Supporting Information

Diverse Reactivity of Nitrones with Electron Deficient Acetylenes

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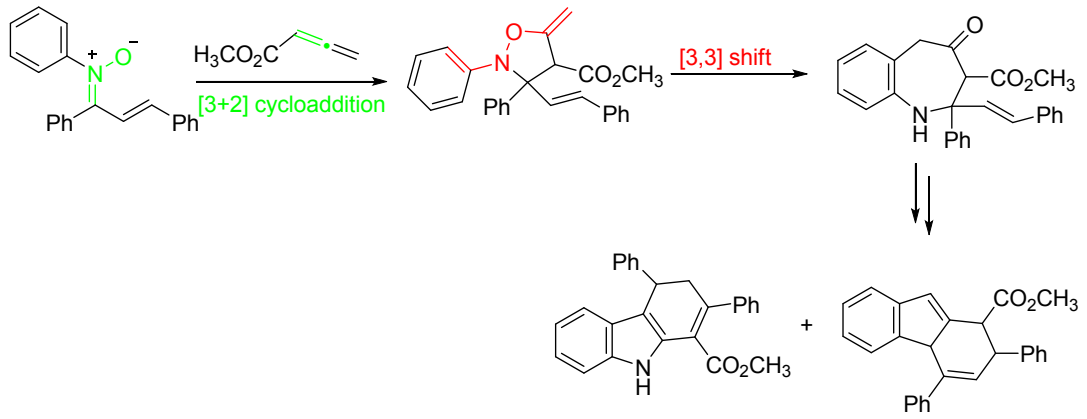
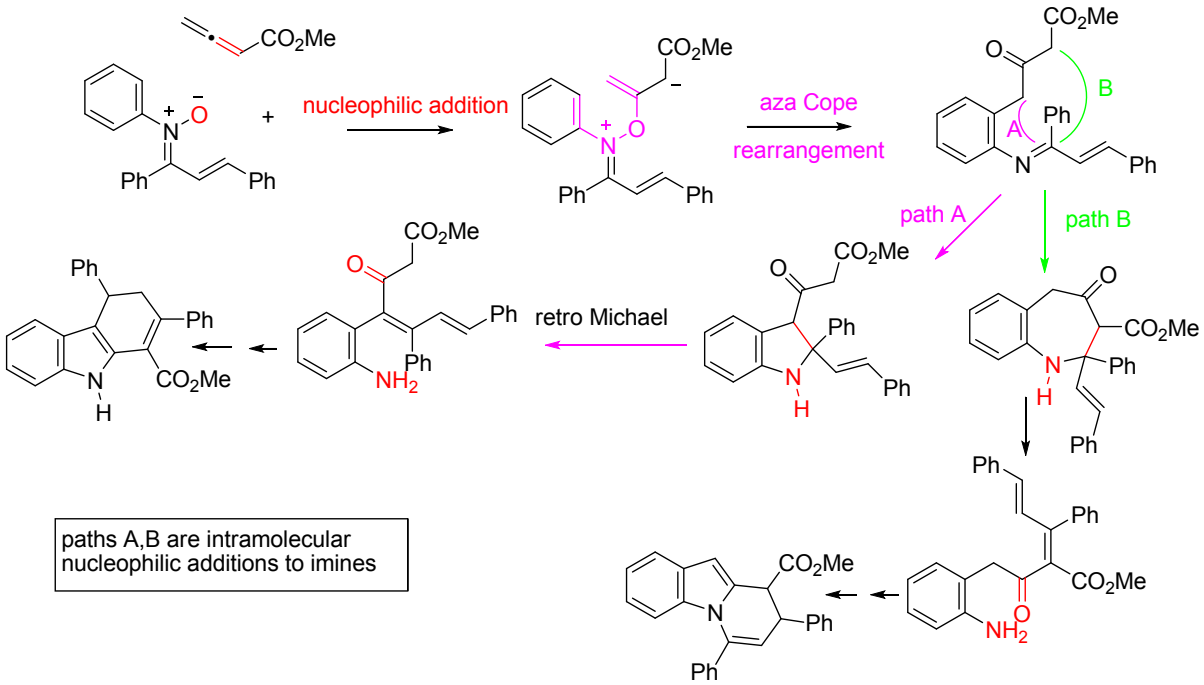
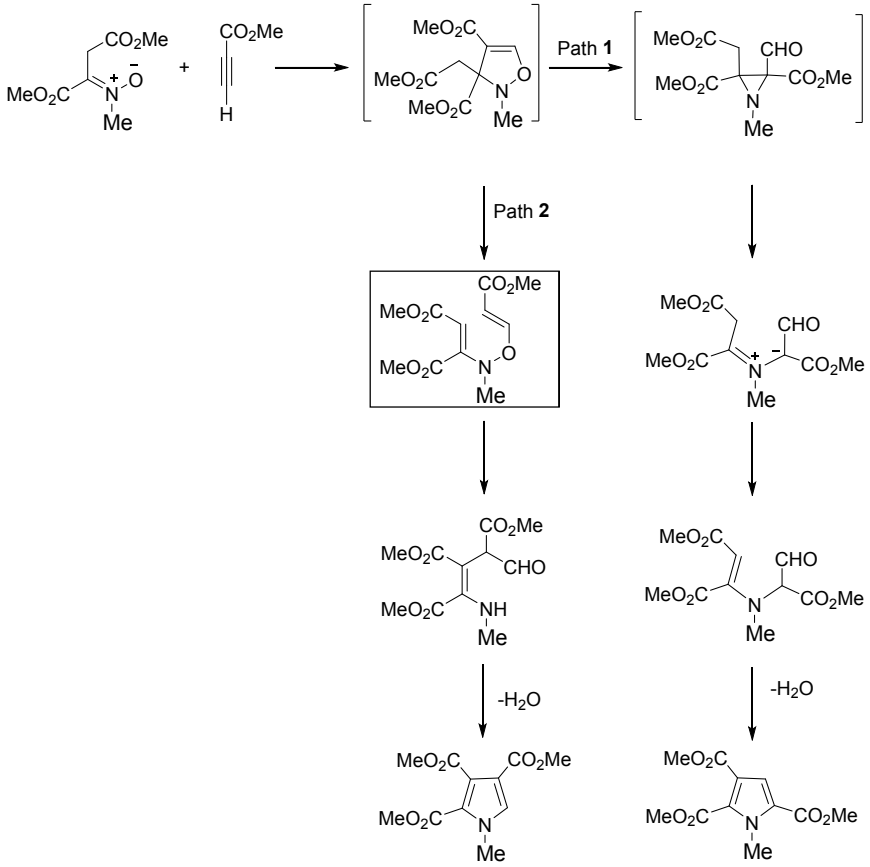
1a. *i*) Reported mechanism for the reaction between (*E*)-*N*-((*E*)-1,3-diphenylallylidene)aniline oxide and methyl buta-2,3-dienoate[2f]



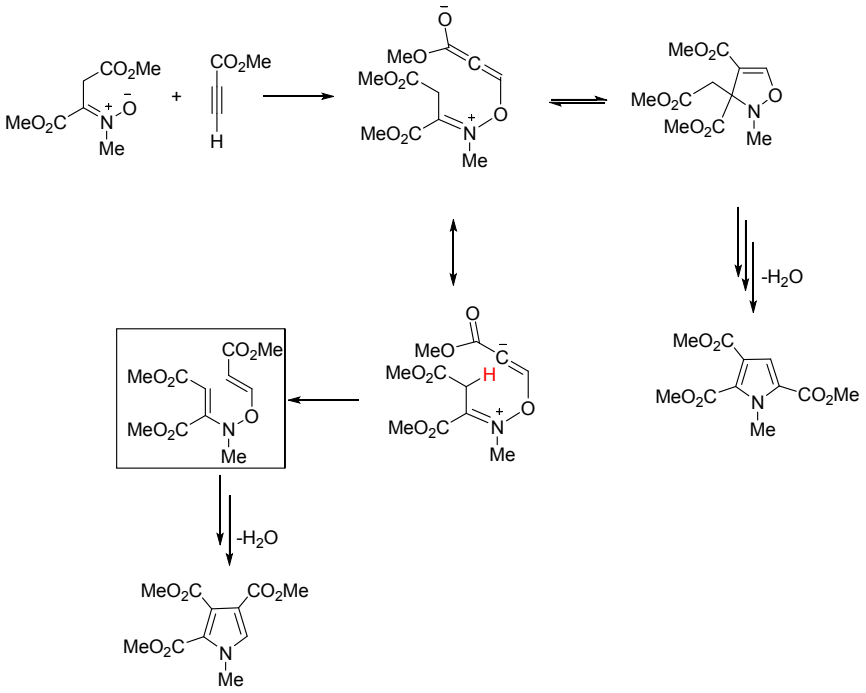
1a. *ii*) Alternate mechanism involving zwitterionic intermediate



1b. *i*) Reported mechanism for the reaction between (*E*)-*N*-(1,4-dimethoxy-1,4-dioxobutan-2-ylidene)methanamine oxide and methyl propiolate[13]



1b. *ii*) Alternate mechanism involving zwitterionic intermediate



1. Crystal data and structure refinement of compound **15**

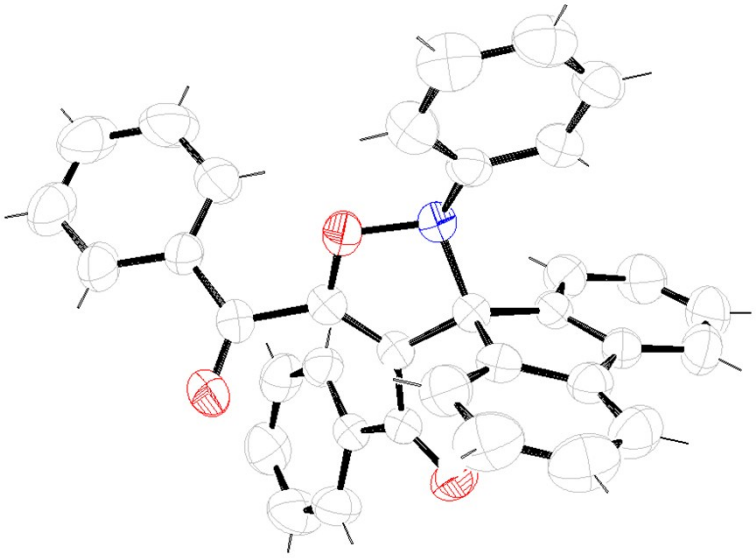


Table 1. Crystal data and structure refinement for Compound **15**.

Identification code	**15**
Empirical formula	C35 H23 N O3
Formula weight	505.54
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P12(1)/c1
Unit cell dimensions	a = 9.9946(4) A alpha = 90 deg.
	b = 20.4122(9) A beta = 102.181(2) deg.
	c = 13.4281(5) A gamma = 90 deg.
Volume	2677.81(19) A^3
Z, Calculated density	4, 1.254 Mg/m^3

Absorption coefficient	0.080 mm^-1
F(000)	1056
Crystal size	0.30 x 0.25 x 0.20 mm
Theta range for data collection	1.84 to 28.24 deg.
Limiting indices	-13<=h<=11, -11<=k<=27, -16<=l<=17
Reflections collected / unique	15195 / 6417 [R(int) = 0.0256]
Completeness to theta = 28.24	96.9 %
Max. and min. transmission	0.9842 and 0.9765
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6417 / 0 / 352
Goodness-of-fit on F^2	1.002
Final R indices [I>2sigma(I)]	R1 = 0.0473, wR2 = 0.1222
R indices (all data)	R1 = 0.0922, wR2 = 0.1541
Largest diff. peak and hole	0.188 and -0.220 e.A^-3

Table 2. Bond lengths [A] and angles [deg] for Compound **15**.

O(1)-C(7)	1.3517(19)
O(1)-N(1)	1.4763(17)
O(2)-C(25)	1.2250(18)
O(3)-C(8)	1.218(2)
N(1)-C(16)	1.428(2)
N(1)-C(5)	1.511(2)
C(1)-C(2)	1.364(3)
C(1)-C(17)	1.384(3)
C(1)-H(1)	0.9300

C(2)-C(3)	1.387(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.380(2)
C(3)-H(3)	0.9300
C(4)-C(18)	1.389(2)
C(4)-C(5)	1.524(2)
C(5)-C(24)	1.515(2)
C(5)-C(6)	1.517(2)
C(6)-C(7)	1.337(2)
C(6)-C(25)	1.475(2)
C(7)-C(8)	1.502(2)
C(8)-C(9)	1.471(2)
C(9)-C(32)	1.384(3)
C(9)-C(10)	1.385(2)
C(10)-C(11)	1.373(3)
C(10)-H(10)	0.9300
C(11)-C(12)	1.360(3)
C(11)-H(11)	0.9300
C(12)-C(33)	1.372(3)
C(12)-H(12)	0.9300
C(13)-C(14)	1.363(3)
C(13)-C(35)	1.374(3)
C(13)-H(13)	0.9300
C(14)-C(15)	1.394(3)
C(14)-H(14)	0.9300
C(15)-C(16)	1.379(2)
C(15)-H(15)	0.9300
C(16)-C(34)	1.384(2)
C(17)-C(18)	1.386(2)

C(17)-H(17)	0.9300
C(18)-C(19)	1.471(2)
C(19)-C(20)	1.380(2)
C(19)-C(24)	1.397(2)
C(20)-C(21)	1.374(3)
C(20)-H(20)	0.9300
C(21)-C(22)	1.379(3)
C(21)-H(21)	0.9300
C(22)-C(23)	1.377(3)
C(22)-H(22)	0.9300
C(23)-C(24)	1.380(2)
C(23)-H(23)	0.9300
C(25)-C(26)	1.489(2)
C(26)-C(31)	1.382(2)
C(26)-C(27)	1.387(2)
C(27)-C(28)	1.382(3)
C(27)-H(27)	0.9300
C(28)-C(29)	1.359(3)
C(28)-H(28)	0.9300
C(29)-C(30)	1.368(3)
C(29)-H(29)	0.9300
C(30)-C(31)	1.369(3)
C(30)-H(30)	0.9300
C(31)-H(31)	0.9300
C(32)-C(33)	1.378(3)
C(32)-H(32)	0.9300
C(33)-H(33)	0.9300
C(34)-C(35)	1.383(3)
C(34)-H(34)	0.9300

C(35)-H(35)	0.9300
C(7)-O(1)-N(1)	104.03(11)
C(16)-N(1)-O(1)	108.61(12)
C(16)-N(1)-C(5)	118.81(12)
O(1)-N(1)-C(5)	104.48(11)
C(2)-C(1)-C(17)	121.74(19)
C(2)-C(1)-H(1)	119.1
C(17)-C(1)-H(1)	119.1
C(1)-C(2)-C(3)	120.73(19)
C(1)-C(2)-H(2)	119.6
C(3)-C(2)-H(2)	119.6
C(4)-C(3)-C(2)	118.12(19)
C(4)-C(3)-H(3)	120.9
C(2)-C(3)-H(3)	120.9
C(3)-C(4)-C(18)	121.21(16)
C(3)-C(4)-C(5)	128.75(16)
C(18)-C(4)-C(5)	110.04(14)
N(1)-C(5)-C(24)	110.15(12)
N(1)-C(5)-C(6)	98.63(12)
C(24)-C(5)-C(6)	116.75(13)
N(1)-C(5)-C(4)	115.72(13)
C(24)-C(5)-C(4)	102.24(12)
C(6)-C(5)-C(4)	114.00(12)
C(7)-C(6)-C(25)	129.64(16)
C(7)-C(6)-C(5)	107.57(14)
C(25)-C(6)-C(5)	122.62(14)
C(6)-C(7)-O(1)	114.20(15)
C(6)-C(7)-C(8)	130.80(16)
O(1)-C(7)-C(8)	114.75(14)

