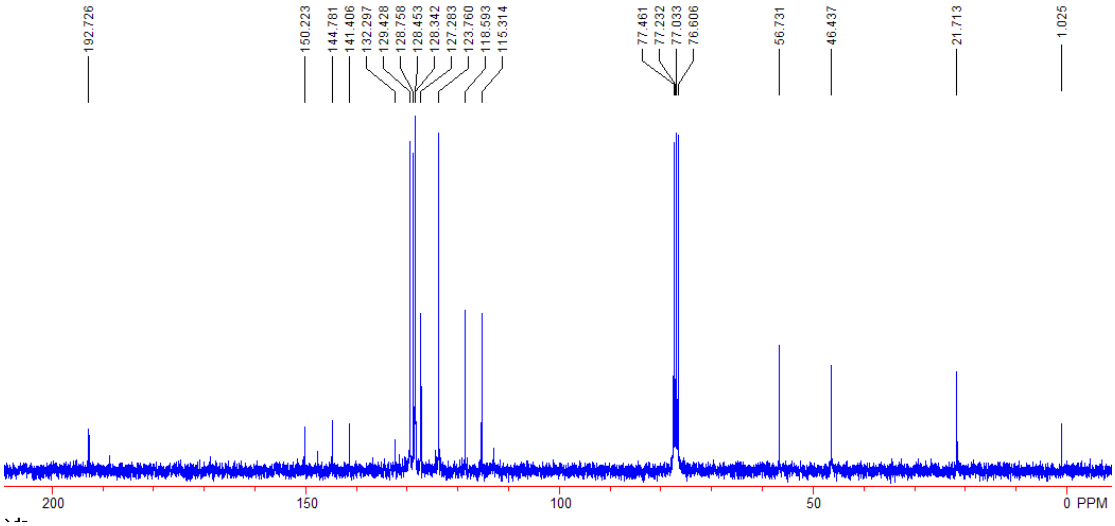




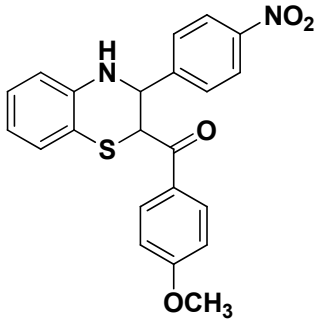
^{1}H and ^{13}C NMR spectra of 4eb

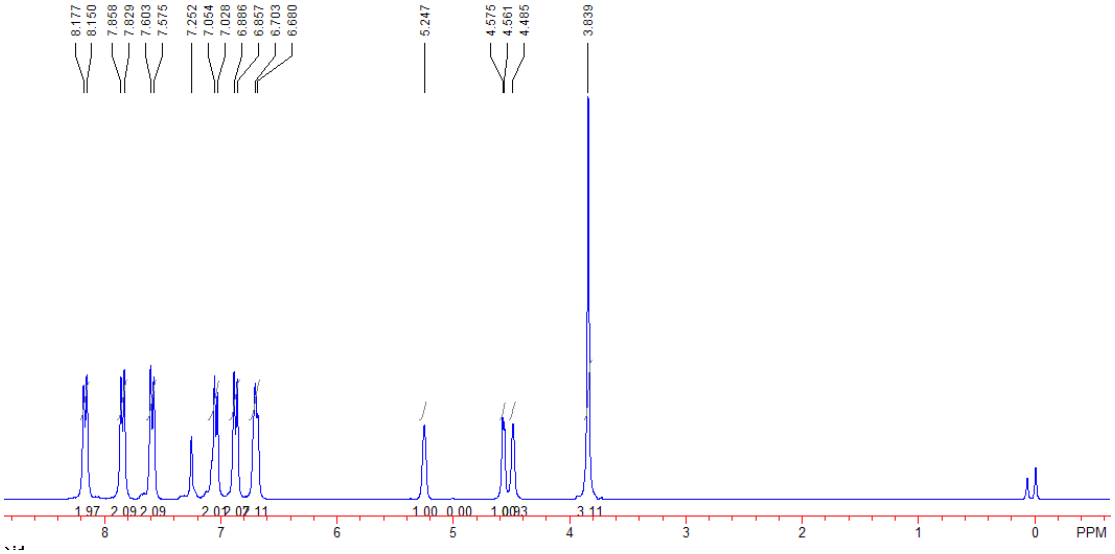


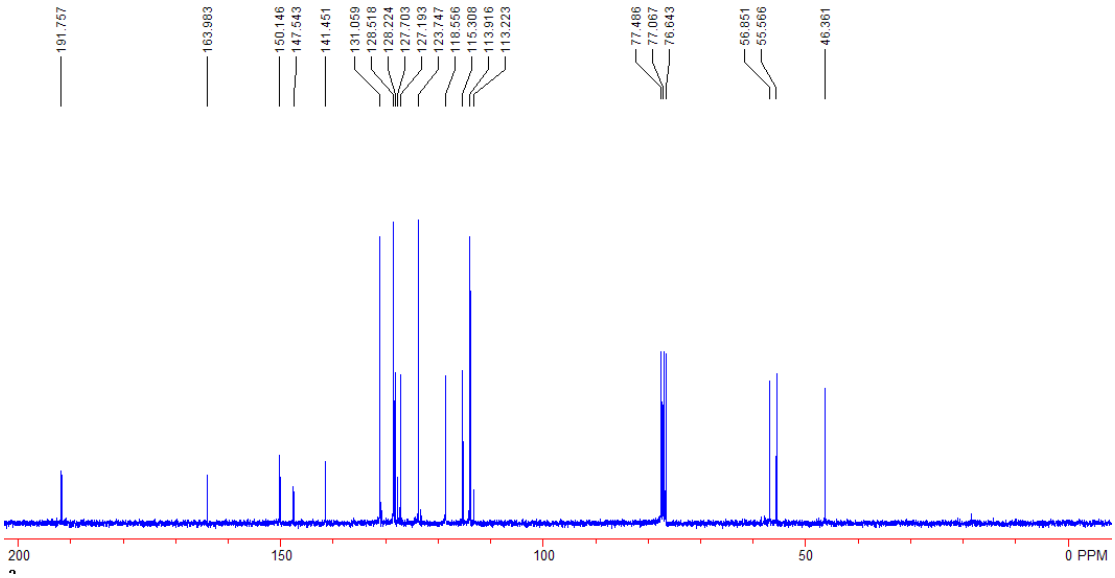




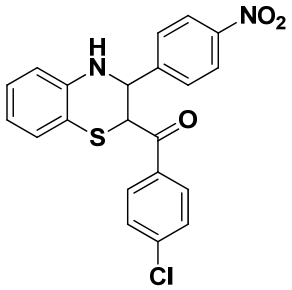
^{1}H and ^{13}C NMR spectra of 4ec

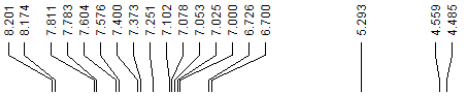


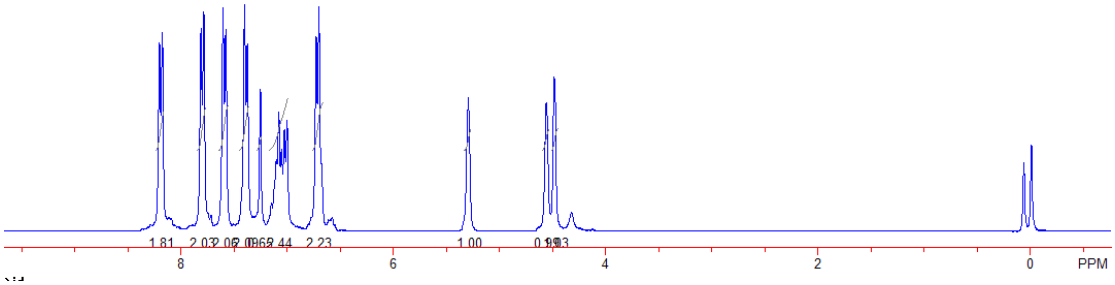


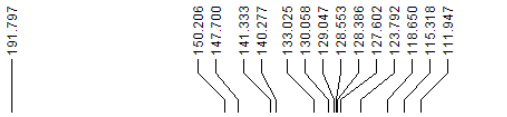


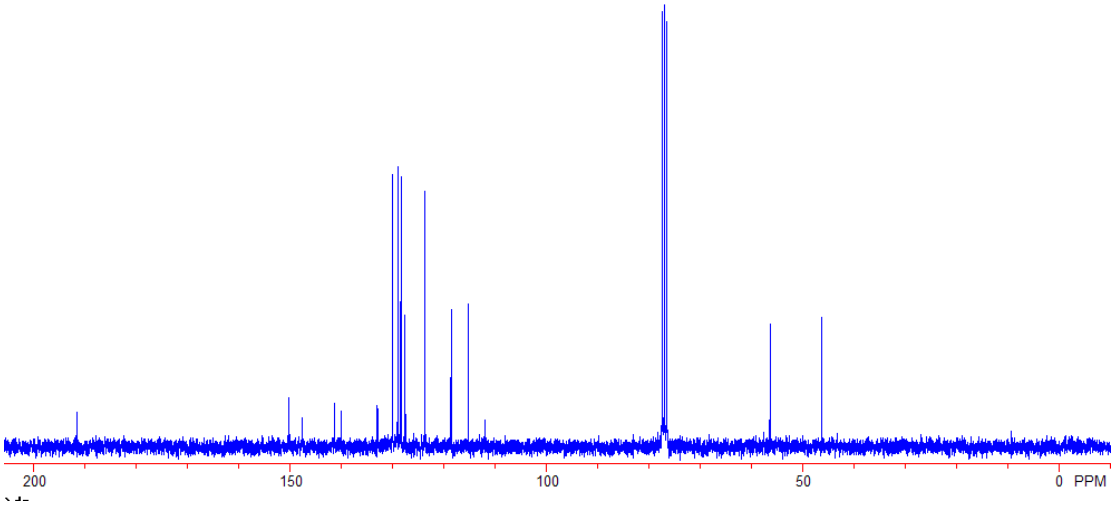
^{1}H and ^{13}C NMR spectra of 4ed



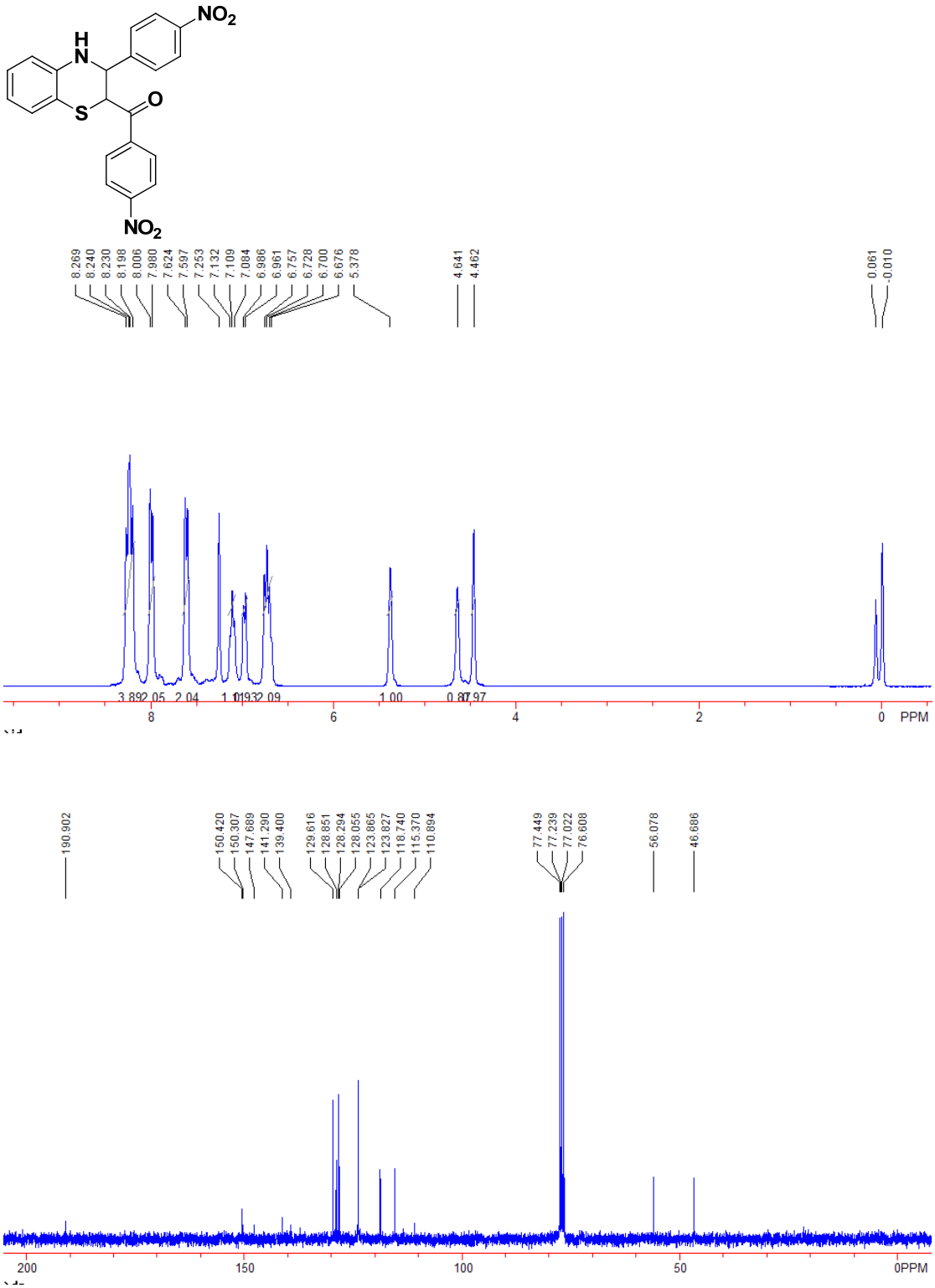




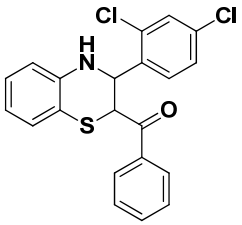


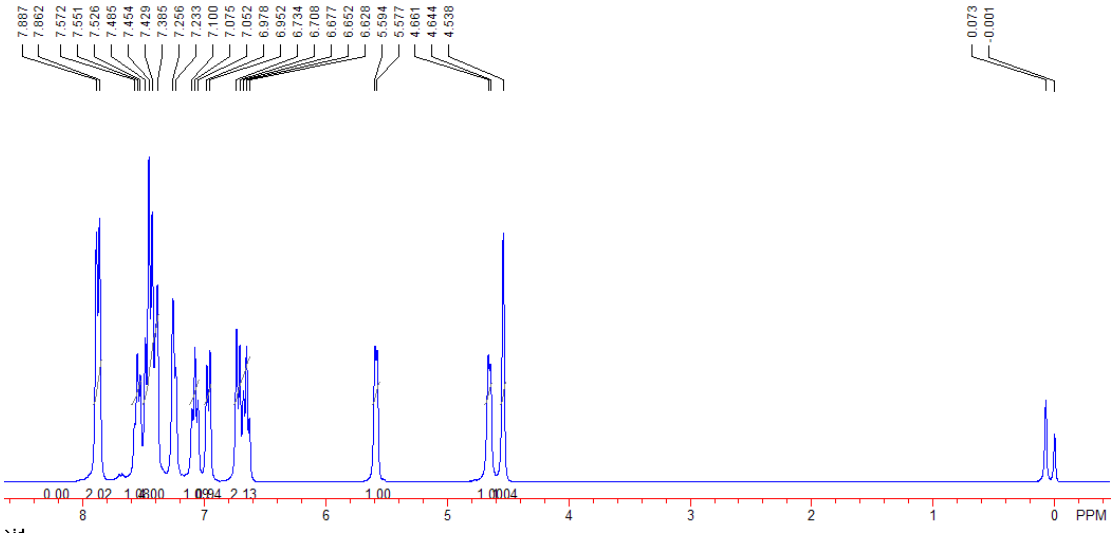


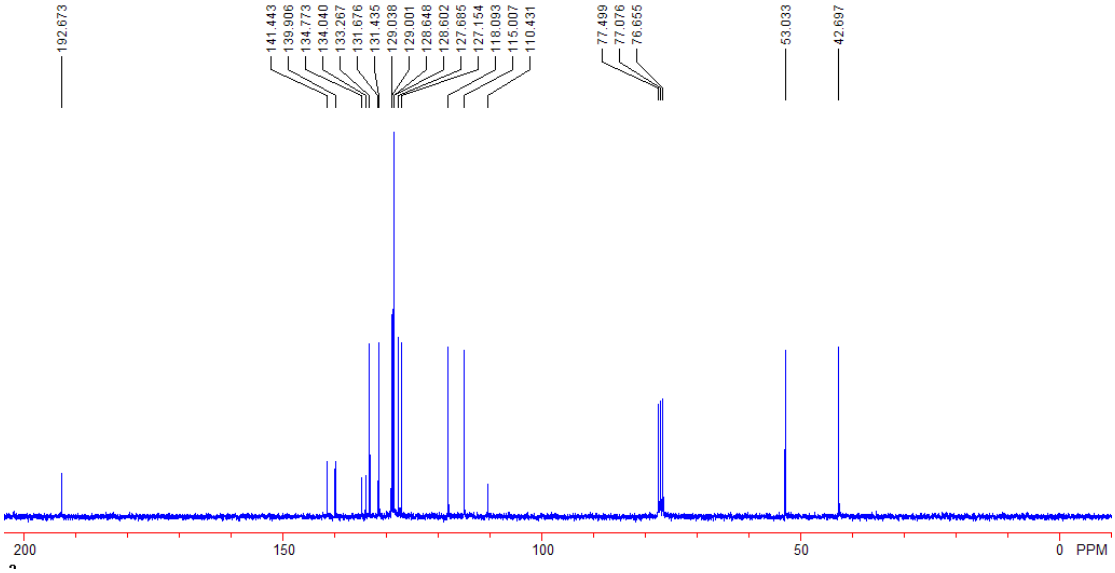
^{1}H and ^{13}C NMR spectra of 4ee



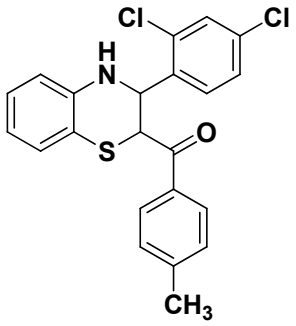
^{1}H and ^{13}C NMR spectra of 4fa

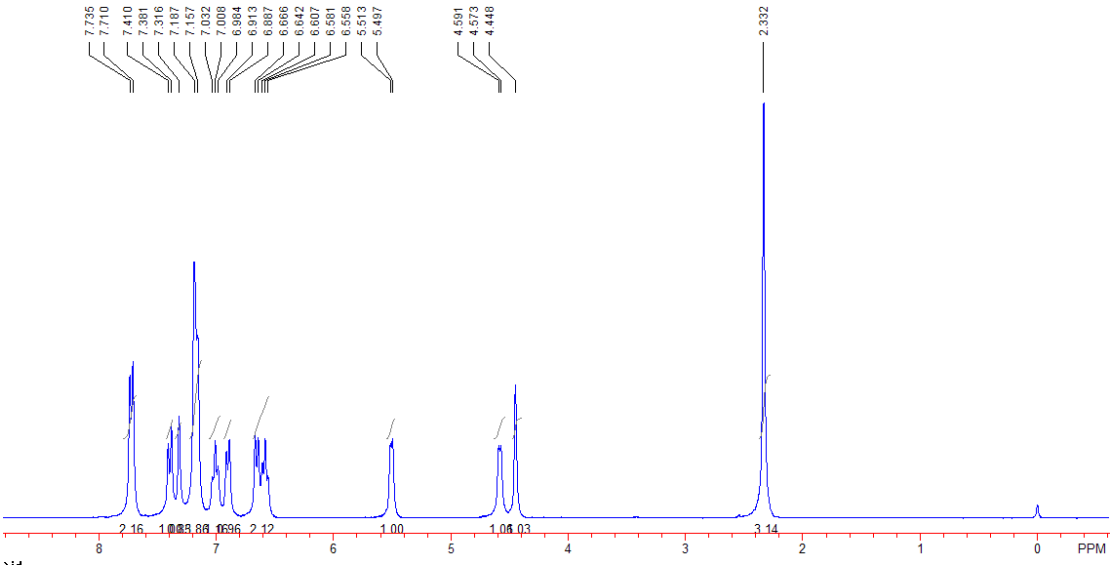


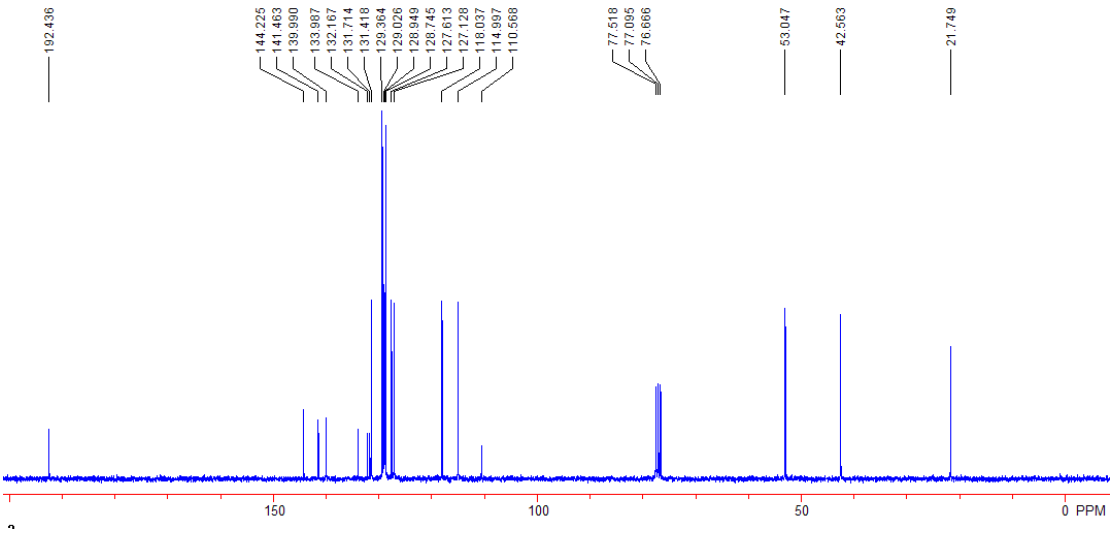




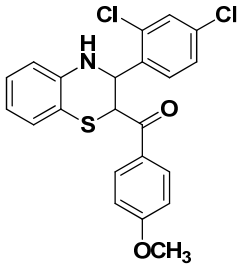
^{1}H and ^{13}C NMR spectra of 4fb

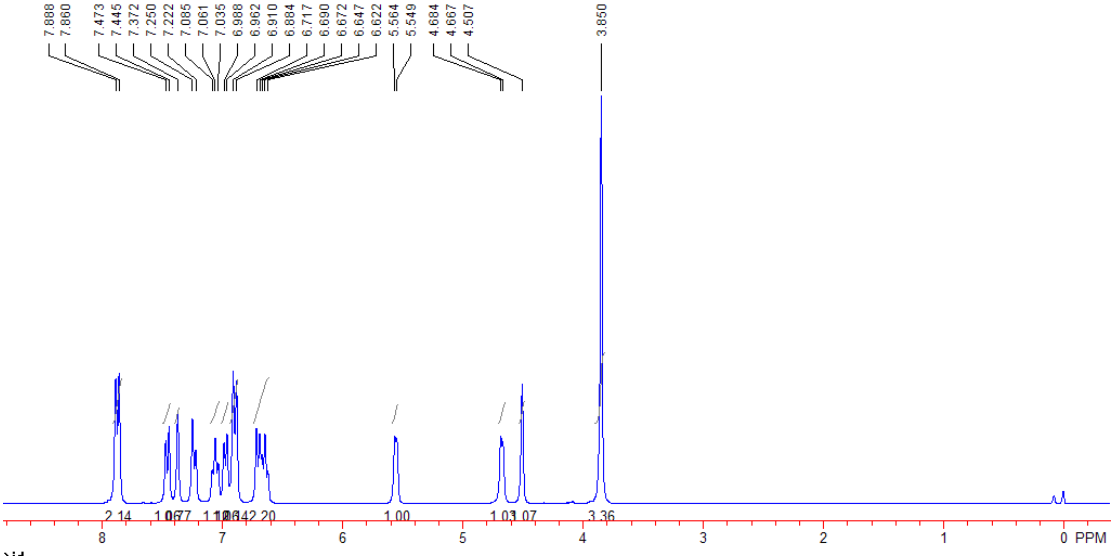


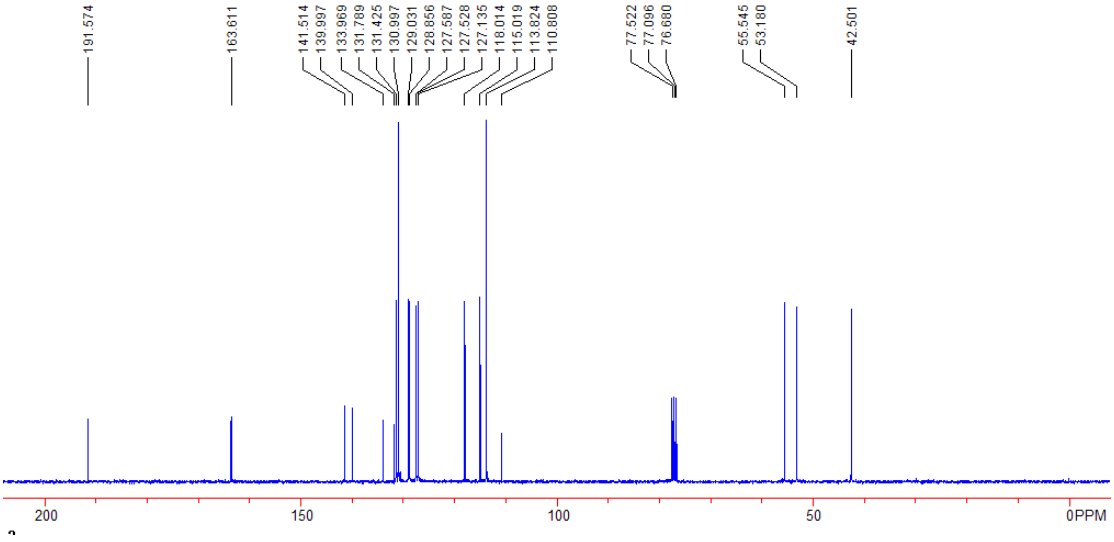




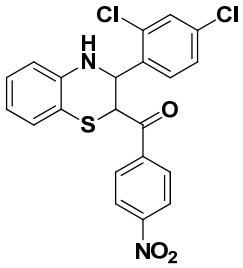
^{1}H and ^{13}C NMR spectra of 4fc

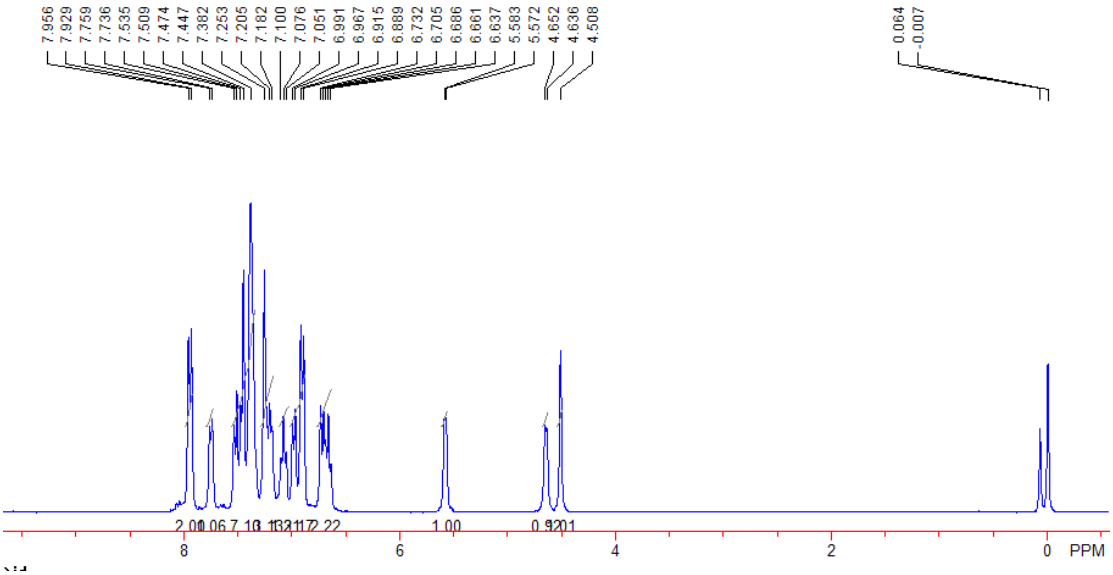


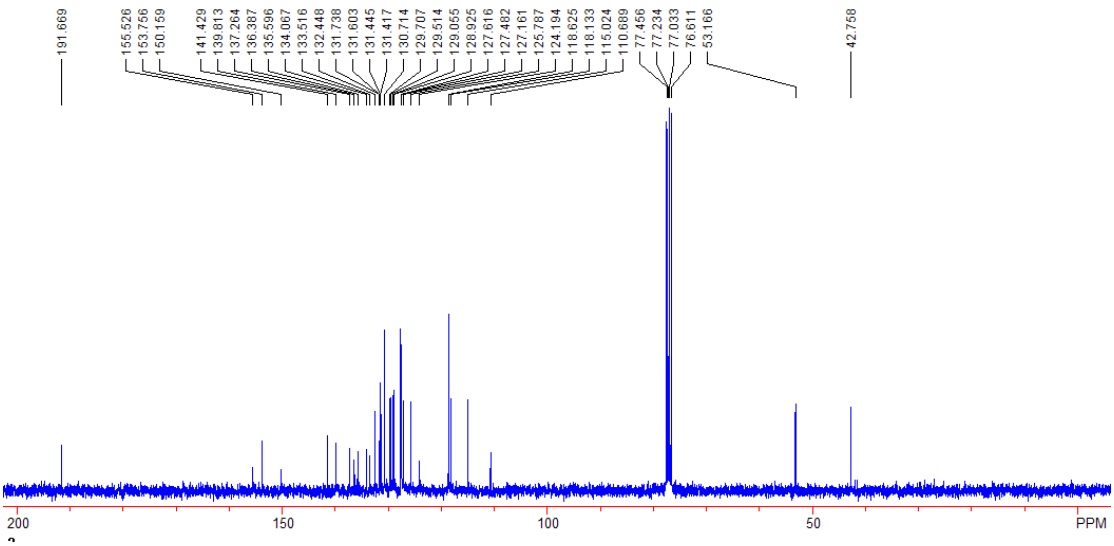




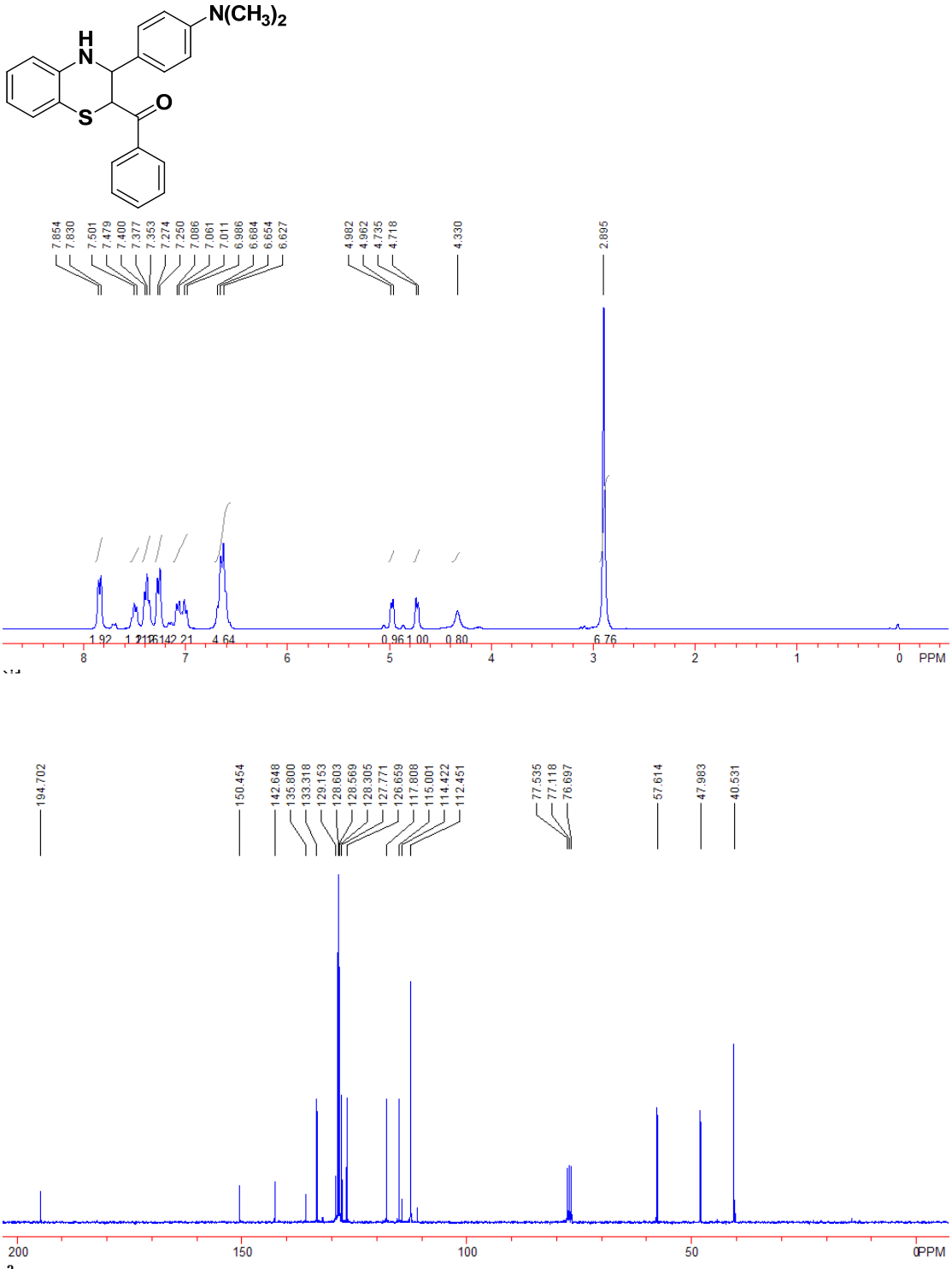
^{1}H and ^{13}C NMR spectra of 4fe



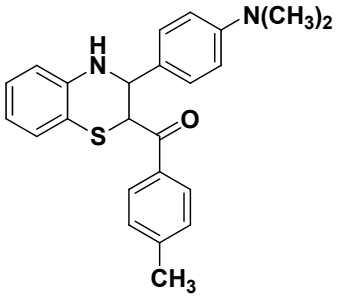


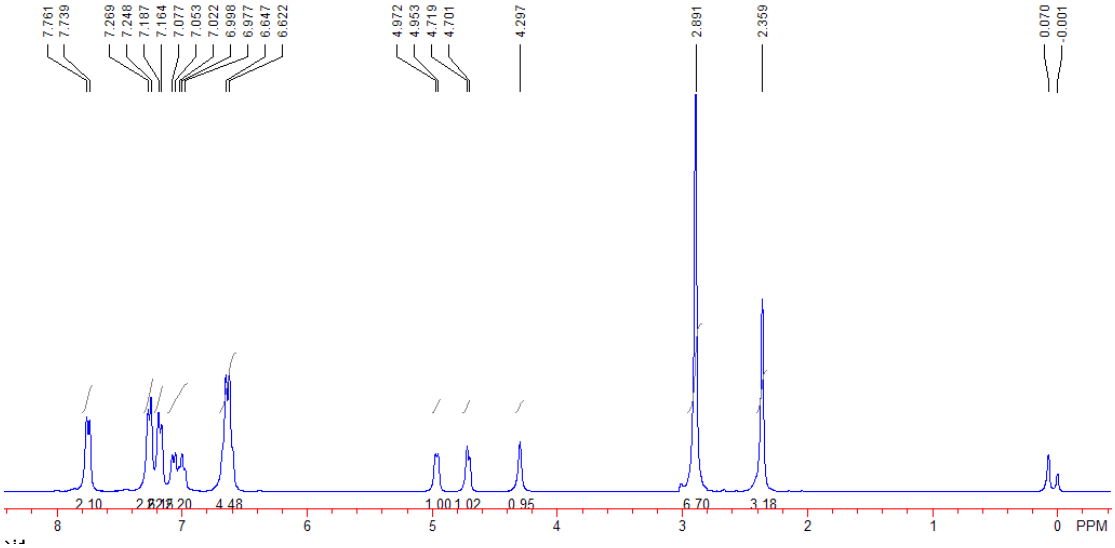


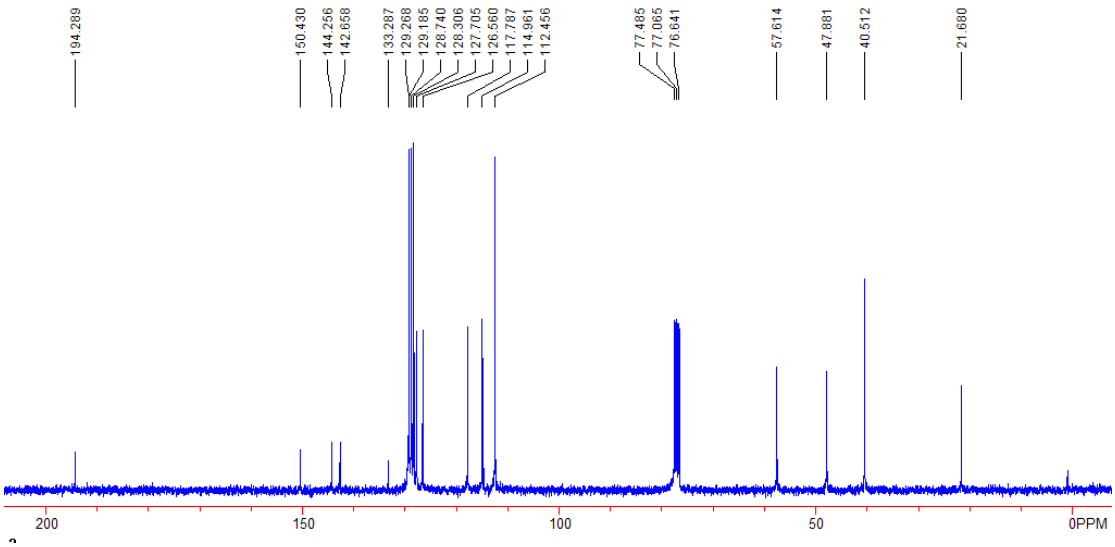
^{1}H and ^{13}C NMR spectra of 4ga



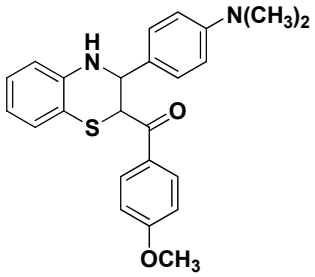
^{1}H and ^{13}C NMR spectra of 4gb