O(3)-C(8)-C(9)	122.55(17)
O(3)-C(8)-C(7)	117.45(15)
C(9)-C(8)-C(7)	119.98(15)
C(32)-C(9)-C(10)	119.14(17)
C(32)-C(9)-C(8)	122.23(17)
C(10)-C(9)-C(8)	118.59(16)
C(11)-C(10)-C(9)	120.5(2)
C(11)-C(10)-H(10)	119.7
C(9)-C(10)-H(10)	119.7
C(12)-C(11)-C(10)	119.9(2)
C(12)-C(11)-H(11)	120.0
C(10)-C(11)-H(11)	120.0
C(11)-C(12)-C(33)	120.5(2)
C(11)-C(12)-H(12)	119.7
C(33)-C(12)-H(12)	119.7
C(14)-C(13)-C(35)	119.51(19)
C(14)-C(13)-H(13)	120.2
C(35)-C(13)-H(13)	120.2
C(13)-C(14)-C(15)	121.0(2)
C(13)-C(14)-H(14)	119.5
C(15)-C(14)-H(14)	119.5
C(16)-C(15)-C(14)	119.30(19)
C(16)-C(15)-H(15)	120.4
C(14)-C(15)-H(15)	120.4
C(15)-C(16)-C(34)	119.66(17)
C(15)-C(16)-N(1)	122.83(16)
C(34)-C(16)-N(1)	117.29(15)
C(1)-C(17)-C(18)	118.0(2)
C(1)-C(17)-H(17)	121.0

C(18)-C(17)-H(17)	121.0
C(17)-C(18)-C(4)	120.18(16)
C(17)-C(18)-C(19)	130.86(17)
C(4)-C(18)-C(19)	108.95(14)
C(20)-C(19)-C(24)	119.74(16)
C(20)-C(19)-C(18)	131.70(16)
C(24)-C(19)-C(18)	108.55(14)
C(21)-C(20)-C(19)	118.76(18)
C(21)-C(20)-H(20)	120.6
C(19)-C(20)-H(20)	120.6
C(20)-C(21)-C(22)	121.38(19)
C(20)-C(21)-H(21)	119.3
C(22)-C(21)-H(21)	119.3
C(23)-C(22)-C(21)	120.55(18)
C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(22)-C(23)-C(24)	118.42(17)
C(22)-C(23)-H(23)	120.8
C(24)-C(23)-H(23)	120.8
C(23)-C(24)-C(19)	121.13(16)
C(23)-C(24)-C(5)	128.68(15)
C(19)-C(24)-C(5)	110.18(13)
O(2)-C(25)-C(6)	119.43(15)
O(2)-C(25)-C(26)	120.90(15)
C(6)-C(25)-C(26)	119.63(13)
C(31)-C(26)-C(27)	118.29(16)
C(31)-C(26)-C(25)	118.96(15)
C(27)-C(26)-C(25)	122.70(15)
C(28)-C(27)-C(26)	120.11(18)

C(28)-C(27)-H(27)	119.9
C(26)-C(27)-H(27)	119.9
C(29)-C(28)-C(27)	120.55(18)
C(29)-C(28)-H(28)	119.7
C(27)-C(28)-H(28)	119.7
C(28)-C(29)-C(30)	119.9(2)
C(28)-C(29)-H(29)	120.1
C(30)-C(29)-H(29)	120.1
C(29)-C(30)-C(31)	120.3(2)
C(29)-C(30)-H(30)	119.9
C(31)-C(30)-H(30)	119.9
C(30)-C(31)-C(26)	120.87(18)
C(30)-C(31)-H(31)	119.6
C(26)-C(31)-H(31)	119.6
C(9)-C(32)-C(33)	119.7(2)
C(9)-C(32)-H(32)	120.2
C(33)-C(32)-H(32)	120.2
C(12)-C(33)-C(32)	120.2(2)
C(12)-C(33)-H(33)	119.9
C(32)-C(33)-H(33)	119.9
C(16)-C(34)-C(35)	120.05(18)
C(16)-C(34)-H(34)	120.0
C(35)-C(34)-H(34)	120.0
C(13)-C(35)-C(34)	120.4(2)
C(13)-C(35)-H(35)	119.8
C(34)-C(35)-H(35)	119.8

Symmetry transformations used to generate equivalent atoms:

2. *ORTEP* Diagram of Compound **17**

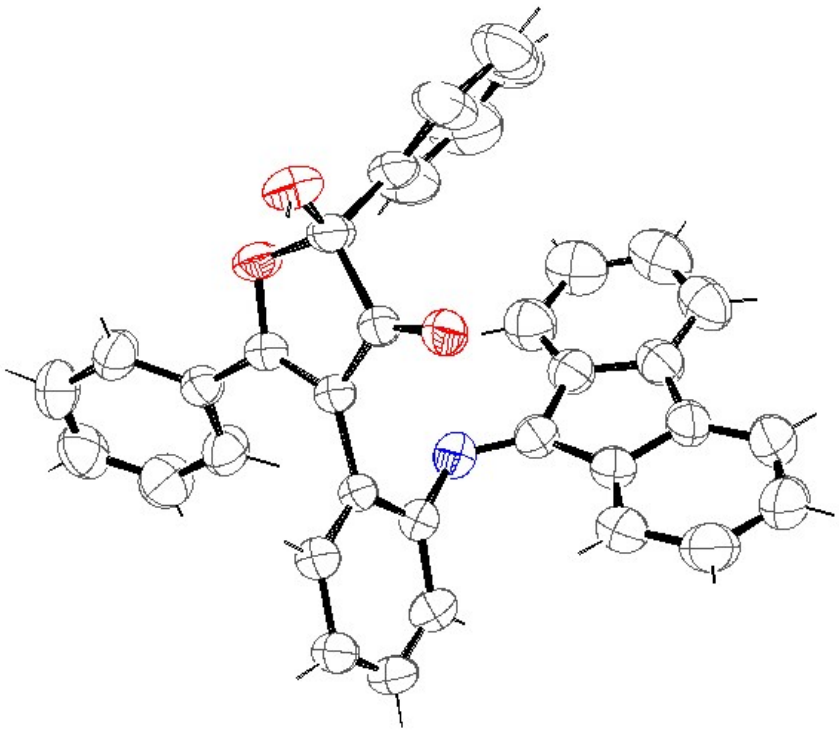


Table 1. Crystal data and structure refinement for compound **17**.

Identification code	compound **17**
Empirical formula	C35 H23 N O3
Formula weight	505.67
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 10.992(2) A alpha = 109.668(2) deg.
	b = 11.411(3) A beta = 106.721(4) deg.
	c = 13.062(3) A gamma = 104.309(3) deg.
Volume	1365.6(5) A^3
Z, Calculated density	2, 1.230 Mg/m^3
Absorption coefficient	0.078 mm^-1
F(000)	528
Crystal size	0.50 x 0.45 x 0.30 mm

Theta range for data collection	1.81 to 26.02 deg.
Limiting indices	-13<=h<=13, -14<=k<=14, -16<=l<=16
Reflections collected / unique	14311 / 5348 [R(int) = 0.0322]
Completeness to theta = 26.00	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9704 and 0.9551
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5348 / 0 / 462
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0447, wR2 = 0.0986
R indices (all data)	R1 = 0.0802, wR2 = 0.1099
Extinction coefficient	0.0044(13)
Largest diff. peak and hole	0.177 and -0.141 e.A^-3

Table 2. Bond lengths [A] and angles [deg] for compound **17**.

O(1)-C(21)	1.2276(17)
O(2)-C(23)	1.3584(17)
O(2)-C(22)	1.4637(18)
O(3)-C(22)	1.3742(19)
N(1)-C(13)	1.277(2)
N(1)-C(14)	1.416(2)
C(21)-C(20)	1.424(2)
C(21)-C(22)	1.541(2)
C(18)-C(19)	1.387(2)
C(18)-C(17)	1.392(2)
C(19)-C(14)	1.390(2)
C(19)-C(20)	1.489(2)
C(20)-C(23)	1.363(2)

C(14)-C(15)	1.386(2)
C(30)-C(31)	1.361(3)
C(30)-C(35)	1.371(3)
C(30)-C(22)	1.509(2)
C(24)-C(25)	1.386(2)
C(24)-C(29)	1.386(2)
C(24)-C(23)	1.458(2)
C(15)-C(16)	1.375(3)
C(17)-C(16)	1.382(3)
C(13)-C(1)	1.480(2)
C(13)-C(12)	1.489(2)
C(12)-C(11)	1.387(2)
C(12)-C(7)	1.401(2)
C(25)-C(26)	1.382(3)
C(1)-C(2)	1.381(3)
C(1)-C(6)	1.391(2)
C(7)-C(8)	1.380(3)
C(7)-C(6)	1.473(3)
C(29)-C(28)	1.383(3)
C(6)-C(5)	1.388(3)
C(8)-C(9)	1.373(3)
C(10)-C(9)	1.378(3)
C(10)-C(11)	1.391(3)
C(28)-C(27)	1.361(3)
C(27)-C(26)	1.366(3)
C(5)-C(4)	1.382(3)
C(35)-C(34)	1.371(3)
C(2)-C(3)	1.390(3)
C(3)-C(4)	1.372(3)

C(31)-C(32)	1.385(4)
C(33)-C(34)	1.345(4)
C(33)-C(32)	1.360(4)
C(23)-O(2)-C(22)	108.20(10)
C(13)-N(1)-C(14)	120.61(14)
O(1)-C(21)-C(20)	130.52(13)
O(1)-C(21)-C(22)	122.09(13)
C(20)-C(21)-C(22)	107.39(12)
C(19)-C(18)-C(17)	121.94(17)
C(18)-C(19)-C(14)	119.19(14)
C(18)-C(19)-C(20)	120.84(14)
C(14)-C(19)-C(20)	119.96(13)
C(23)-C(20)-C(21)	106.83(13)
C(23)-C(20)-C(19)	126.55(13)
C(21)-C(20)-C(19)	126.55(13)
C(15)-C(14)-C(19)	119.22(16)
C(15)-C(14)-N(1)	121.90(16)
C(19)-C(14)-N(1)	118.52(13)
C(31)-C(30)-C(35)	118.6(2)
C(31)-C(30)-C(22)	122.39(18)
C(35)-C(30)-C(22)	118.87(17)
C(25)-C(24)-C(29)	118.93(16)
C(25)-C(24)-C(23)	120.97(15)
C(29)-C(24)-C(23)	120.10(16)
O(2)-C(23)-C(20)	114.69(13)
O(2)-C(23)-C(24)	114.76(12)
C(20)-C(23)-C(24)	130.54(14)
C(16)-C(15)-C(14)	120.37(19)
C(16)-C(17)-C(18)	117.37(17)

O(3)-C(22)-O(2)	108.97(12)
O(3)-C(22)-C(30)	110.50(13)
O(2)-C(22)-C(30)	109.20(13)
O(3)-C(22)-C(21)	113.75(13)
O(2)-C(22)-C(21)	102.66(11)
C(30)-C(22)-C(21)	111.39(13)
N(1)-C(13)-C(1)	121.28(15)
N(1)-C(13)-C(12)	133.08(16)
C(1)-C(13)-C(12)	105.63(14)
C(11)-C(12)-C(7)	119.63(17)
C(11)-C(12)-C(13)	132.57(16)
C(7)-C(12)-C(13)	107.79(15)
C(26)-C(25)-C(24)	120.02(19)
C(2)-C(1)-C(6)	121.09(18)
C(2)-C(1)-C(13)	129.67(17)
C(6)-C(1)-C(13)	109.23(16)
C(8)-C(7)-C(12)	120.96(19)
C(8)-C(7)-C(6)	129.83(18)
C(12)-C(7)-C(6)	109.21(15)
C(15)-C(16)-C(17)	121.68(17)
C(28)-C(29)-C(24)	120.1(2)
C(5)-C(6)-C(1)	120.08(19)
C(5)-C(6)-C(7)	131.78(19)
C(1)-C(6)-C(7)	108.09(15)
C(9)-C(8)-C(7)	118.7(2)
C(9)-C(10)-C(11)	120.6(2)
C(27)-C(28)-C(29)	120.4(2)
C(12)-C(11)-C(10)	118.8(2)
C(28)-C(27)-C(26)	120.2(2)

C(27)-C(26)-C(25)	120.4(2)
C(4)-C(5)-C(6)	118.4(2)
C(30)-C(35)-C(34)	121.2(3)
C(8)-C(9)-C(10)	121.3(2)
C(1)-C(2)-C(3)	118.4(2)
C(4)-C(3)-C(2)	120.5(2)
C(30)-C(31)-C(32)	119.8(3)
C(3)-C(4)-C(5)	121.6(2)
C(34)-C(33)-C(32)	119.8(3)
C(33)-C(34)-C(35)	120.0(3)
C(33)-C(32)-C(31)	120.6(3)

Symmetry transformations used to generate equivalent atoms:

3. Crystal data and structure refinement of compound **22**

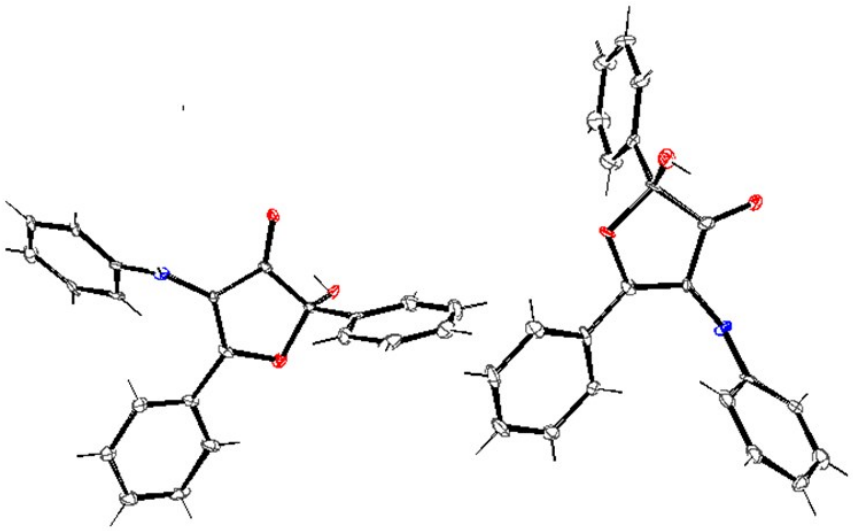


Table 1. Crystal data and structure refinement for Compound **22**

Identification code	**22**	
Empirical formula	$C_{22}H_{17}NO_3$	
Formula weight	343.37	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 27.608(2) Å	α= 90°.
	b = 5.5963(5) Å	β= 90°.
	c = 21.6736(19) Å	γ = 90°.
Volume	3348.6(5) $Å^3$	
Z	8	
Density (calculated)	1.362 Mg/m^3	
Absorption coefficient	0.091 mm^{-1}	
F(000)	1440	
Crystal size	0.47 x 0.39 x 0.37 mm^3	
Theta range for data collection	2.95 to 25.00°.	
Index ranges	$-32\leq h\leq 32$, $-6\leq k\leq 6$, $-25\leq l\leq 24$	
Reflections collected	93166	
Independent reflections	5857 [R(int) = 0.0755]	
Completeness to theta = 25.00°	99.9 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9671 and 0.9582
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5857 / 1 / 439
Goodness-of-fit on F^2	1.152
Final R indices [I>2sigma(I)]	R1 = 0.0902, wR2 = 0.2349
R indices (all data)	R1 = 0.0925, wR2 = 0.2365
Absolute structure parameter	-0.2(19)
Largest diff. peak and hole	0.934 and -0.546 e.$Å^{-3}$

Table 2. Bond lengths [Å] and angles [°] for Compound **22**.