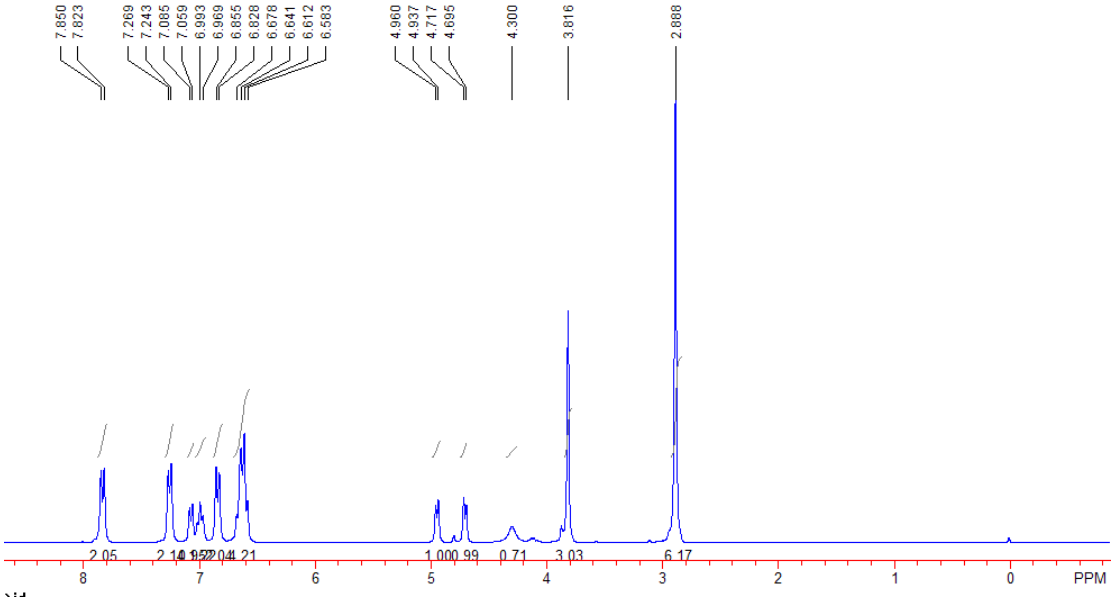


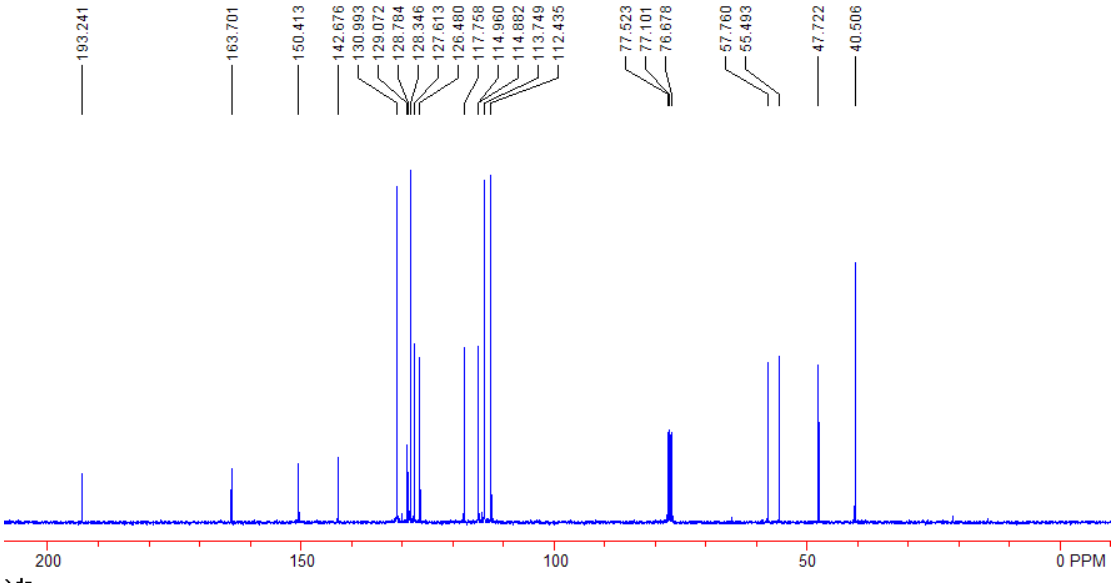




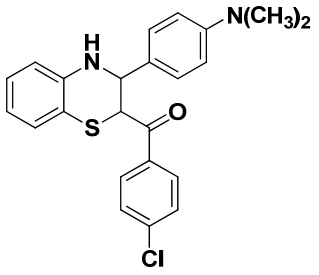
^{1}H and ^{13}C NMR spectra of 4gc

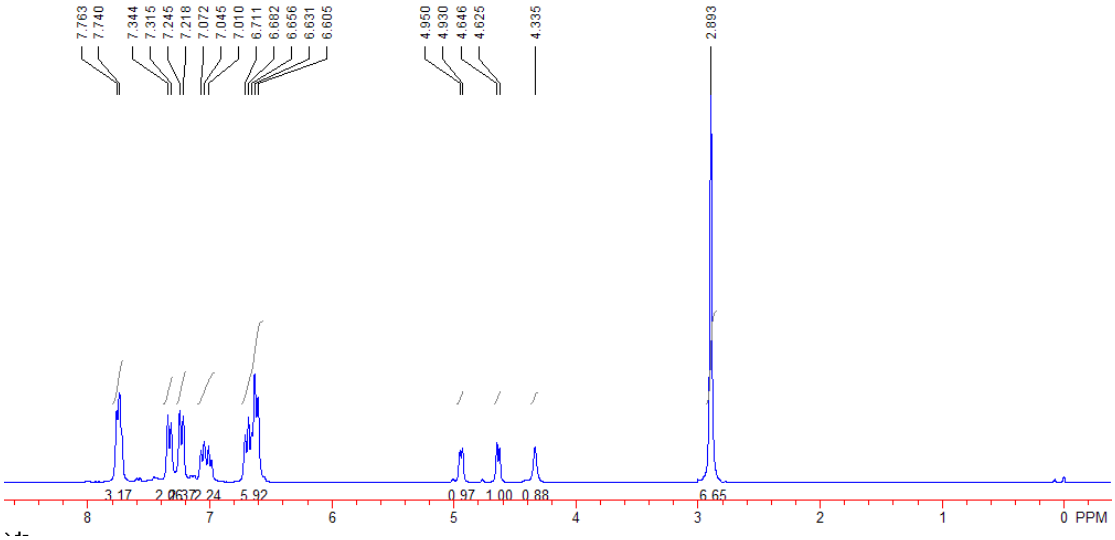


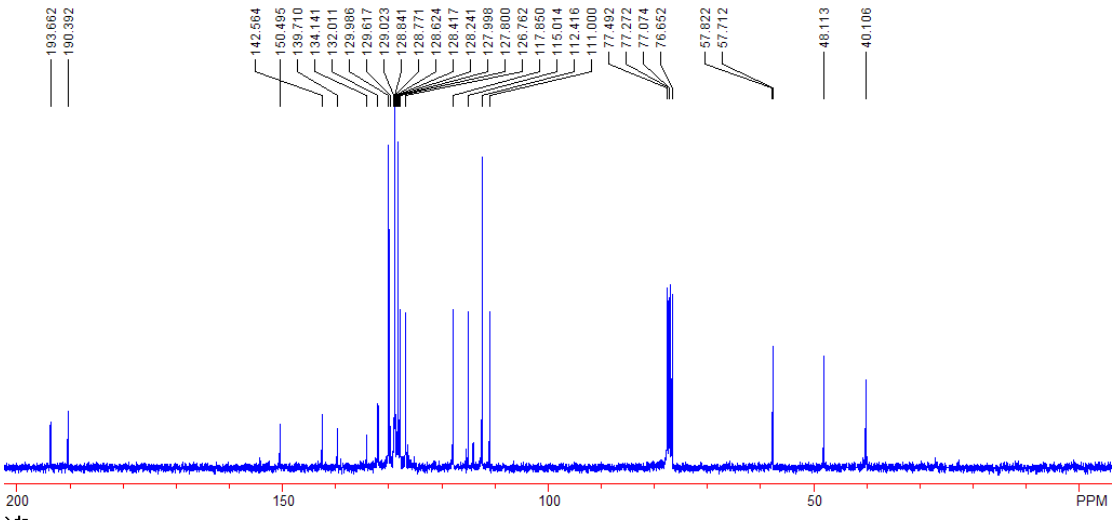




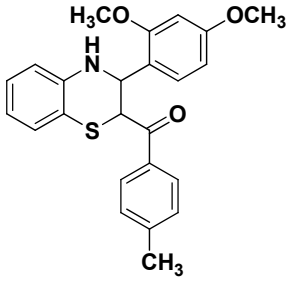
^{1}H and ^{13}C NMR spectra of 4gd

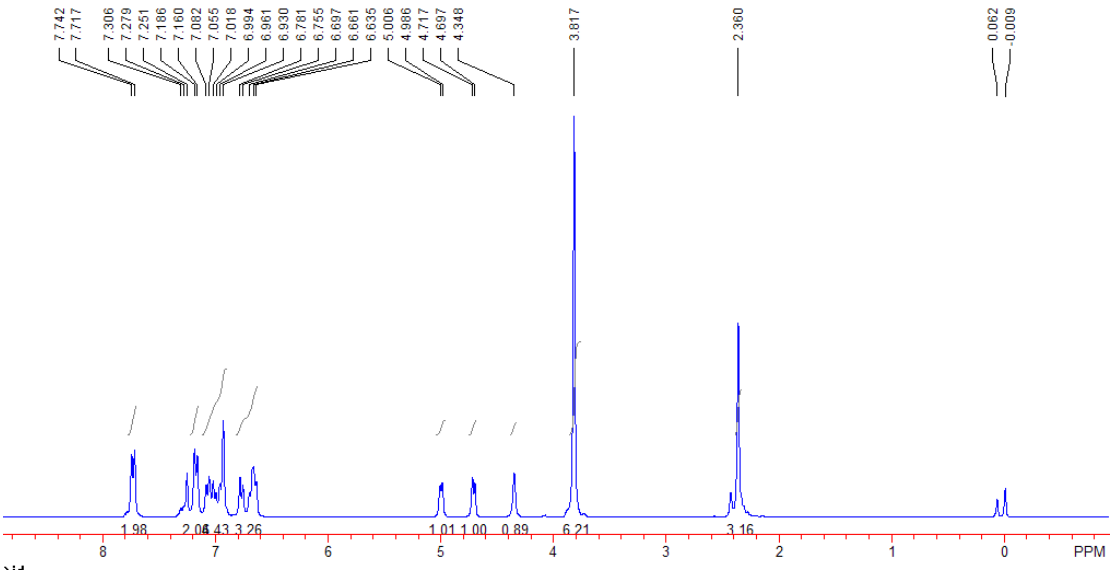


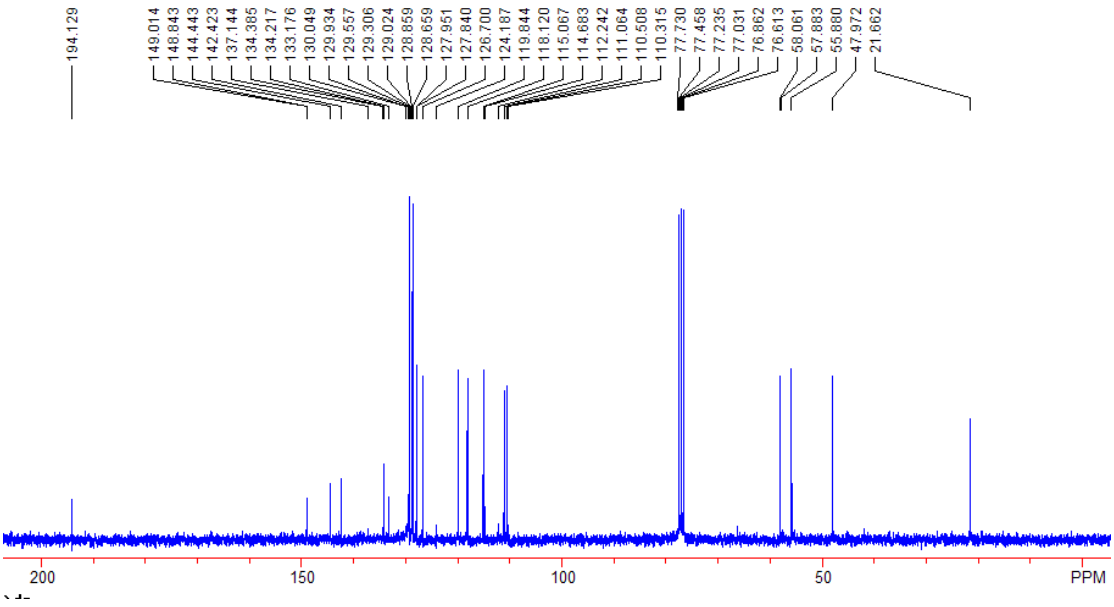




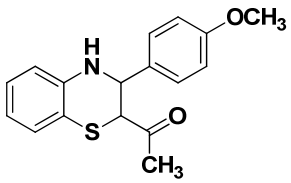
^{1}H and ^{13}C NMR spectra of 4hb

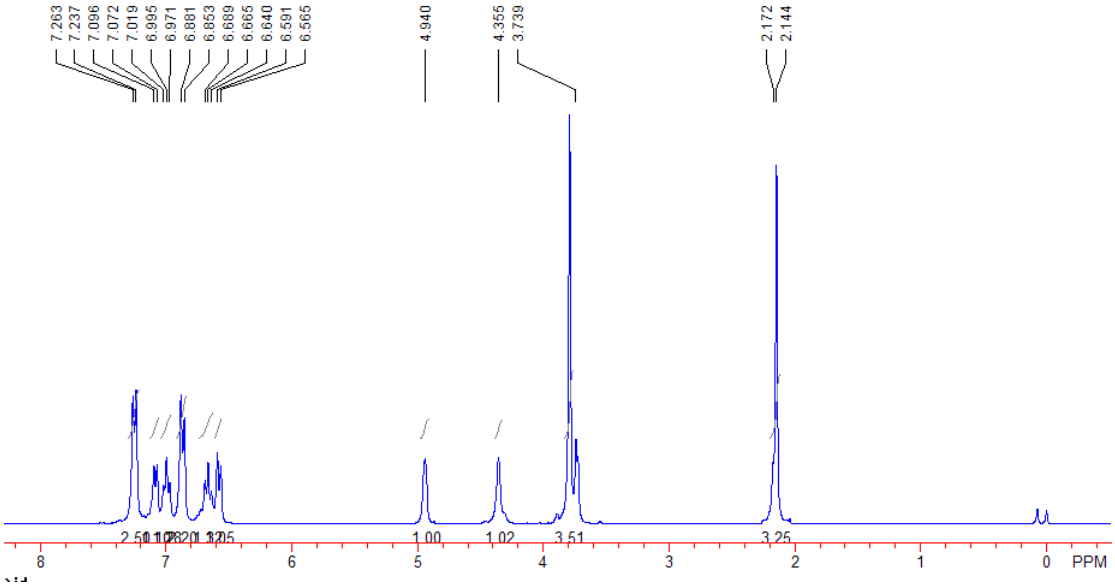


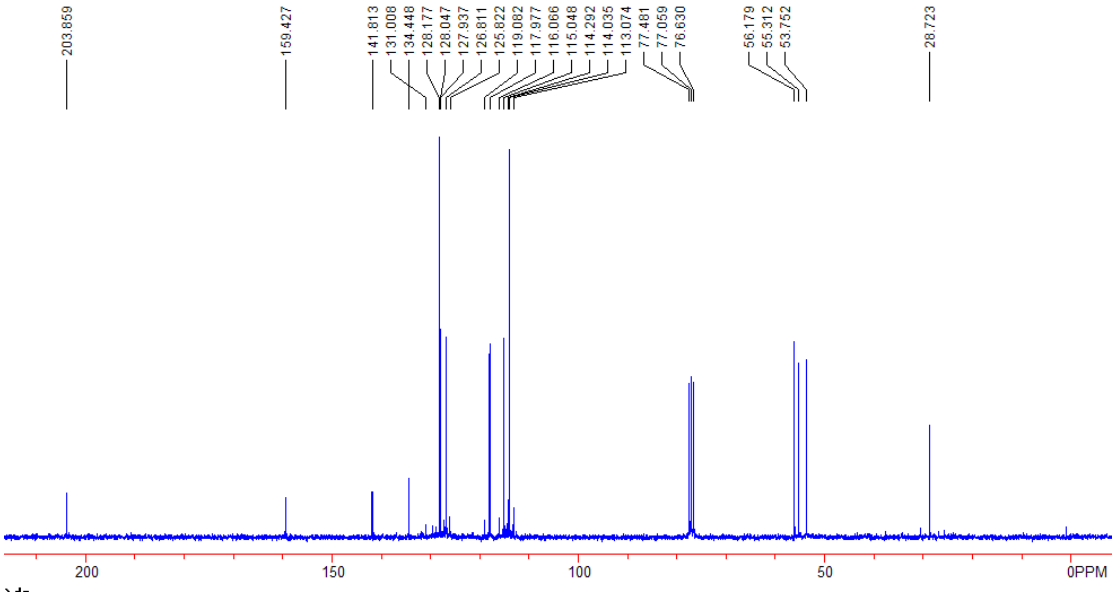




^{1}H and ^{13}C NMR spectra of 4cf







X-ray Crystallography

The diffraction data for **4fb** were collected on a Bruker SMART APEX diffractometer using Mo K α (λ = 0.71073 Å). The crystallographic data are listed in Table S1. The CIF deposition number: **CCDC-847691**.

Table S1. Crystal data and structure refinement for **4fb**.

Identification code	101130b_0m
Empirical formula	C22 H17 Cl2 N O S
Formula weight	414.33
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 10.1879(10) A alpha = 95.3630(10) deg. b = 10.7179(10) A beta = 109.8910(10) deg. c = 11.0530(11) A gamma = 115.9520(10) deg.
Volume	977.64(16) A^3
Z, Calculated density	2, 1.407 Mg/m^3
Absorption coefficient	0.451 mm^-1
F (000)	428
Crystal size	0.14 x 0.12 x 0.11 mm
Theta range for data collection	2.05 to 26.00 deg.
Limiting indices	-12<=h<=12, -12<=k<=13, -13<=l<=13.
Reflections collected / unique	7592 / 3797 [R(int) = 0.0186]
Completeness to theta = 26.00	98.9 %
Absorption correction	None
Max. and min. transmission	0.9521 and 0.9396
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3797 / 0 / 246
Goodness-of-fit on F^2	1.043
Final R indices [I>2 sigma (I)]	R1 = 0.0380, wR2 = 0.1012
R indices (all data)	R1 = 0.0446, wR2 = 0.1077
Largest diff. peak and hole	0.263 and -0.302 e.A^-3

Table S2. Selected Bond lengths [Å] and angles [°] for **4fb**.

Cl(1)-C(18)	1.7451(19)
Cl(2)-C(20)	1.742(2)
S(1)-C(6)	1.7581(19)
S(1)-C(7)	1.8184(19)
O(1)-C(8)	1.219(2)
N(1)-C(1)	1.374(2)
N(1)-C(16)	1.449(2)
N(1)-H(1)	0.8600
C(1)-C(6)	1.397(3)
C(1)-C(2)	1.402(3)
C(2)-C(3)	1.372(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.378(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.373(3)