O(1)-C(4)	1.363(6)
O(1)-C(1)	1.461(6)
O(2)-C(2)	1.211(6)
O(3)-C(1)	1.381(6)
O(3)-H(3A)	0.8400
O(4)-C(26)	1.347(6)
O(4)-C(23)	1.484(6)
N(1)-C(3)	1.391(7)
N(1)-C(11)	1.410(7)
N(1)-H(1A)	0.8800
C(1)-C(5)	1.510(7)
C(1)-C(2)	1.528(7)
C(2)-C(3)	1.444(7)
C(3)-C(4)	1.364(7)
C(4)-C(17)	1.466(7)
C(5)-C(10)	1.372(8)
C(5)-C(6)	1.393(8)
C(6)-C(7)	1.424(8)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.361(9)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.384(9)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.400(9)
C(9)-H(9A)	0.9500
C(10)-H(10A)	0.9500

C(11)-C(16)	1.366(8)
C(11)-C(12)	1.396(8)
C(12)-C(13)	1.388(8)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.380(9)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.368(8)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.433(8)
C(15)-H(15A)	0.9500
C(16)-H(16A)	0.9500
C(17)-C(18)	1.389(8)
C(17)-C(22)	1.390(8)
C(18)-C(19)	1.380(7)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.391(9)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.378(9)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.383(8)
C(21)-H(21A)	0.9500
C(22)-H(22A)	0.9500
N(2)-C(25)	1.387(7)
N(2)-C(33)	1.418(7)
N(2)-H(2A)	0.8800
O(5)-C(24)	1.255(6)
O(6)-C(23)	1.379(6)
O(6)-H(6B)	0.8400
C(23)-C(27)	1.501(7)
C(23)-C(24)	1.524(7)
C(24)-C(25)	1.430(7)
C(25)-C(26)	1.377(7)
C(26)-C(39)	1.476(7)
C(27)-C(28)	1.380(8)
C(27)-C(32)	1.387(8)
C(28)-C(29)	1.388(8)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.375(9)

C(29)-H(29A)	0.9500
C(30)-C(31)	1.384(9)
C(30)-H(30A)	0.9500
C(31)-C(32)	1.386(8)
C(31)-H(31A)	0.9500
C(32)-H(32A)	0.9500
C(33)-C(34)	1.379(8)
C(33)-C(38)	1.385(7)
C(34)-C(35)	1.409(8)
C(34)-H(34A)	0.9500
C(35)-C(36)	1.369(9)
C(35)-H(35A)	0.9500
C(36)-C(37)	1.381(8)
C(36)-H(36A)	0.9500
C(37)-C(38)	1.397(8)
C(37)-H(37A)	0.9500
C(38)-H(38A)	0.9500
C(39)-C(40)	1.356(8)
C(39)-C(44)	1.400(8)
C(40)-C(41)	1.391(7)
C(40)-H(40A)	0.9500
C(41)-C(42)	1.401(8)
C(41)-H(41A)	0.9500
C(42)-C(43)	1.373(9)
C(42)-H(42A)	0.9500
C(43)-C(44)	1.394(8)
C(43)-H(43A)	0.9500
C(44)-H(44A)	0.9500

C(4)-O(1)-C(1)	109.2(4)
C(1)-O(3)-H(3A)	109.5
C(26)-O(4)-C(23)	107.7(4)
C(3)-N(1)-C(11)	125.8(4)
C(3)-N(1)-H(1A)	117.1
C(11)-N(1)-H(1A)	117.1
O(3)-C(1)-O(1)	108.6(4)
O(3)-C(1)-C(5)	110.6(4)
O(1)-C(1)-C(5)	110.1(4)

O(3)-C(1)-C(2)	113.6(4)
O(1)-C(1)-C(2)	102.4(4)
C(5)-C(1)-C(2)	111.2(4)
O(2)-C(2)-C(3)	127.9(5)
O(2)-C(2)-C(1)	124.1(5)
C(3)-C(2)-C(1)	107.9(4)
C(4)-C(3)-N(1)	131.9(5)
C(4)-C(3)-C(2)	106.3(5)
N(1)-C(3)-C(2)	121.7(4)
O(1)-C(4)-C(3)	114.1(4)
O(1)-C(4)-C(17)	113.7(4)
C(3)-C(4)-C(17)	132.2(5)
C(10)-C(5)-C(6)	119.9(5)
C(10)-C(5)-C(1)	120.9(5)
C(6)-C(5)-C(1)	119.1(5)
C(5)-C(6)-C(7)	119.7(5)
C(5)-C(6)-H(6A)	120.2
C(7)-C(6)-H(6A)	120.2
C(8)-C(7)-C(6)	119.0(5)
C(8)-C(7)-H(7A)	120.5
C(6)-C(7)-H(7A)	120.5
C(7)-C(8)-C(9)	121.6(5)
C(7)-C(8)-H(8A)	119.2
C(9)-C(8)-H(8A)	119.2
C(8)-C(9)-C(10)	119.2(5)
C(8)-C(9)-H(9A)	120.4
C(10)-C(9)-H(9A)	120.4
C(5)-C(10)-C(9)	120.6(6)
C(5)-C(10)-H(10A)	119.7
C(9)-C(10)-H(10A)	119.7
C(16)-C(11)-C(12)	121.0(5)
C(16)-C(11)-N(1)	121.8(5)
C(12)-C(11)-N(1)	117.2(5)
C(13)-C(12)-C(11)	119.8(5)
C(13)-C(12)-H(12A)	120.1
C(11)-C(12)-H(12A)	120.1
C(14)-C(13)-C(12)	120.3(6)
C(14)-C(13)-H(13A)	119.9

C(12)-C(13)-H(13A)	119.9
C(15)-C(14)-C(13)	119.9(6)
C(15)-C(14)-H(14A)	120.1
C(13)-C(14)-H(14A)	120.1
C(14)-C(15)-C(16)	120.7(6)
C(14)-C(15)-H(15A)	119.6
C(16)-C(15)-H(15A)	119.6
C(11)-C(16)-C(15)	118.2(5)
C(11)-C(16)-H(16A)	120.9
C(15)-C(16)-H(16A)	120.9
C(18)-C(17)-C(22)	120.1(5)
C(18)-C(17)-C(4)	121.5(5)
C(22)-C(17)-C(4)	118.4(5)
C(19)-C(18)-C(17)	119.5(5)
C(19)-C(18)-H(18A)	120.2
C(17)-C(18)-H(18A)	120.2
C(18)-C(19)-C(20)	120.2(5)
C(18)-C(19)-H(19A)	119.9
C(20)-C(19)-H(19A)	119.9
C(21)-C(20)-C(19)	120.2(5)
C(21)-C(20)-H(20A)	119.9
C(19)-C(20)-H(20A)	119.9
C(20)-C(21)-C(22)	119.9(5)
C(20)-C(21)-H(21A)	120.0
C(22)-C(21)-H(21A)	120.0
C(21)-C(22)-C(17)	120.0(5)
C(21)-C(22)-H(22A)	120.0
C(17)-C(22)-H(22A)	120.0
C(25)-N(2)-C(33)	125.6(4)
C(25)-N(2)-H(2A)	117.2
C(33)-N(2)-H(2A)	117.2
C(23)-O(6)-H(6B)	109.5
O(6)-C(23)-O(4)	108.6(4)
O(6)-C(23)-C(27)	110.7(4)
O(4)-C(23)-C(27)	107.9(4)
O(6)-C(23)-C(24)	112.6(4)
O(4)-C(23)-C(24)	102.8(4)
C(27)-C(23)-C(24)	113.8(4)

O(5)-C(24)-C(25)	127.3(5)
O(5)-C(24)-C(23)	124.3(4)
C(25)-C(24)-C(23)	108.4(4)
C(26)-C(25)-N(2)	129.1(4)
C(26)-C(25)-C(24)	105.7(4)
N(2)-C(25)-C(24)	125.2(4)
O(4)-C(26)-C(25)	115.5(4)
O(4)-C(26)-C(39)	113.4(4)
C(25)-C(26)-C(39)	131.1(5)
C(28)-C(27)-C(32)	120.1(5)
C(28)-C(27)-C(23)	121.0(5)
C(32)-C(27)-C(23)	118.8(5)
C(27)-C(28)-C(29)	119.8(5)
C(27)-C(28)-H(28A)	120.1
C(29)-C(28)-H(28A)	120.1
C(30)-C(29)-C(28)	120.3(5)
C(30)-C(29)-H(29A)	119.8
C(28)-C(29)-H(29A)	119.8
C(29)-C(30)-C(31)	119.9(5)
C(29)-C(30)-H(30A)	120.1
C(31)-C(30)-H(30A)	120.1
C(30)-C(31)-C(32)	120.1(5)
C(30)-C(31)-H(31A)	119.9
C(32)-C(31)-H(31A)	119.9
C(31)-C(32)-C(27)	119.7(6)
C(31)-C(32)-H(32A)	120.1
C(27)-C(32)-H(32A)	120.1
C(34)-C(33)-C(38)	120.3(5)
C(34)-C(33)-N(2)	117.8(5)
C(38)-C(33)-N(2)	121.9(5)
C(33)-C(34)-C(35)	119.0(5)
C(33)-C(34)-H(34A)	120.5
C(35)-C(34)-H(34A)	120.5
C(36)-C(35)-C(34)	120.9(5)
C(36)-C(35)-H(35A)	119.5
C(34)-C(35)-H(35A)	119.5
C(35)-C(36)-C(37)	119.8(5)
C(35)-C(36)-H(36A)	120.1

C(37)-C(36)-H(36A)	120.1
C(36)-C(37)-C(38)	120.1(5)
C(36)-C(37)-H(37A)	119.9
C(38)-C(37)-H(37A)	119.9
C(33)-C(38)-C(37)	119.9(5)
C(33)-C(38)-H(38A)	120.0
C(37)-C(38)-H(38A)	120.0
C(40)-C(39)-C(44)	120.4(5)
C(40)-C(39)-C(26)	120.8(5)
C(44)-C(39)-C(26)	118.6(5)
C(39)-C(40)-C(41)	119.8(5)
C(39)-C(40)-H(40A)	120.1
C(41)-C(40)-H(40A)	120.1
C(40)-C(41)-C(42)	120.5(5)
C(40)-C(41)-H(41A)	119.8
C(42)-C(41)-H(41A)	119.8
C(43)-C(42)-C(41)	119.5(5)
C(43)-C(42)-H(42A)	120.2
C(41)-C(42)-H(42A)	120.2
C(42)-C(43)-C(44)	119.8(5)
C(42)-C(43)-H(43A)	120.1
C(44)-C(43)-H(43A)	120.1
C(43)-C(44)-C(39)	119.9(5)
C(43)-C(44)-H(44A)	120.0
C(39)-C(44)-H(44A)	120.0

4. Crystal data and structure refinement of compound **32**

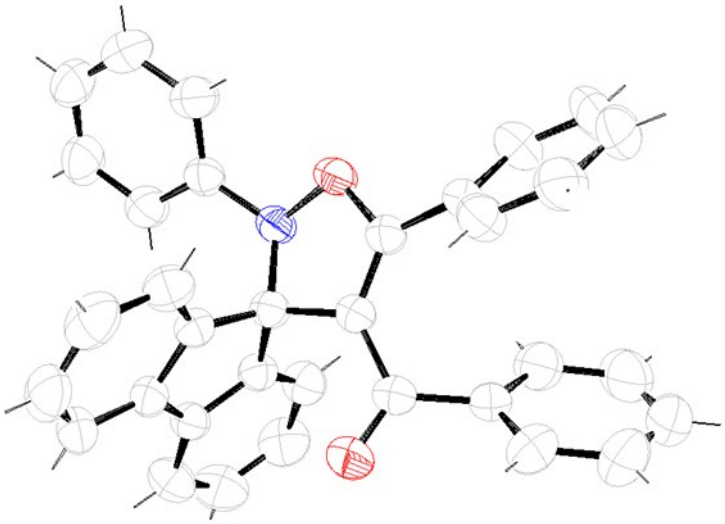


Table 1. Crystal data and structure refinement for Compound **32**.

Identification code	**32**
Empirical formula	C34 H23 N O2
Formula weight	477.53
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	triclinic, P-1
Unit cell dimensions	a = 8.1615(4) A alpha = 100.324(2) deg. b = 11.8152(8) A beta = 91.527(2) deg. c = 13.6440(10) A gamma = 102.577(2) deg.
Volume	1260.37(14) A^3
Z, Calculated density	2, 1.258 Mg/m^3
Absorption coefficient	0.078 mm^-1
F(000)	500
Crystal size	.35 x .3 x .25 mm

Theta range for data collection	1.52 to 27.50 deg.
Limiting indices	-9<=h<=5, -15<=k<=15, -17<=l<=17
Reflections collected / unique	9742 / 5531 [R(int) = 0.0210]
Completeness to theta = 27.50	95.4 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5531 / 0 / 334
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0469, wR2 = 0.1239
R indices (all data)	R1 = 0.0793, wR2 = 0.1562
Largest diff. peak and hole	0.147 and -0.199 e.A^-3

Table 2. Bond lengths [A] and angles [deg] for Compound **32**.

O(1)-C(3)	1.3594(19)
O(1)-N(1)	1.4710(17)
O(2)-C(22)	1.2159(19)
N(1)-C(4)	1.423(2)
N(1)-C(1)	1.508(2)
C(1)-C(2)	1.518(2)
C(1)-C(21)	1.522(2)
C(1)-C(10)	1.523(2)
C(2)-C(3)	1.340(2)
C(2)-C(22)	1.471(2)
C(3)-C(29)	1.472(2)
C(4)-C(5)	1.377(3)
C(4)-C(9)	1.389(2)
C(5)-C(6)	1.383(3)
C(5)-H(5)	0.9300
C(6)-C(7)	1.362(3)
C(6)-H(6)	0.9300
C(7)-C(8)	1.369(3)
C(7)-H(7)	0.9300
C(8)-C(9)	1.380(3)
C(8)-H(8)	0.9300
C(9)-H(9)	0.9300
C(10)-C(11)	1.380(3)
C(10)-C(15)	1.399(2)
C(11)-C(12)	1.386(3)
C(11)-H(11)	0.9300
C(12)-C(13)	1.380(3)
C(12)-H(12)	0.9300
C(13)-C(14)	1.373(3)
C(13)-H(13)	0.9300
C(14)-C(15)	1.388(2)
C(14)-H(14)	0.9300
C(15)-C(16)	1.468(2)
C(16)-C(17)	1.382(2)
C(16)-C(21)	1.390(2)
C(17)-C(18)	1.378(3)
C(17)-H(17)	0.9300

C(18)-C(19)	1.376(3)
C(18)-H(18)	0.9300
C(19)-C(20)	1.388(3)
C(19)-H(19)	0.9300
C(20)-C(21)	1.374(3)
C(20)-H(20)	0.9300
C(22)-C(23)	1.490(2)
C(23)-C(24)	1.371(3)
C(23)-C(28)	1.378(3)
C(24)-C(25)	1.392(3)
C(24)-H(24)	0.9300
C(25)-C(26)	1.368(4)
C(25)-H(25)	0.9300
C(26)-C(27)	1.347(4)
C(26)-H(26)	0.9300
C(27)-C(28)	1.374(3)
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300
C(29)-C(30)	1.380(2)
C(29)-C(34)	1.386(2)
C(30)-C(31)	1.382(3)
C(30)-H(30)	0.9300
C(31)-C(32)	1.366(3)
C(31)-H(31)	0.9300
C(32)-C(33)	1.376(3)
C(32)-H(32)	0.9300
C(33)-C(34)	1.381(3)
C(33)-H(33)	0.9300
C(34)-H(34)	0.9300

C(3)-O(1)-N(1)	105.45(11)
C(4)-N(1)-O(1)	108.11(12)
C(4)-N(1)-C(1)	119.83(13)
O(1)-N(1)-C(1)	106.19(11)
N(1)-C(1)-C(2)	99.15(12)
N(1)-C(1)-C(21)	110.71(13)
C(2)-C(1)-C(21)	114.20(14)
N(1)-C(1)-C(10)	117.52(13)

C(2)-C(1)-C(10)	113.81(13)
C(21)-C(1)-C(10)	102.06(13)
C(3)-C(2)-C(22)	128.17(15)
C(3)-C(2)-C(1)	109.05(14)
C(22)-C(2)-C(1)	122.68(14)
C(2)-C(3)-O(1)	113.26(14)
C(2)-C(3)-C(29)	132.70(15)
O(1)-C(3)-C(29)	113.89(13)
C(5)-C(4)-C(9)	119.31(17)
C(5)-C(4)-N(1)	122.74(16)
C(9)-C(4)-N(1)	117.77(15)
C(4)-C(5)-C(6)	119.8(2)
C(4)-C(5)-H(5)	120.1
C(6)-C(5)-H(5)	120.1
C(7)-C(6)-C(5)	121.0(2)
C(7)-C(6)-H(6)	119.5
C(5)-C(6)-H(6)	119.5
C(6)-C(7)-C(8)	119.30(19)
C(6)-C(7)-H(7)	120.3
C(8)-C(7)-H(7)	120.3
C(7)-C(8)-C(9)	121.0(2)
C(7)-C(8)-H(8)	119.5
C(9)-C(8)-H(8)	119.5
C(8)-C(9)-C(4)	119.58(19)
C(8)-C(9)-H(9)	120.2
C(4)-C(9)-H(9)	120.2
C(11)-C(10)-C(15)	120.57(16)
C(11)-C(10)-C(1)	129.29(16)
C(15)-C(10)-C(1)	110.06(14)
C(10)-C(11)-C(12)	118.60(19)
C(10)-C(11)-H(11)	120.7
C(12)-C(11)-H(11)	120.7
C(13)-C(12)-C(11)	120.39(19)
C(13)-C(12)-H(12)	119.8
C(11)-C(12)-H(12)	119.8
C(14)-C(13)-C(12)	121.81(19)
C(14)-C(13)-H(13)	119.1
C(12)-C(13)-H(13)	119.1

C(13)-C(14)-C(15)	118.14(19)
C(13)-C(14)-H(14)	120.9
C(15)-C(14)-H(14)	120.9
C(14)-C(15)-C(10)	120.47(16)
C(14)-C(15)-C(16)	130.88(16)
C(10)-C(15)-C(16)	108.61(14)
C(17)-C(16)-C(21)	119.81(17)
C(17)-C(16)-C(15)	131.19(17)
C(21)-C(16)-C(15)	109.00(14)
C(18)-C(17)-C(16)	118.50(19)
C(18)-C(17)-H(17)	120.8
C(16)-C(17)-H(17)	120.8
C(19)-C(18)-C(17)	121.60(19)
C(19)-C(18)-H(18)	119.2
C(17)-C(18)-H(18)	119.2
C(18)-C(19)-C(20)	120.2(2)
C(18)-C(19)-H(19)	119.9
C(20)-C(19)-H(19)	119.9
C(21)-C(20)-C(19)	118.26(18)
C(21)-C(20)-H(20)	120.9
C(19)-C(20)-H(20)	120.9
C(20)-C(21)-C(16)	121.57(16)
C(20)-C(21)-C(1)	128.15(15)
C(16)-C(21)-C(1)	110.23(14)
O(2)-C(22)-C(2)	120.78(16)
O(2)-C(22)-C(23)	120.45(15)
C(2)-C(22)-C(23)	118.74(14)
C(24)-C(23)-C(28)	118.67(18)
C(24)-C(23)-C(22)	123.20(17)
C(28)-C(23)-C(22)	118.12(17)
C(23)-C(24)-C(25)	119.8(2)
C(23)-C(24)-H(24)	120.1
C(25)-C(24)-H(24)	120.1
C(26)-C(25)-C(24)	120.1(2)
C(26)-C(25)-H(25)	120.0
C(24)-C(25)-H(25)	120.0
C(27)-C(26)-C(25)	120.4(2)
C(27)-C(26)-H(26)	119.8

C(25)-C(26)-H(26)	119.8
C(26)-C(27)-C(28)	120.0(3)
C(26)-C(27)-H(27)	120.0
C(28)-C(27)-H(27)	120.0
C(27)-C(28)-C(23)	121.1(2)
C(27)-C(28)-H(28)	119.4
C(23)-C(28)-H(28)	119.4
C(30)-C(29)-C(34)	119.39(16)
C(30)-C(29)-C(3)	119.21(15)
C(34)-C(29)-C(3)	121.40(16)
C(29)-C(30)-C(31)	120.65(18)
C(29)-C(30)-H(30)	119.7
C(31)-C(30)-H(30)	119.7
C(32)-C(31)-C(30)	119.9(2)
C(32)-C(31)-H(31)	120.0
C(30)-C(31)-H(31)	120.0
C(31)-C(32)-C(33)	119.77(19)
C(31)-C(32)-H(32)	120.1
C(33)-C(32)-H(32)	120.1
C(32)-C(33)-C(34)	120.97(19)
C(32)-C(33)-H(33)	119.5
C(34)-C(33)-H(33)	119.5
C(33)-C(34)-C(29)	119.26(19)
C(33)-C(34)-H(34)	120.4
C(29)-C(34)-H(34)	120.4

Symmetry transformations used to generate equivalent atoms:

4. Crystal data and structure refinement of compound **36**

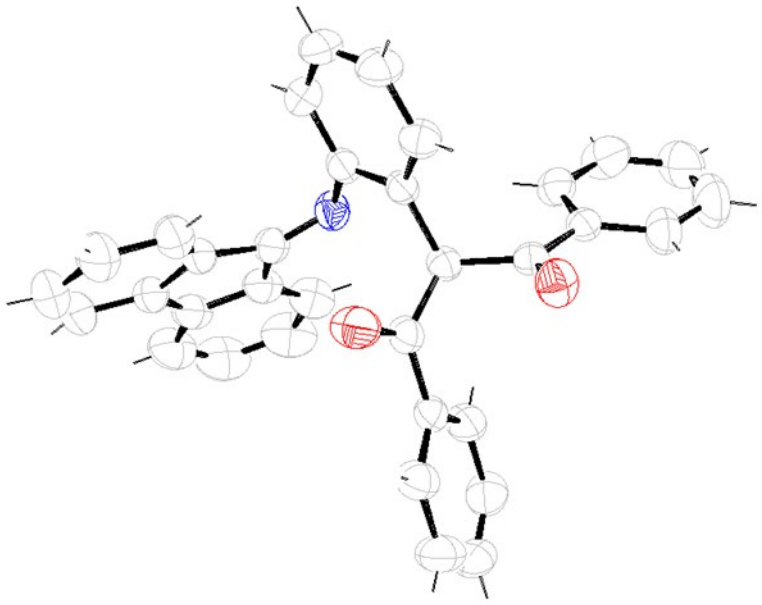


Table 1. Crystal data and structure refinement for Compound **36**.

Identification code	**36**
Empirical formula	C34 H23 N O2
Formula weight	477.53
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	monoclinic, P21/n
Unit cell dimensions	a = 12.7719(7) A alpha = 90 deg.
	b = 8.2486(3) A beta = 102.757(2) deg.
	c = 24.3125(14) A gamma = 90 deg.
Volume	2498.1(2) A^3
Z, Calculated density	4, 1.270 Mg/m^3
Absorption coefficient	0.078 mm^-1
F(000)	1000
Crystal size	.4 x .3 x .2 mm
Theta range for data collection	1.67 to 27.50 deg.
Limiting indices	-16<=h<=15, -10<=k<=5, -15<=l<=31
Reflections collected / unique	8669 / 5560 [R(int) = 0.0187]
Completeness to theta = 27.50	96.9 %
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	5560 / 0 / 334
Goodness-of-fit on F^2	1.012
Final R indices [I>2sigma(I)]	R1 = 0.0480, wR2 = 0.1271
R indices (all data)	R1 = 0.0903, wR2 = 0.1670
Largest diff. peak and hole	0.170 and -0.182 e.A^-3

Table 2. Bond lengths [A] and angles [deg] for Compound **36**.

C(1)-N(1)	1.277(2)
C(1)-C(2)	1.482(3)
C(1)-C(13)	1.486(3)
C(2)-C(3)	1.380(3)
C(2)-C(7)	1.392(3)
C(3)-C(4)	1.384(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.365(4)
C(4)-H(4)	0.9300
C(5)-C(6)	1.376(4)
C(5)-H(5)	0.9300
C(6)-C(7)	1.389(3)
C(6)-H(6)	0.9300
C(7)-C(8)	1.467(3)
C(8)-C(9)	1.382(3)
C(8)-C(13)	1.407(3)
C(9)-C(10)	1.376(4)
C(9)-H(9)	0.9300
C(10)-C(11)	1.374(4)
C(10)-H(10)	0.9300
C(11)-C(12)	1.386(3)
C(11)-H(11)	0.9300
C(12)-C(13)	1.379(3)
C(12)-H(12)	0.9300
C(14)-C(15)	1.394(3)
C(14)-C(19)	1.396(2)
C(14)-N(1)	1.414(2)
C(15)-C(16)	1.375(3)
C(15)-H(15)	0.9300

C(16)-C(17)	1.373(3)
C(16)-H(16)	0.9300
C(17)-C(18)	1.379(3)
C(17)-H(17)	0.9300
C(18)-C(19)	1.384(2)
C(18)-H(18)	0.9300
C(19)-C(20)	1.515(2)
C(20)-C(21)	1.520(2)
C(20)-C(28)	1.537(2)
C(20)-H(20)	0.9800
C(21)-O(1)	1.214(2)
C(21)-C(22)	1.487(2)
C(22)-C(27)	1.388(3)
C(22)-C(23)	1.390(3)
C(23)-C(24)	1.373(3)
C(23)-H(23)	0.9300
C(24)-C(25)	1.362(4)
C(24)-H(24)	0.9300
C(25)-C(26)	1.369(4)
C(25)-H(25)	0.9300
C(26)-C(27)	1.384(3)
C(26)-H(26)	0.9300
C(27)-H(27)	0.9300
C(28)-O(2)	1.207(2)
C(28)-C(29)	1.491(2)
C(29)-C(30)	1.382(3)
C(29)-C(34)	1.391(3)
C(30)-C(31)	1.378(3)
C(30)-H(30)	0.9300
C(31)-C(32)	1.369(3)
C(31)-H(31)	0.9300
C(32)-C(33)	1.367(3)
C(32)-H(32)	0.9300
C(33)-C(34)	1.387(3)
C(33)-H(33)	0.9300
C(34)-H(34)	0.9300

N(1)-C(1)-C(2)	121.14(17)

N(1)-C(1)-C(13)	133.35(17)
C(2)-C(1)-C(13)	105.51(16)
C(3)-C(2)-C(7)	121.19(19)
C(3)-C(2)-C(1)	129.7(2)
C(7)-C(2)-C(1)	109.08(18)
C(2)-C(3)-C(4)	117.6(2)
C(2)-C(3)-H(3)	121.2
C(4)-C(3)-H(3)	121.2
C(5)-C(4)-C(3)	121.4(3)
C(5)-C(4)-H(4)	119.3
C(3)-C(4)-H(4)	119.3
C(4)-C(5)-C(6)	121.4(2)
C(4)-C(5)-H(5)	119.3
C(6)-C(5)-H(5)	119.3
C(5)-C(6)-C(7)	118.1(3)
C(5)-C(6)-H(6)	120.9
C(7)-C(6)-H(6)	120.9
C(6)-C(7)-C(2)	120.2(2)
C(6)-C(7)-C(8)	131.4(2)
C(2)-C(7)-C(8)	108.33(17)
C(9)-C(8)-C(13)	120.4(2)
C(9)-C(8)-C(7)	130.6(2)
C(13)-C(8)-C(7)	108.96(17)
C(10)-C(9)-C(8)	118.8(2)
C(10)-C(9)-H(9)	120.6
C(8)-C(9)-H(9)	120.6
C(11)-C(10)-C(9)	120.9(2)
C(11)-C(10)-H(10)	119.5
C(9)-C(10)-H(10)	119.5
C(10)-C(11)-C(12)	121.2(2)
C(10)-C(11)-H(11)	119.4
C(12)-C(11)-H(11)	119.4
C(13)-C(12)-C(11)	118.5(2)
C(13)-C(12)-H(12)	120.8
C(11)-C(12)-H(12)	120.8
C(12)-C(13)-C(8)	120.19(19)
C(12)-C(13)-C(1)	131.86(18)
C(8)-C(13)-C(1)	107.88(17)

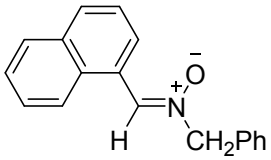
C(15)-C(14)-C(19)	119.52(16)
C(15)-C(14)-N(1)	122.27(17)
C(19)-C(14)-N(1)	117.95(14)
C(16)-C(15)-C(14)	120.18(19)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(17)-C(16)-C(15)	120.43(17)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(16)-C(17)-C(18)	119.85(18)
C(16)-C(17)-H(17)	120.1
C(18)-C(17)-H(17)	120.1
C(17)-C(18)-C(19)	120.91(19)
C(17)-C(18)-H(18)	119.5
C(19)-C(18)-H(18)	119.5
C(18)-C(19)-C(14)	119.10(15)
C(18)-C(19)-C(20)	122.58(16)
C(14)-C(19)-C(20)	118.32(14)
C(19)-C(20)-C(21)	111.50(13)
C(19)-C(20)-C(28)	112.29(13)
C(21)-C(20)-C(28)	110.14(14)
C(19)-C(20)-H(20)	107.6
C(21)-C(20)-H(20)	107.6
C(28)-C(20)-H(20)	107.6
O(1)-C(21)-C(22)	120.84(17)
O(1)-C(21)-C(20)	120.18(16)
C(22)-C(21)-C(20)	118.98(15)
C(27)-C(22)-C(23)	118.66(18)
C(27)-C(22)-C(21)	122.74(17)
C(23)-C(22)-C(21)	118.60(17)
C(24)-C(23)-C(22)	120.7(2)
C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6
C(25)-C(24)-C(23)	120.0(2)
C(25)-C(24)-H(24)	120.0
C(23)-C(24)-H(24)	120.0
C(24)-C(25)-C(26)	120.6(2)
C(24)-C(25)-H(25)	119.7

C(26)-C(25)-H(25)	119.7
C(25)-C(26)-C(27)	120.1(2)
C(25)-C(26)-H(26)	119.9
C(27)-C(26)-H(26)	119.9
C(26)-C(27)-C(22)	119.9(2)
C(26)-C(27)-H(27)	120.1
C(22)-C(27)-H(27)	120.1
O(2)-C(28)-C(29)	121.21(16)
O(2)-C(28)-C(20)	121.08(15)
C(29)-C(28)-C(20)	117.71(14)
C(30)-C(29)-C(34)	118.62(17)
C(30)-C(29)-C(28)	118.77(16)
C(34)-C(29)-C(28)	122.61(16)
C(31)-C(30)-C(29)	120.3(2)
C(31)-C(30)-H(30)	119.9
C(29)-C(30)-H(30)	119.9
C(32)-C(31)-C(30)	120.5(2)
C(32)-C(31)-H(31)	119.7
C(30)-C(31)-H(31)	119.7
C(33)-C(32)-C(31)	120.37(18)
C(33)-C(32)-H(32)	119.8
C(31)-C(32)-H(32)	119.8
C(32)-C(33)-C(34)	119.5(2)
C(32)-C(33)-H(33)	120.2
C(34)-C(33)-H(33)	120.2
C(33)-C(34)-C(29)	120.7(2)
C(33)-C(34)-H(34)	119.7
C(29)-C(34)-H(34)	119.7
C(1)-N(1)-C(14)	122.58(16)

Symmetry transformations used to generate equivalent atoms:

Copies of ^{1}H and ^{13}C NMR spectra for reported compounds:-

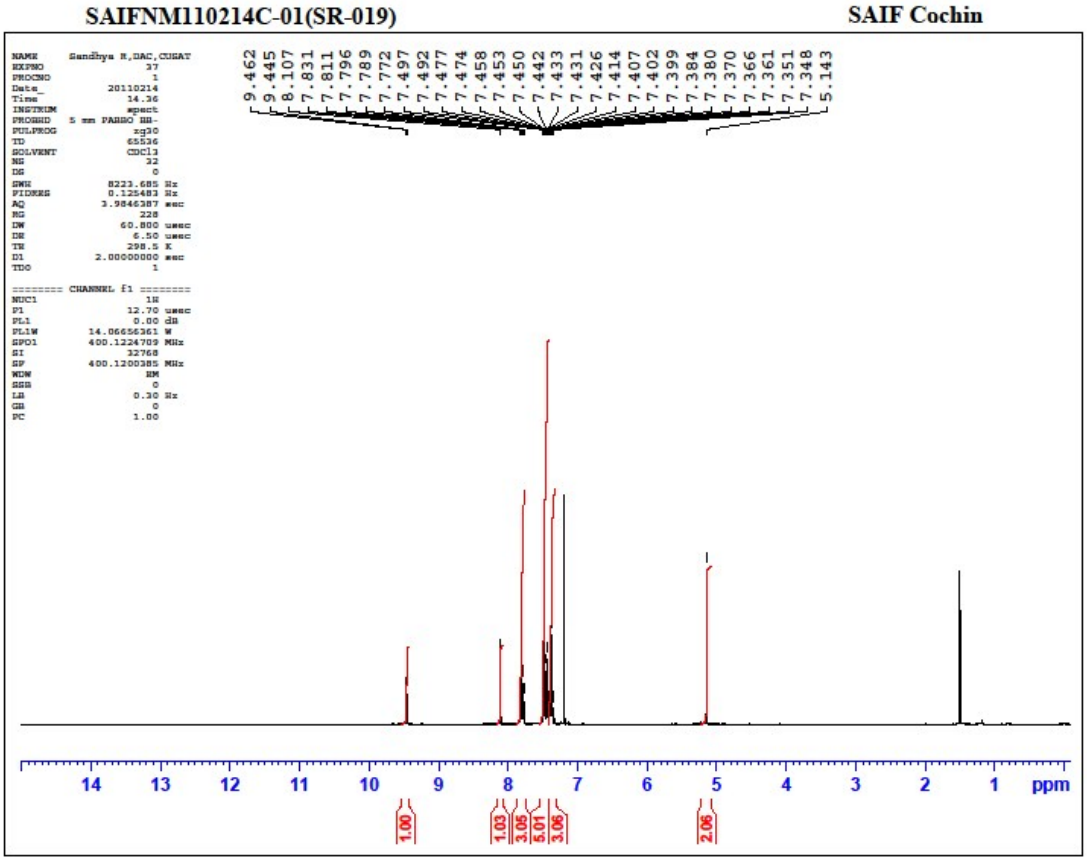
(Z)-N-(naphthalen-1-ylmethylene)-1-phenylmethanamine oxide **(6b)**



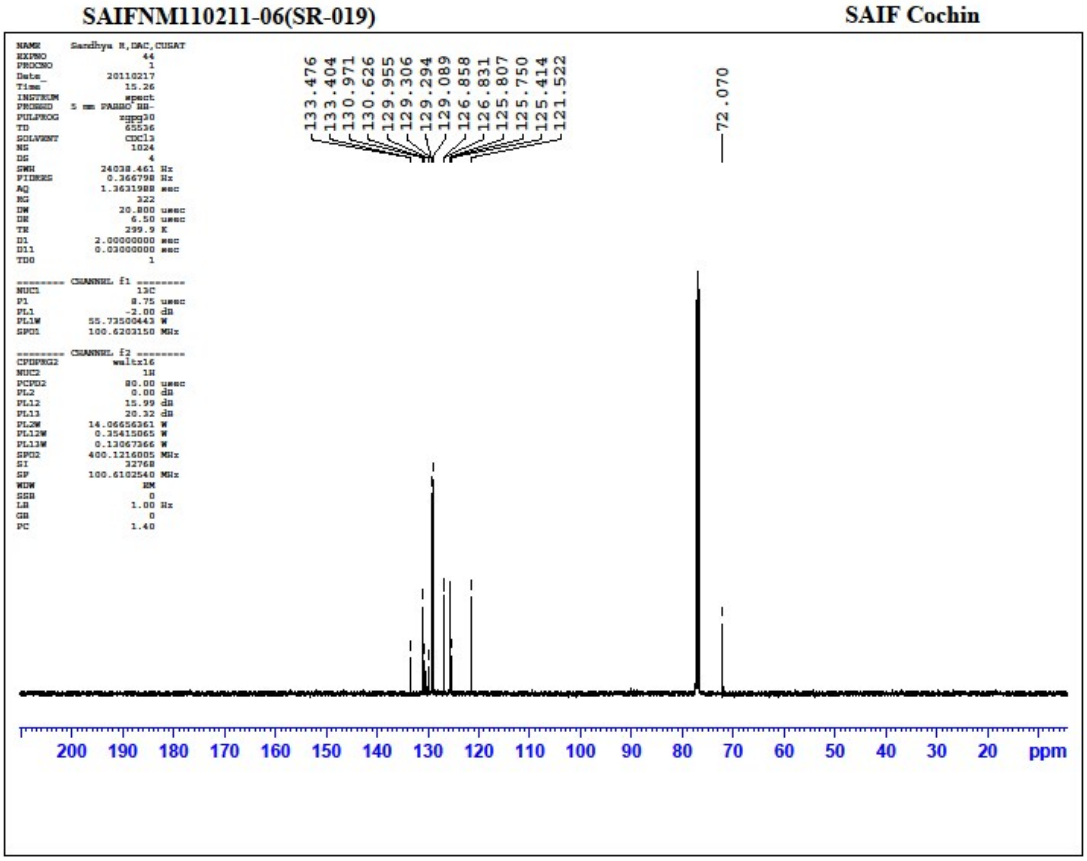
6b

^{1}H NMR Spectrum of Compound 6b Yield = 77%

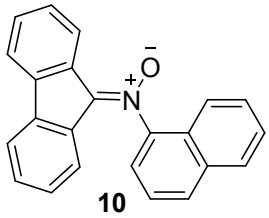
White solid, mp: 82°C



^{13}C NMR Spectrum of Compound 6b



N-(9H-fluoren-9-ylidene)naphthalen-1-amine oxide **(10)**

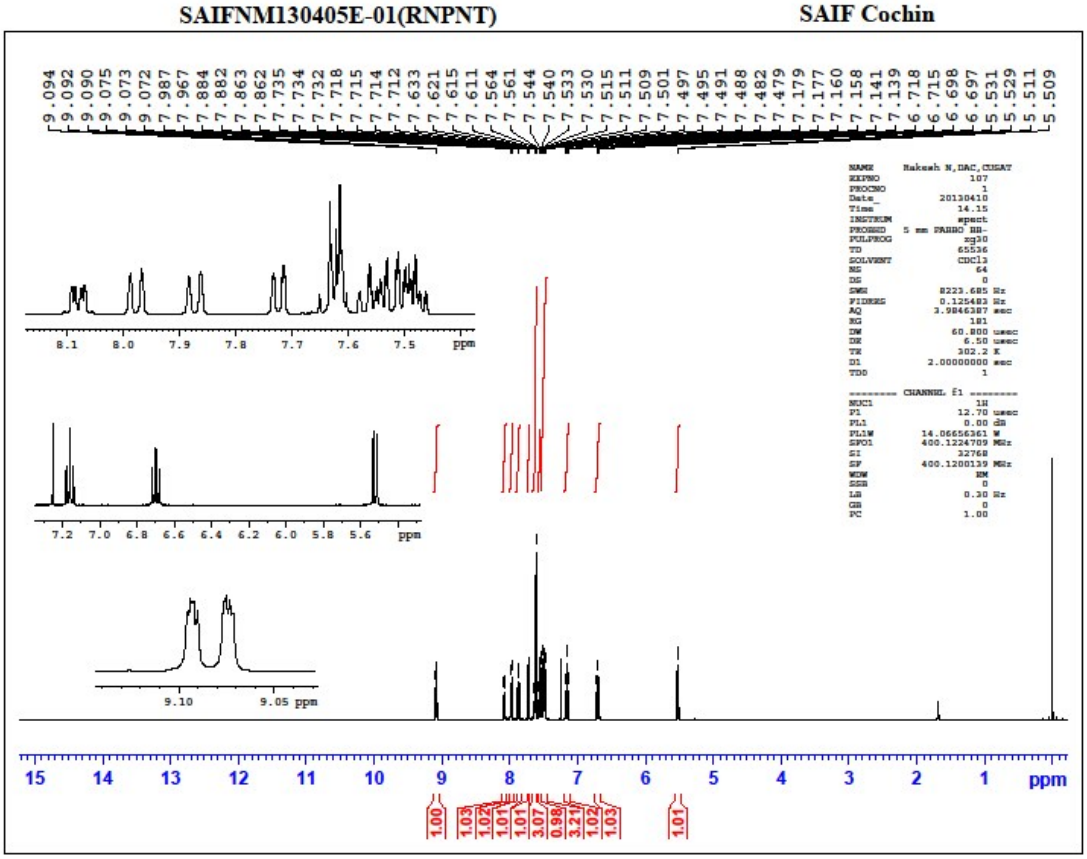


10

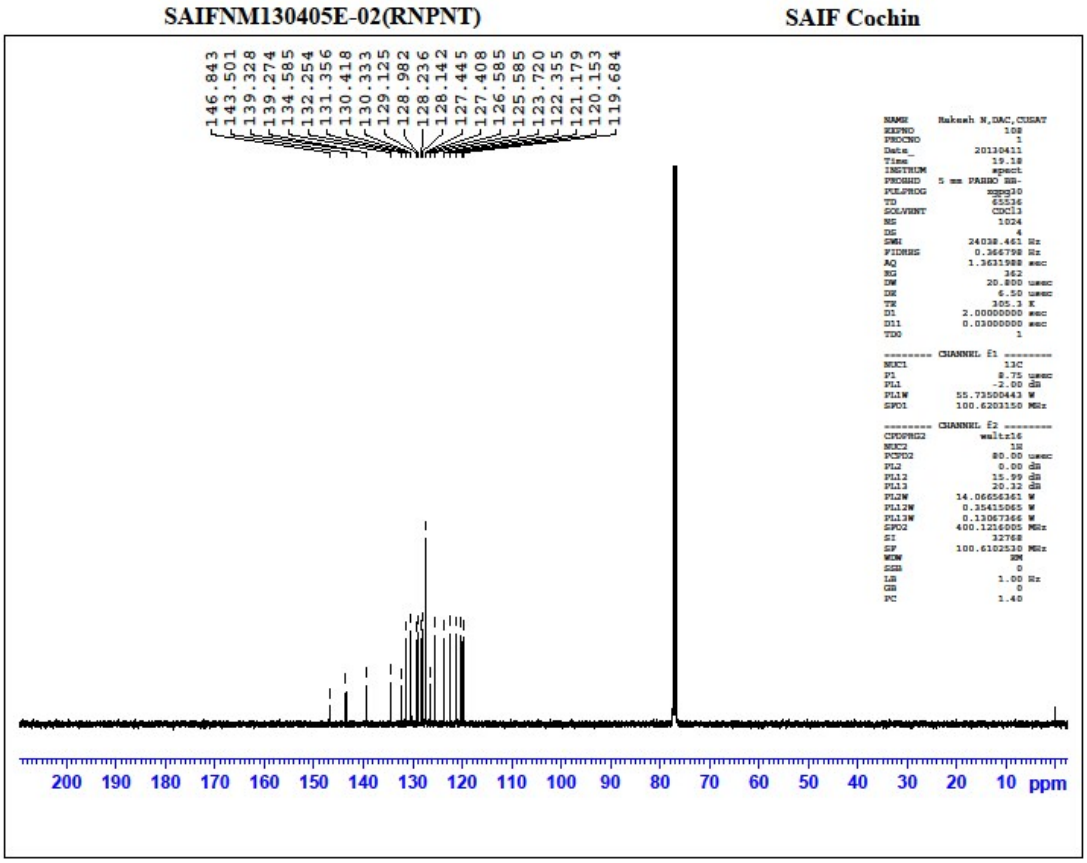
Yield = 79%

Yellow solid, mp: 157°C

^{1}H NMR Spectrum of Compound 10



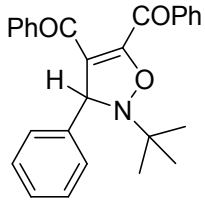
^{13}C NMR Spectrum of Compound 10



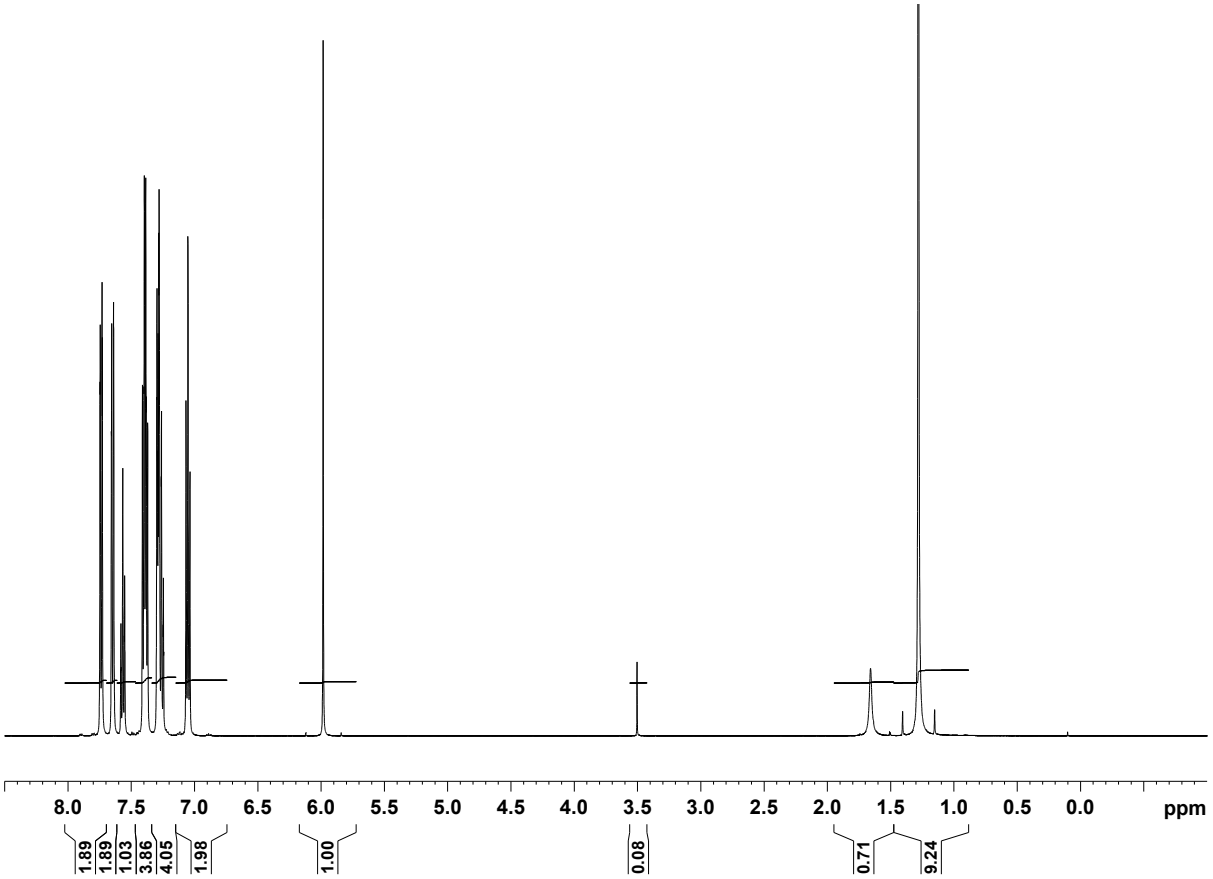
(2-tert-butyl-3-phenyl-2,3-dihydroisoxazole-4,5-diyl)bis(phenylmethanone) **(13a)**