C(4)-H(4)	0.9300
C(5)-C(6)	1.388(3)
C(5)-H(5)	0.9300
C(7)-C(8)	1.517(3)
C(7)-C(16)	1.540(2)
C(7)-H(7)	0.9800
C(8)-C(9)	1.482(3)
C(9)-C(10)	1.390(3)
C(9)-C(14)	1.391(3)
C(10)-C(11)	1.378(3)
C(10)-H(10)	0.9300
C(11)-C(12)	1.387(3)
C(11)-H(11)	0.9300
C(12)-C(13)	1.378(3)
C(12)-C(15)	1.508(3)
C(13)-C(14)	1.377(3)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-C(17)	1.516(3)
C(16)-H(16)	0.9800
C(17)-C(18)	1.385(3)
C(17)-C(22)	1.392(3)
C(18)-C(19)	1.383(3)
C(19)-C(20)	1.372(3)

C(19)-H(19)	0.9300
C(20)-C(21)	1.370(3)
C(21)-C(22)	1.375(3)
C(21)-H(21)	0.9300
C(22)-H(22)	0.9300

C(6)-S(1)-C(7)	98.55(8)
C(1)-N(1)-C(16)	127.18(16)
C(1)-N(1)-H(1)	116.4
C(16)-N(1)-H(1)	116.4
N(1)-C(1)-C(6)	122.93(17)
N(1)-C(1)-C(2)	119.26(18)
C(6)-C(1)-C(2)	117.79(18)