Yield = 85%

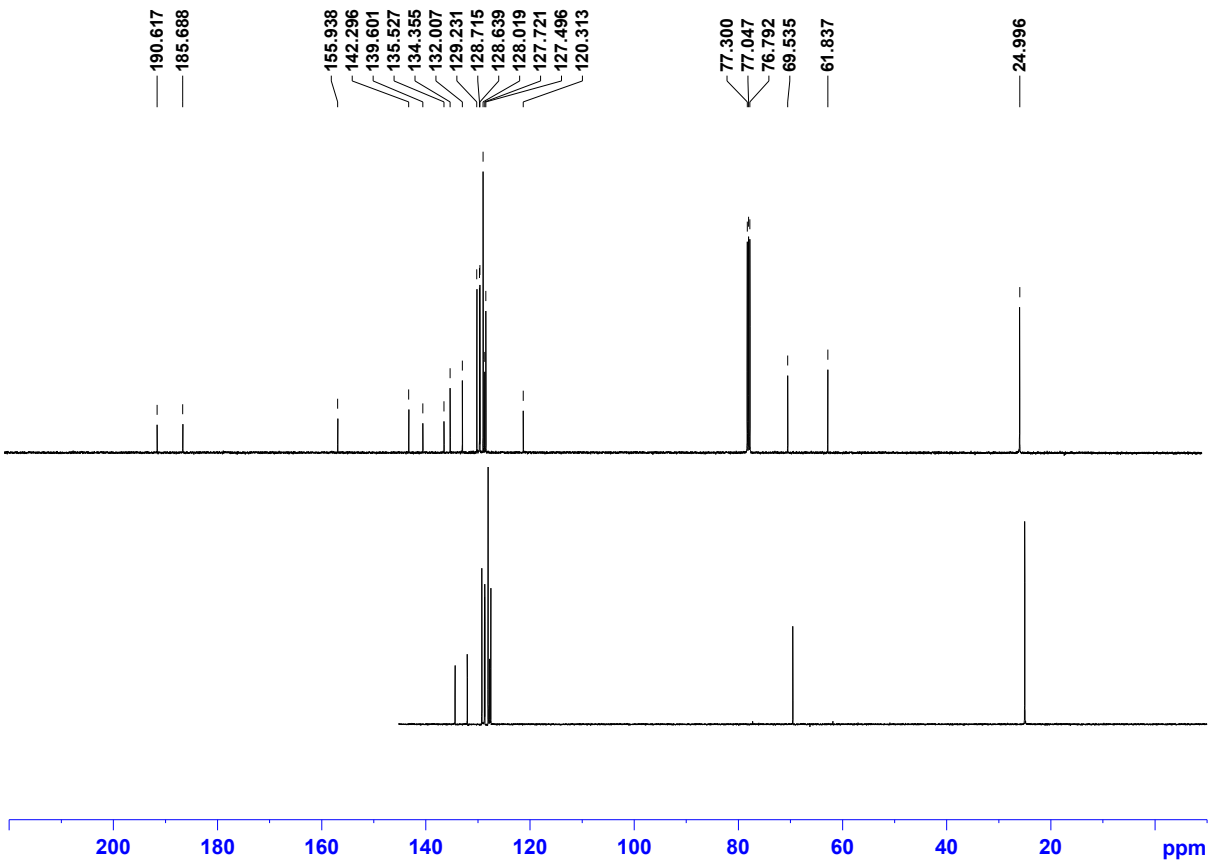
Pale Yellow solid, mp: 110°C



^{1}H NMR Spectrum of Compound 13a



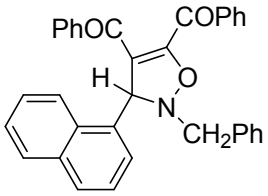
^{13}C NMR Spectrum of Compound 13a



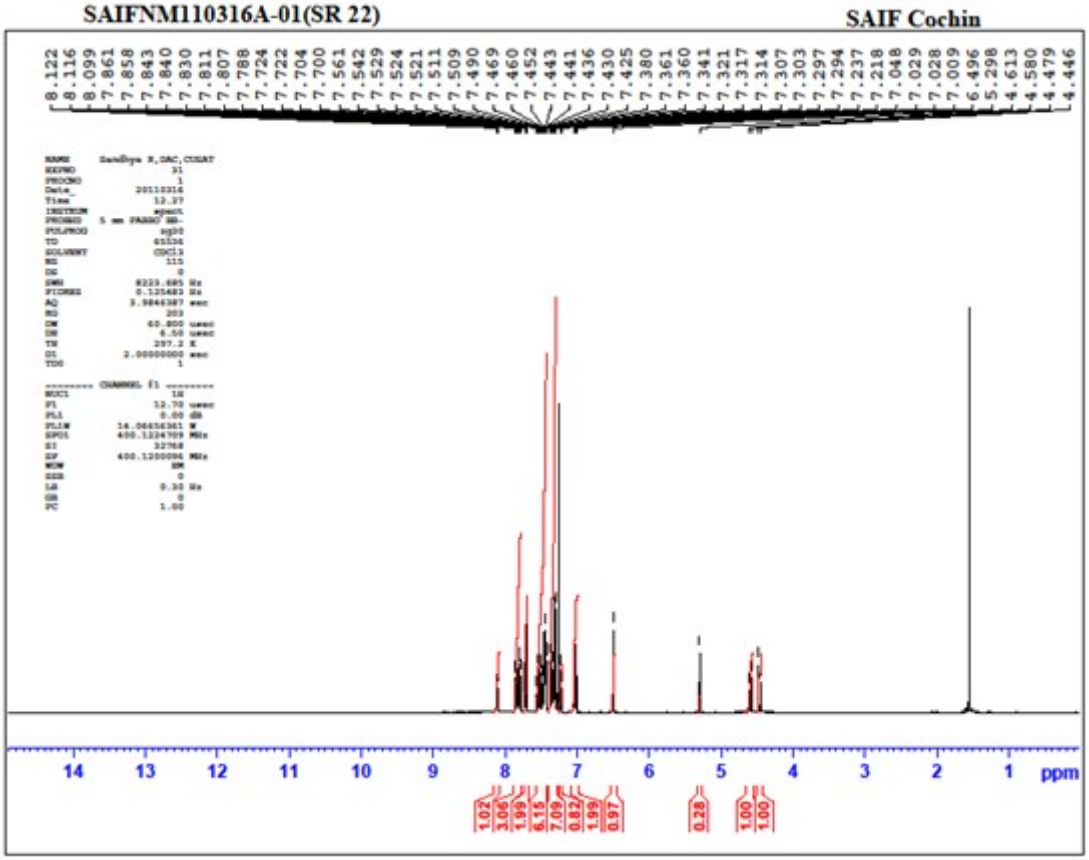
(*2-benzyl-3-(naphthalen-1-yl)-2,3-dihydroisoxazole-4,5-diyl)bis(phenylmethanone)* (13b)

Yield = 83%

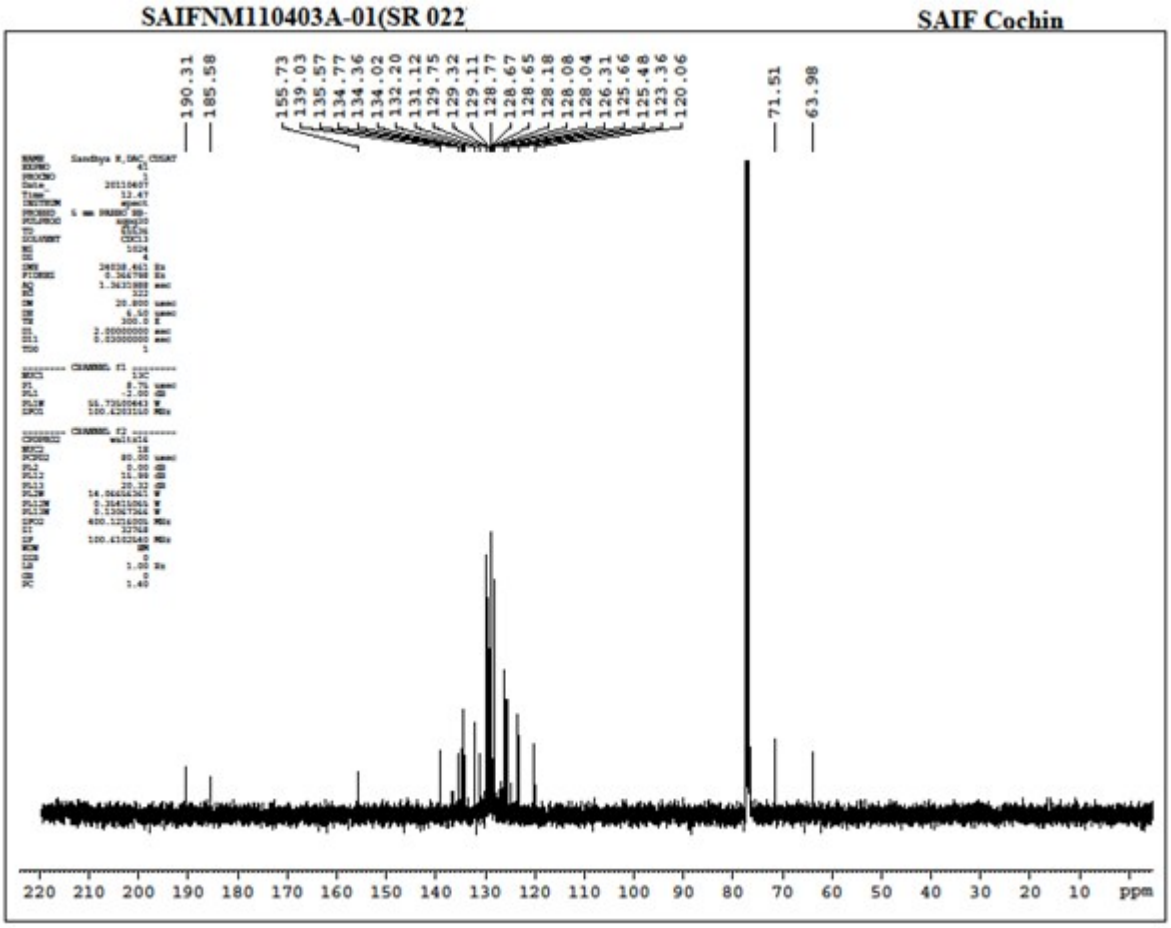
Pale Yellow solid, mp: 134°C



^{1}H NMR Spectrum of Compound 13b



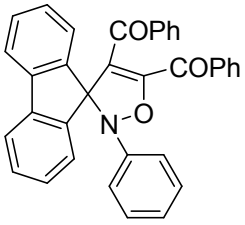
^{13}C NMR Spectrum of Compound 13b



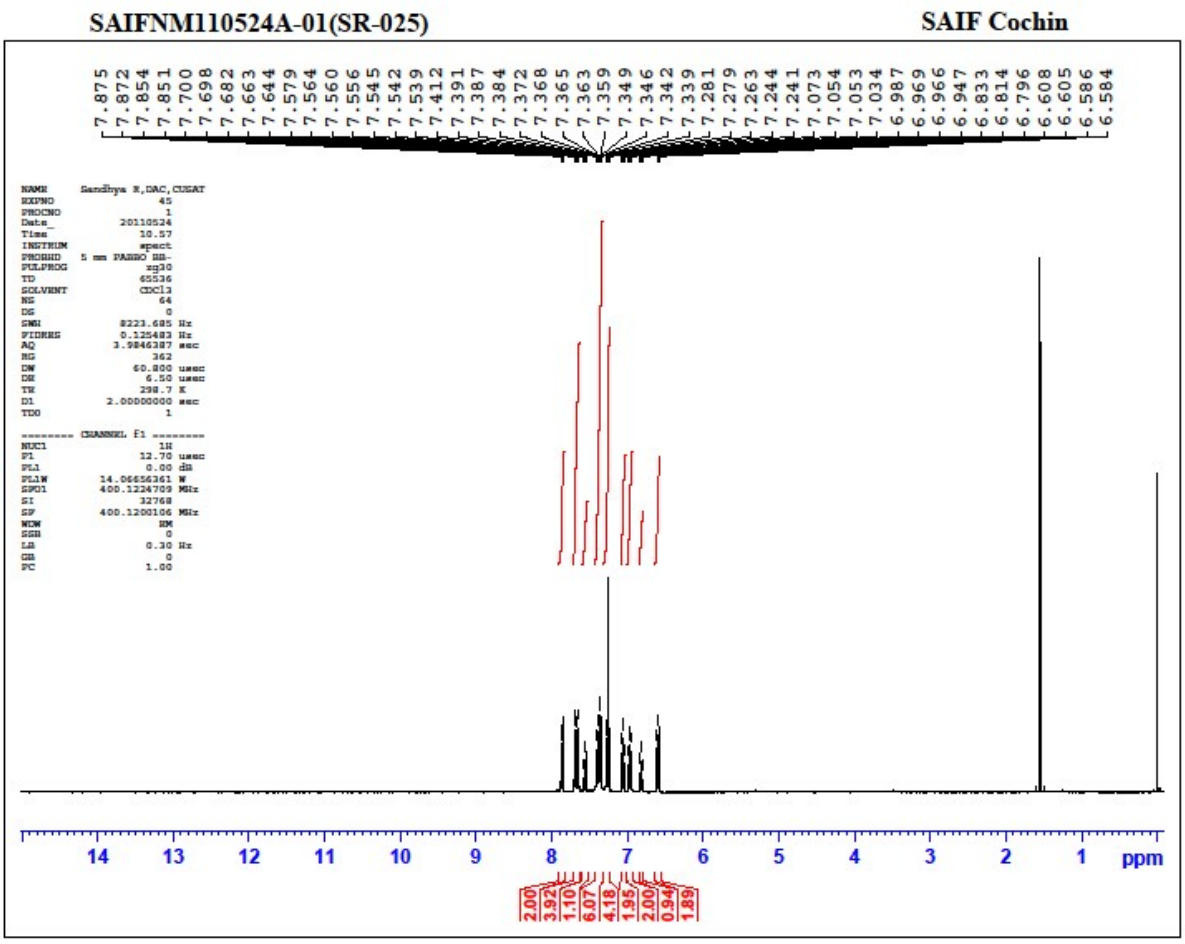
***(2'-phenyl-2'H-spiro[fluorene-9,3'-isoxazole]-4',5'-diyl)bis(phenylmethanone)* (15)**

Yield = 18%

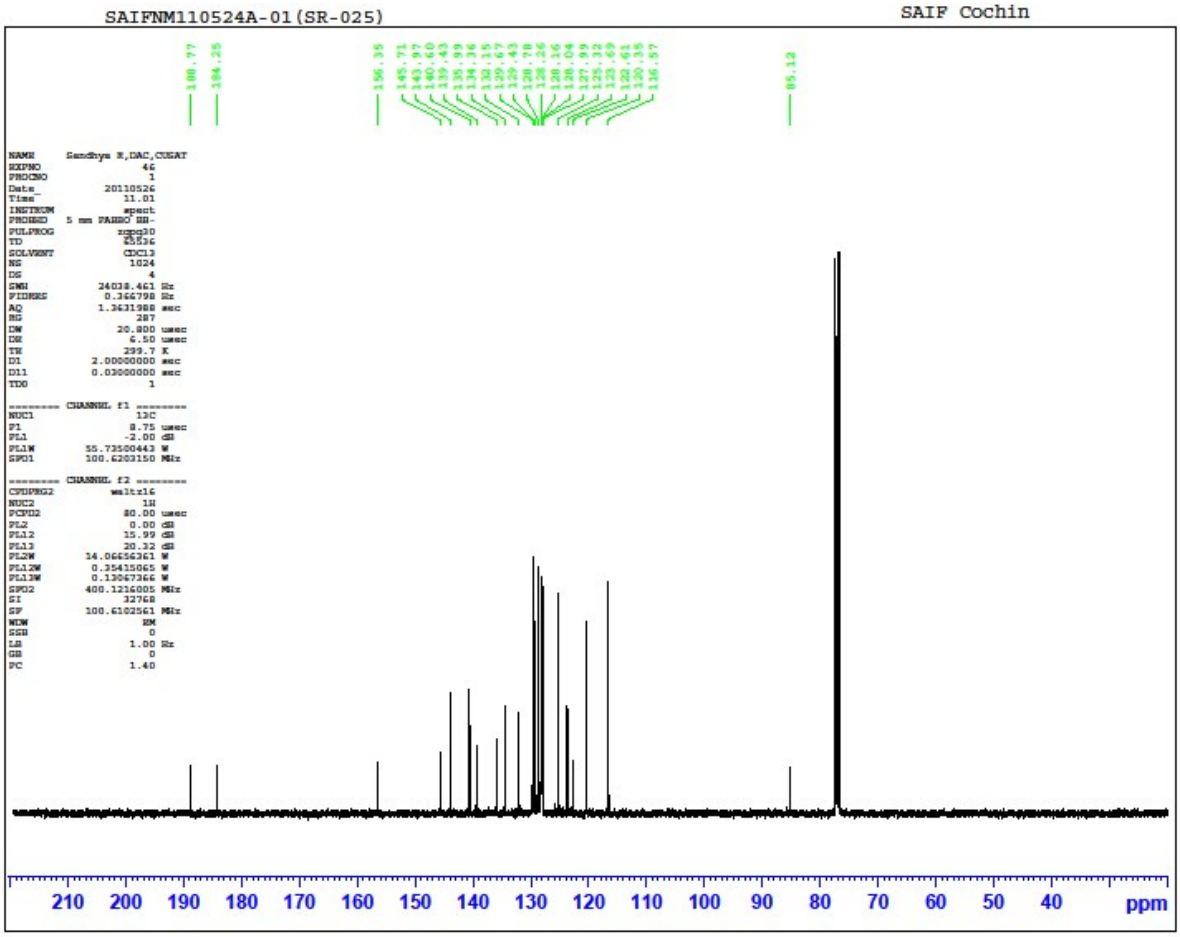
Yellow solid, mp: 120°C



^{1}H NMR Spectrum of Compound 15



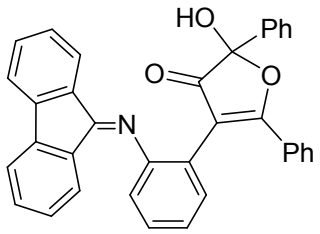
^{13}C NMR Spectrum of Compound 15



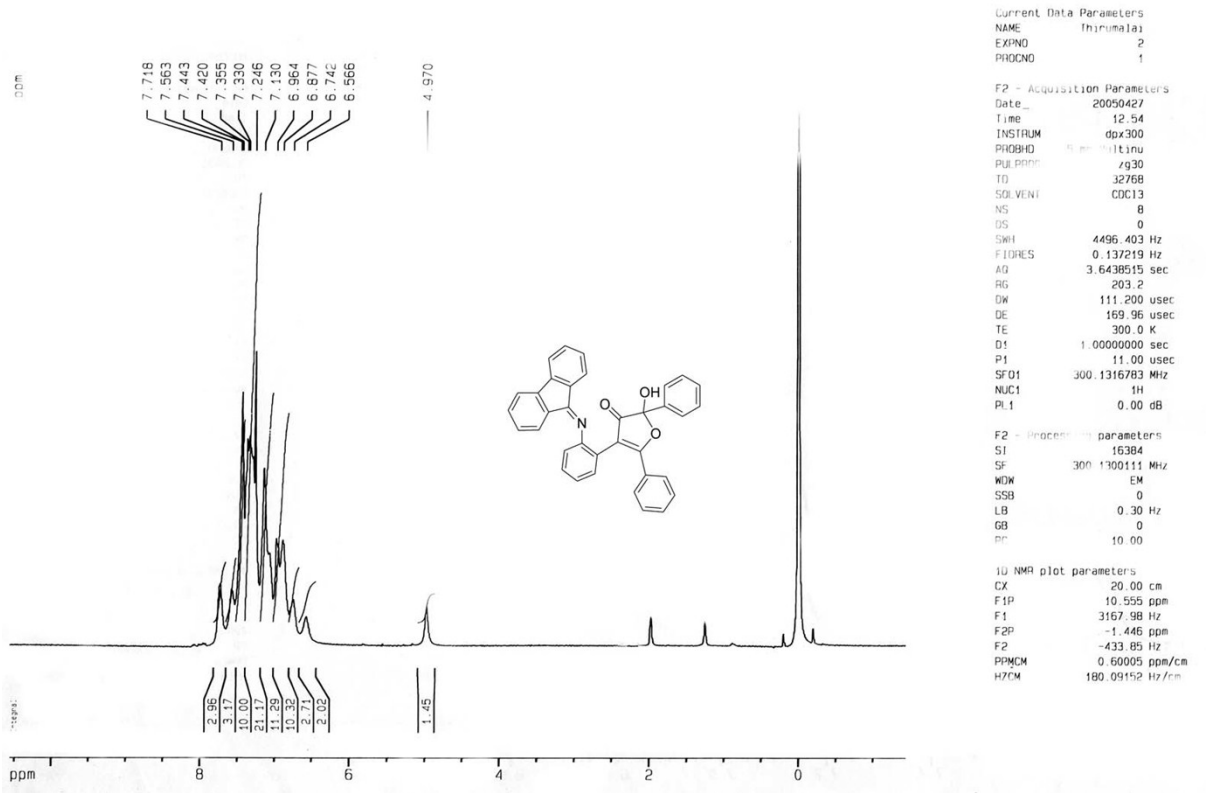
***4-(2-(9H-fluoren-9-ylideneamino)phenyl)-2-hydroxy-2,5-diphenylfuran-3(2H)-one* (17)**

Yield = 72%

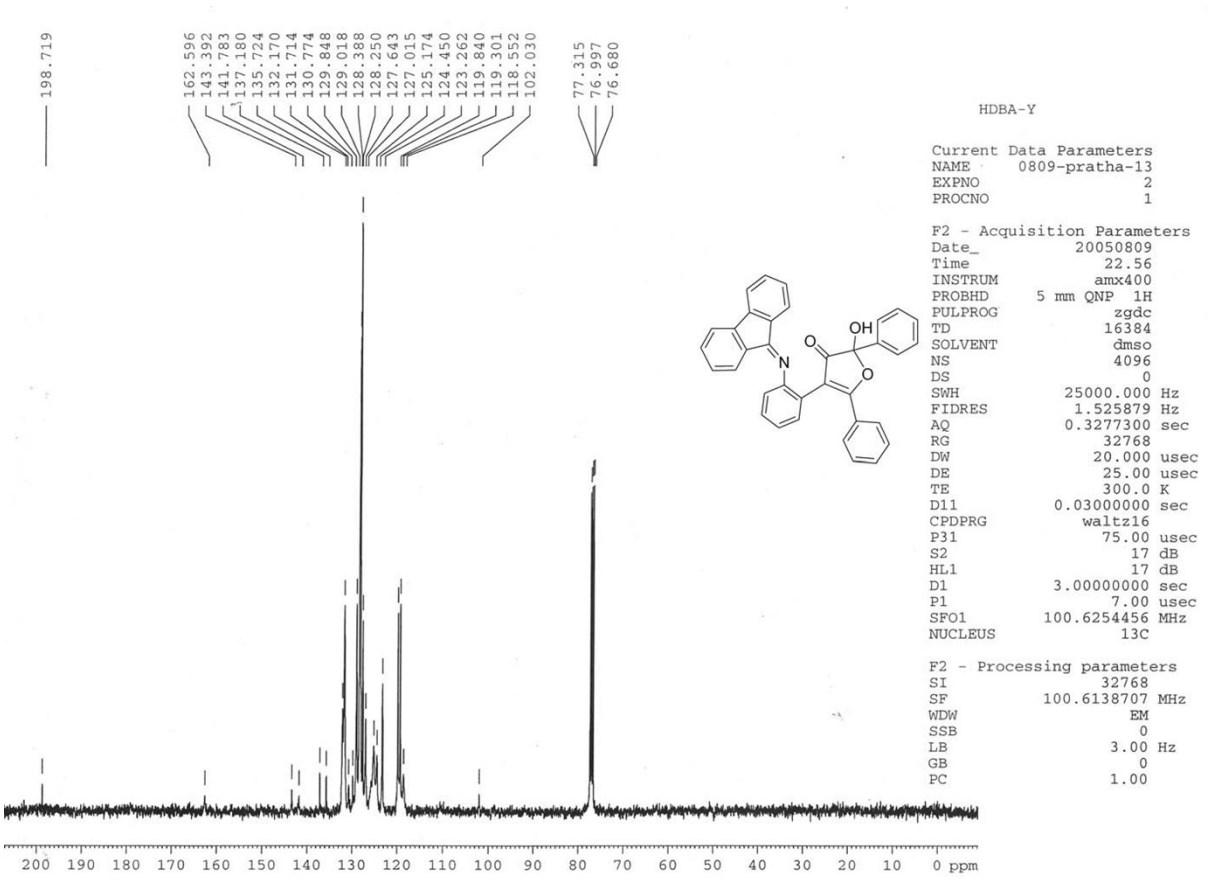
Yellow solid, mp: 206°C



^{1}H NMR Spectrum of Compound 17



^{13}C NMR Spectrum of Compound 17

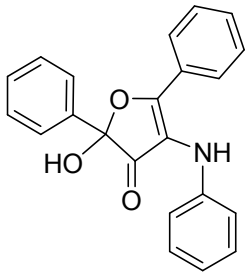


Note: Aromatic region in the NMR spectra (^{1}H and ^{13}C) of rearranged 1:1 adducts ***17***, ***25*** and ***28*** *are poorly resolved. We recorded the spectra of analytically pure samples on 300, 400 and 500 MHz instruments with no improvement in resolution. Structure of adducts was assigned on the basis single crystal XRD analysis.*

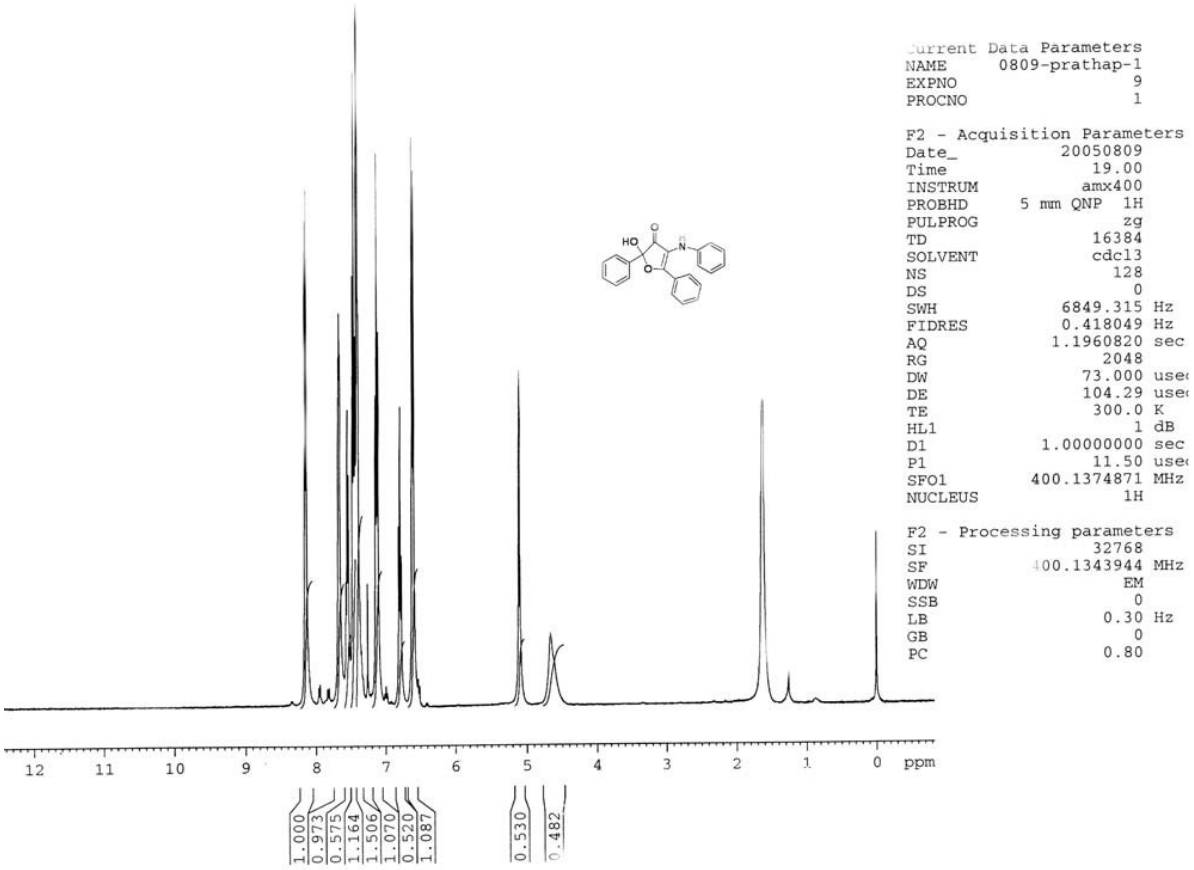
2-hydroxy-2,5-diphenyl-4-(phenylamino)furan-3(2H)-one **(22)**

Yield = 19%

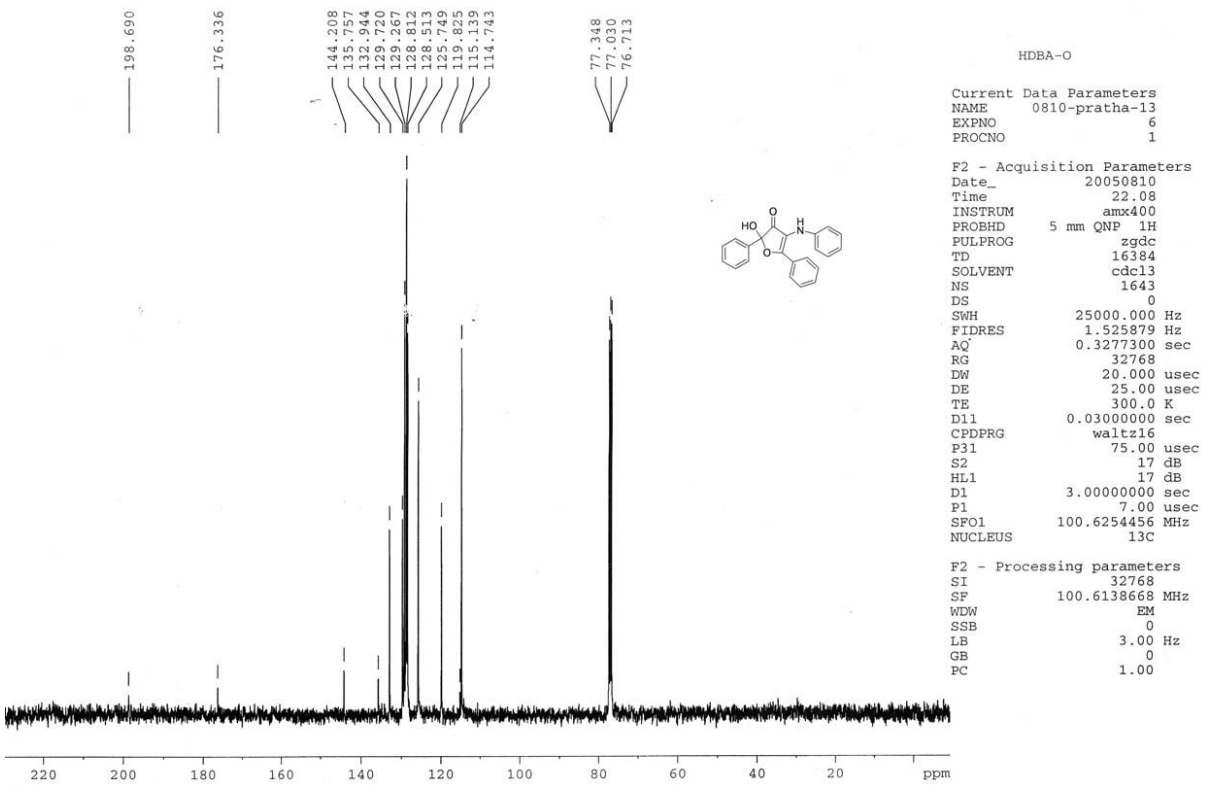
Orange solid, mp: 150 °C



^{1}H NMR Spectrum of Compound 22



^{13}C NMR Spectrum of Compound 22



HDBA-O

Current Data Parameters

NAME	0810-pratha-13
EXPNO	6
PROCNO	1

F2 - Acquisition Parameters

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Time	22.08
INSTRUM	amx400
PROBHD	5 mm QNP 1H
PULPROG	zgdc
TD	16384
SOLVENT	cdcl3
NS	1643
DS	0
SWH	25000.000 Hz
FIDRES	1.525879 Hz
AQ	0.3277300 sec
RG	32768
DW	20.000 usec
DE	25.00 usec
TE	300.0 K
D11	0.03000000 sec
CPDPRG	waltz16
P31	75.00 usec
S2	17 dB
HL1	17 dB
D1	3.00000000 sec
P1	7.00 usec
SFO1	100.6254456 MHz
NUCLEUS	13C