C(3)-C(2)-C(1)	120.9(2)
C(3)-C(2)-H(2)	119.6
C(1)-C(2)-H(2)	119.6
C(2)-C(3)-C(4)	120.8(2)
C(2)-C(3)-H(3)	119.6
C(4)-C(3)-H(3)	119.6
C(5)-C(4)-C(3)	119.3(2)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	120.7(2)
C(4)-C(5)-H(5)	119.6
C(6)-C(5)-H(5)	119.6
C(5)-C(6)-C(1)	120.42(19)
C(5)-C(6)-S(1)	119.26(16)
C(1)-C(6)-S(1)	120.23(14)
C(8)-C(7)-C(16)	112.48(14)
C(8)-C(7)-S(1)	109.74(12)
C(16)-C(7)-S(1)	111.74(13)
C(8)-C(7)-H(7)	107.5
C(16)-C(7)-H(7)	107.5
S(1)-C(7)-H(7)	107.5
O(1)-C(8)-C(9)	120.74(18)
O(1)-C(8)-C(7)	119.43(17)
C(9)-C(8)-C(7)	119.84(15)
C(10)-C(9)-C(14)	117.88(18)
C(10)-C(9)-C(8)	118.25(17)
C(14)-C(9)-C(8)	123.86(17)
C(11)-C(10)-C(9)	121.38(19)
C(11)-C(10)-H(10)	119.3
C(9)-C(10)-H(10)	119.3
C(10)-C(11)-C(12)	120.6(2)

C(10)-C(11)-H(11)	119.7
C(12)-C(11)-H(11)	119.7
C(13)-C(12)-C(11)	117.90(19)
C(13)-C(12)-C(15)	121.4(2)
C(11)-C(12)-C(15)	120.7(2)
C(14)-C(13)-C(12)	122.08(19)
C(14)-C(13)-H(13)	119.0
C(12)-C(13)-H(13)	119.0
C(13)-C(14)-C(9)	120.16(19)
C(13)-C(14)-H(14)	119.9
C(9)-C(14)-H(14)	119.9
C(12)-C(15)-H(15A)	109.5
C(12)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(12)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
N(1)-C(16)-C(17)	111.80(15)
N(1)-C(16)-C(7)	113.96(15)
C(17)-C(16)-C(7)	110.51(14)
N(1)-C(16)-H(16)	106.7
C(17)-C(16)-H(16)	106.7
C(7)-C(16)-H(16)	106.7
C(18)-C(17)-C(22)	116.41(17)
C(18)-C(17)-C(16)	121.91(16)
C(22)-C(17)-C(16)	121.67(16)
C(19)-C(18)-C(17)	122.62(18)
C(19)-C(18)-Cl(1)	117.09(15)
C(17)-C(18)-Cl(1)	120.24(15)
C(20)-C(19)-C(18)	118.47(19)
C(20)-C(19)-H(19)	120.8
C(18)-C(19)-H(19)	120.8
C(21)-C(20)-C(19)	121.10(19)
C(21)-C(20)-Cl(2)	118.89(17)
C(19)-C(20)-Cl(2)	119.98(17)
C(20)-C(21)-C(22)	119.28(19)
C(20)-C(21)-H(21)	120.4
C(22)-C(21)-H(21)	120.4
C(21)-C(22)-C(17)	122.04(18)
C(21)-C(22)-H(22)	119.0
C(17)-C(22)-H(22)	119.0

The diffraction data for **4ec** were collected on a Bruker SMART APEX diffractometer using Mo K α (λ = 0.71073 Å). The crystallographic data are listed in Table S1. The CIF deposition number: **CCDC-847690**.

Table S1. Crystal data and structure refinement for **4ec**.

Identification code	101130a_0m
Empirical formula	C22 H18 N2 O4 S
Formula weight	406.44
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, Pbca
Unit cell dimensions	a = 10.427(2) A alpha = 90 deg.
	b = 19.086(4) A beta = 90 deg.
	c = 19.748(4) A gamma = 90 deg.
Volume	3929.9(14) A^3
Z, Calculated density	8, 1.374 Mg/m^3
Absorption coefficient	0.197 mm^-1
F (000)	1696
Crystal size	0.14 x 0.12 x 0.11 mm
Theta range for data collection	2.06 to 27.53 deg.
Limiting indices	-13<=h<=13, -24<=k<=24, -22<=l<=25
Reflections collected / unique	32048 / 4512 [R(int) = 0.0286]
Completeness to theta = 26.00	99.6 %
Absorption correction	None
Max. and min. transmission	0.9787 and 0.9730
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4512 / 0 / 263
Goodness-of-fit on F^2	1.024
Final R indices [I>2 sigma (I)]	R1 = 0.0407, wR2 = 0.1047
R indices (all data)	R1 = 0.0549, wR2 = 0.1170
Largest diff. peak and hole	0.397 and -0.386 e.A^-3

Table S2. Selected Bond lengths [Å] and angles [°] for **4ec**.

S(1)-C(6)	1.7610(17)
S(1)-C(7)	1.8205(18)
O(1)-N(2)	1.212(2)
O(2)-N(2)	1.220(2)
O(3)-C(8)	1.209(2)
O(4)-C(19)	1.366(2)
O(4)-C(22)	1.424(3)
N(1)-C(1)	1.383(2)
N(1)-C(15)	1.451(2)
N(1)-H(1)	0.8600
N(2)-C(12)	1.469(2)
C(1)-C(2)	1.394(2)
C(1)-C(6)	1.397(2)
C(2)-C(3)	1.379(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.382(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.371(3)
C(4)-H(4)	0.9300
C(5)-C(6)	1.393(2)
C(5)-H(5)	0.9300
C(7)-C(8)	1.520(2)
C(7)-C(15)	1.535(2)
C(7)-H(7)	0.9800
C(8)-C(9)	1.494(2)
C(9)-C(10)	1.387(2)
C(9)-C(14)	1.389(2)
C(10)-C(11)	1.378(2)
C(10)-H(10)	0.9300
C(11)-C(12)	1.371(2)
C(11)-H(11)	0.9300
C(12)-C(13)	1.372(2)
C(13)-C(14)	1.378(2)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(16)	1.513(2)
C(15)-H(15)	0.9800
C(16)-C(21)	1.381(2)
C(16)-C(17)	1.389(2)
C(17)-C(18)	1.379(3)
C(17)-H(17)	0.9300

C(18)-C(19)	1.376(3)
C(18)-H(18)	0.9300
C(19)-C(20)	1.383(2)
C(20)-C(21)	1.379(3)
C(20)-H(20)	0.9300
C(21)-H(21)	0.9300
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600

C(6)-S(1)-C(7)	101.58(8)
C(19)-O(4)-C(22)	118.18(16)
C(1)-N(1)-C(15)	121.19(13)
C(1)-N(1)-H(1)	119.4
C(15)-N(1)-H(1)	119.4
O(1)-N(2)-O(2)	123.45(17)
O(1)-N(2)-C(12)	118.33(17)
O(2)-N(2)-C(12)	118.22(17)
N(1)-C(1)-C(2)	120.35(15)
N(1)-C(1)-C(6)	121.45(14)
C(2)-C(1)-C(6)	118.19(15)
C(3)-C(2)-C(1)	121.22(17)
C(3)-C(2)-H(2)	119.4
C(1)-C(2)-H(2)	119.4
C(2)-C(3)-C(4)	120.14(18)
C(2)-C(3)-H(3)	119.9
C(4)-C(3)-H(3)	119.9
C(5)-C(4)-C(3)	119.54(18)
C(5)-C(4)-H(4)	120.2
C(3)-C(4)-H(4)	120.2
C(4)-C(5)-C(6)	120.95(18)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
C(5)-C(6)-C(1)	119.93(16)
C(5)-C(6)-S(1)	116.42(13)
C(1)-C(6)-S(1)	123.65(13)
C(8)-C(7)-C(15)	112.85(13)
C(8)-C(7)-S(1)	104.52(11)
C(15)-C(7)-S(1)	111.30(11)
C(8)-C(7)-H(7)	109.3
C(15)-C(7)-H(7)	109.3
S(1)-C(7)-H(7)	109.3
O(3)-C(8)-C(9)	120.54(15)
O(3)-C(8)-C(7)	120.95(15)

C(9)-C(8)-C(7)	118.51(14)
C(10)-C(9)-C(14)	119.55(15)
C(10)-C(9)-C(8)	122.24(14)
C(14)-C(9)-C(8)	118.22(14)
C(11)-C(10)-C(9)	120.66(16)
C(11)-C(10)-H(10)	119.7
C(9)-C(10)-H(10)	119.7
C(12)-C(11)-C(10)	117.98(16)
C(12)-C(11)-H(11)	121.0
C(10)-C(11)-H(11)	121.0
C(11)-C(12)-C(13)	123.22(15)
C(11)-C(12)-N(2)	118.28(16)
C(13)-C(12)-N(2)	118.51(15)
C(12)-C(13)-C(14)	118.18(15)
C(12)-C(13)-H(13)	120.9
C(14)-C(13)-H(13)	120.9
C(13)-C(14)-C(9)	120.39(16)
C(13)-C(14)-H(14)	119.8
C(9)-C(14)-H(14)	119.8
N(1)-C(15)-C(16)	109.81(13)
N(1)-C(15)-C(7)	107.78(13)
C(16)-C(15)-C(7)	111.53(13)
N(1)-C(15)-H(15)	109.2
C(16)-C(15)-H(15)	109.2
C(7)-C(15)-H(15)	109.2
C(21)-C(16)-C(17)	117.56(16)
C(21)-C(16)-C(15)	121.07(14)
C(17)-C(16)-C(15)	121.36(15)
C(18)-C(17)-C(16)	121.17(16)
C(18)-C(17)-H(17)	119.4
C(16)-C(17)-H(17)	119.4
C(19)-C(18)-C(17)	120.26(16)
C(19)-C(18)-H(18)	119.9
C(17)-C(18)-H(18)	119.9
O(4)-C(19)-C(18)	116.06(16)
O(4)-C(19)-C(20)	124.42(17)
C(18)-C(19)-C(20)	119.53(16)
C(21)-C(20)-C(19)	119.58(16)
C(21)-C(20)-H(20)	120.2
C(19)-C(20)-H(20)	120.2
C(20)-C(21)-C(16)	121.89(16)
C(20)-C(21)-H(21)	119.1
C(16)-C(21)-H(21)	119.1
O(4)-C(22)-H(22A)	109.5

O(4)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
O(4)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5