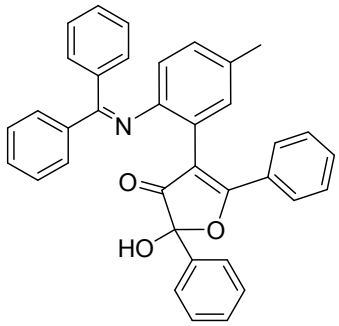
F2 - Processing parameters

SI	32768
SF	100.6138668 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

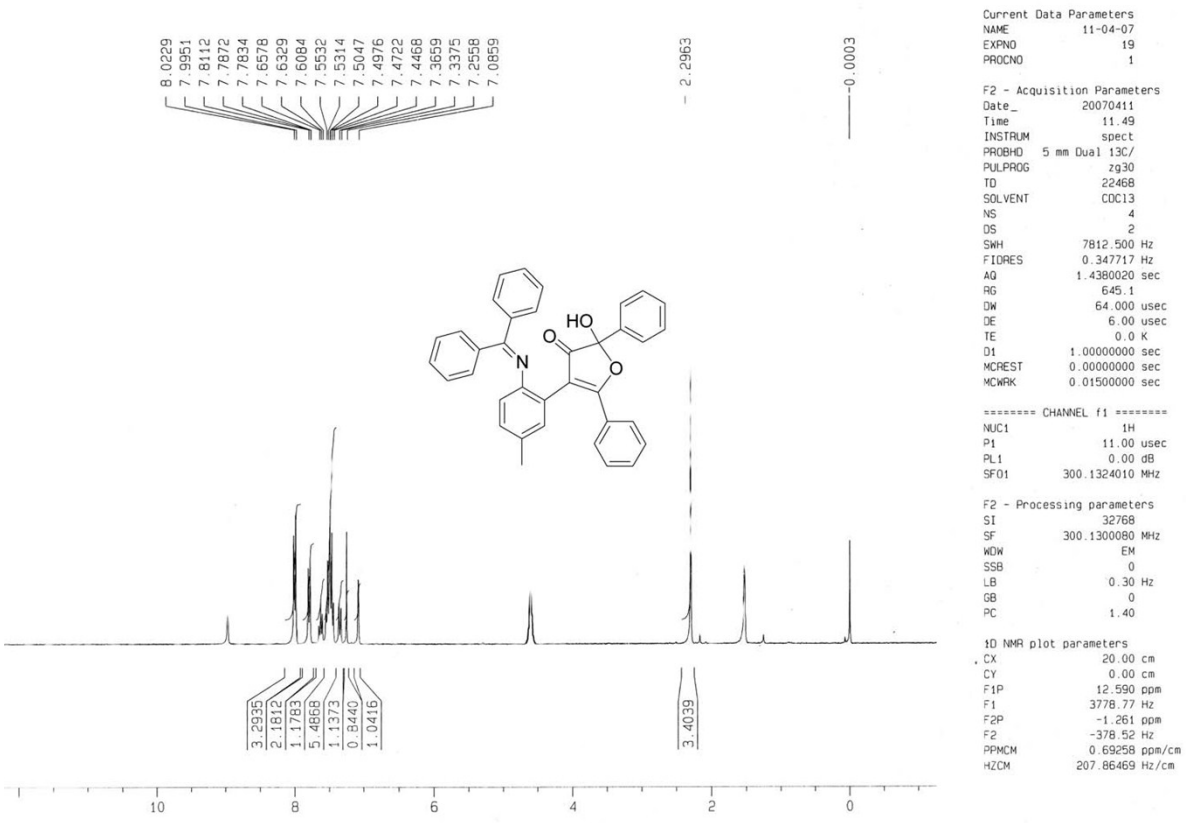
4-(2-(diphenylmethyleneamino)-5-methylphenyl)-2-hydroxy-2,5-diphenylfuran-3(2H)-one (25)

Yield = 61%

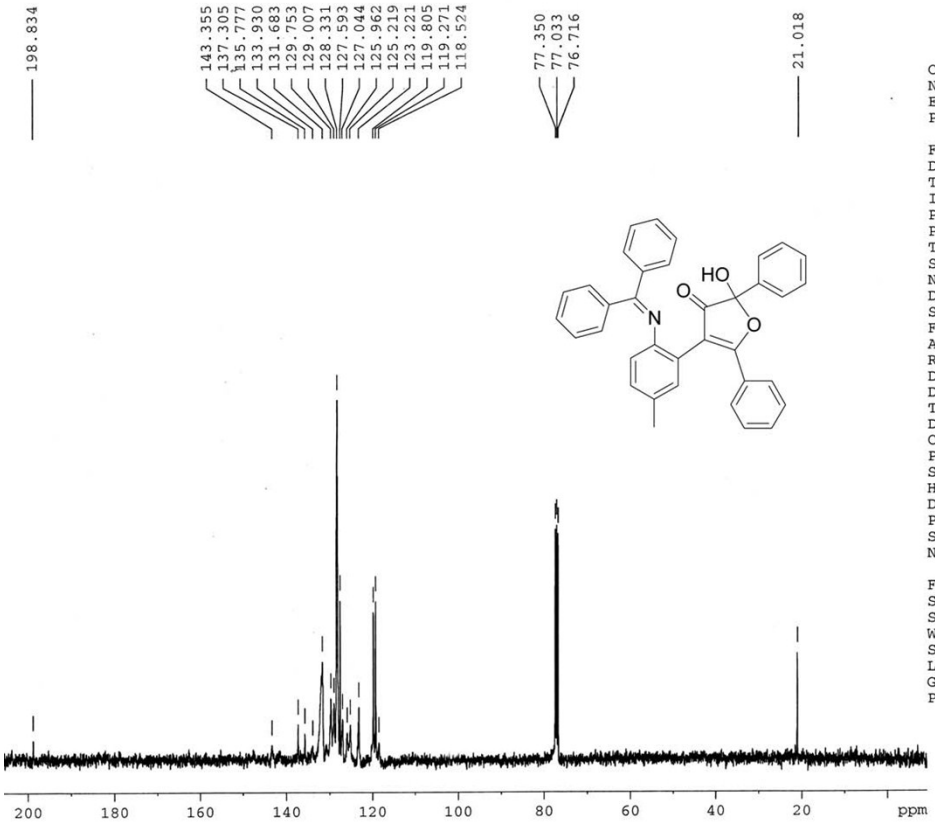
Yellow solid, mp: 134 °C



^{1}H NMR Spectrum of *4-(2-(diphenylmethyleneamino)-5-methylphenyl)-2-hydroxy-2,5-diphenylfuran-3(2H)-one* (*25*)



^{13}C NMR Spectrum of *4-(2-(diphenylmethyleneamino)-5-methylphenyl)-2-hydroxy-2,5-diphenylfuran-3(2H)-one (25)*

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PROCNO                1

F2 - Acquisition Parameters
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TD               16384
SOLVENT          cdcl3
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DS                   0
SWH          25000.000 Hz
FIDRES           1.525879 Hz
AQ            0.3277300 sec
RG                32768
DW               20.000 usec
DE               25.00 usec
TE               300.0 K
D11           0.03000000 sec
CPDPRG           waltz16
P31              75.00 usec
S2                  17 dB
HL1                 17 dB
D1            3.00000000 sec
P1                7.00 usec
SFO1         100.6254456 MHz
NUCLEUS             13C

F2 - Processing parameters
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SF           100.6138668 MHz
WDW                  EM
SSB                   0
LB                 3.00 Hz
GB                    0
PC                 1.00
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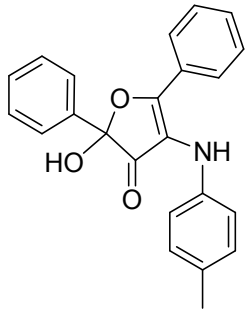
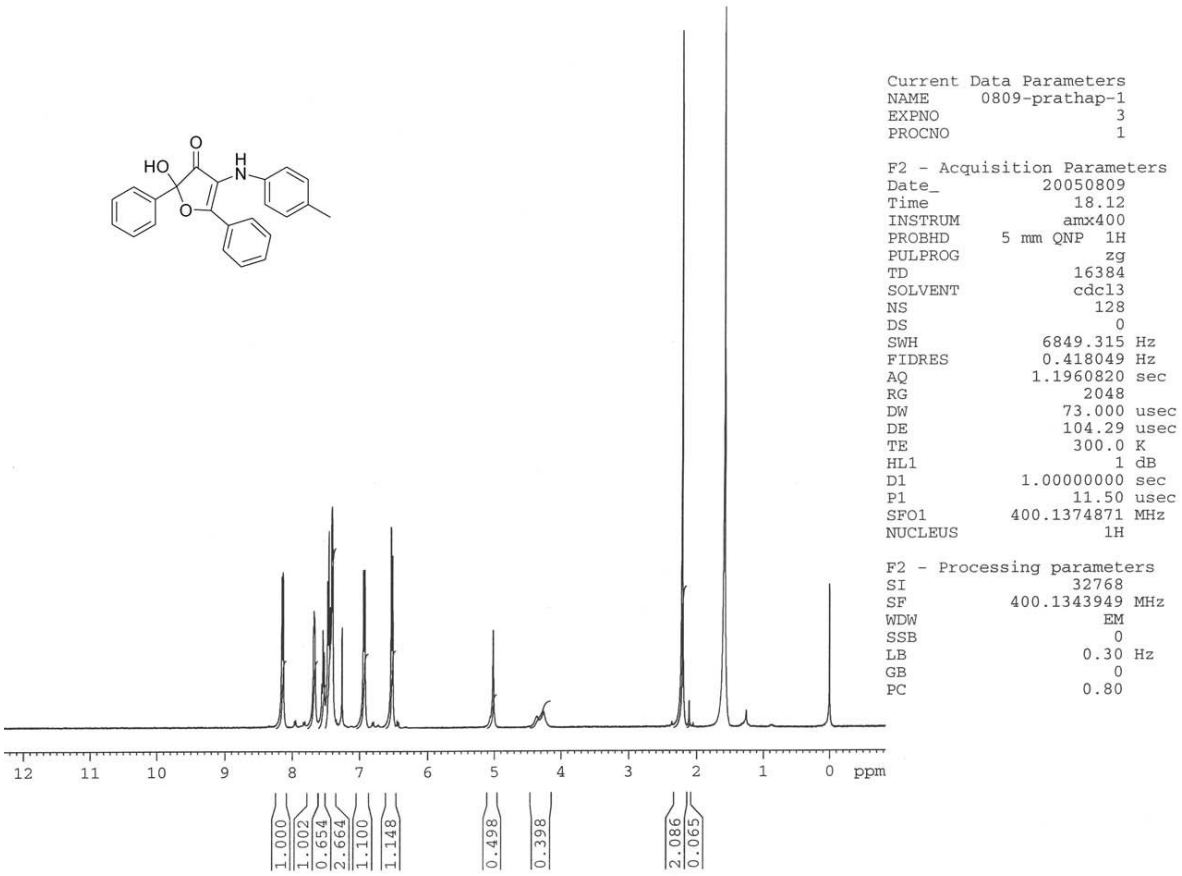
2-hydroxy-2,5-diphenyl-4-(p-tolylamino)furan-3(2H)-one (26)

Yield = 26%

Orange solid, mp: 154 °C



^{1}H NMR Spectrum of *2-hydroxy-2,5-diphenyl-4-(p-tolylamino)furan-3(2H)-one (26)*

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PROCNO                 1

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DS                    0
SWH            6849.315 Hz
FIDRES         0.418049 Hz
AQ             1.1960820 sec
RG                 2048
DW                73.000 usec
DE                104.29 usec
TE                 300.0 K
HL1                    1 dB
D1           1.00000000 sec
P1                11.50 usec
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NUCLEUS              1H

F2 - Processing parameters
SI                 32768
SF           400.1343949 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 0.80
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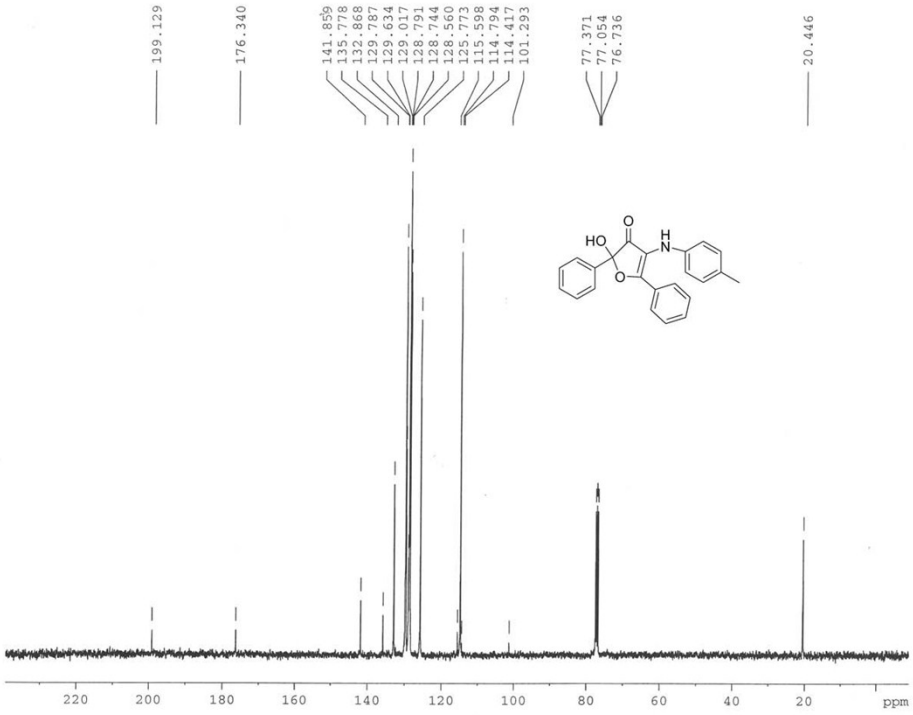
^{13}C NMR Spectrum of *4-(2-(diphenylmethyleneamino)-5-methylphenyl)-2-hydroxy-2,5-diphenylfuran-3(2H)-one (26)*



Current Data Parameters
NAME 0810-pratha-13
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

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FIDRES	1.525879 Hz
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RG	32768
DW	20.000 usec
DE	25.00 usec
TE	300.0 K
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P31	75.00 usec
S2	17 dB
HL1	17 dB
D1	3.00000000 sec
P1	7.00 usec
SFO1	100.6254456 MHz
NUCLEUS	13C

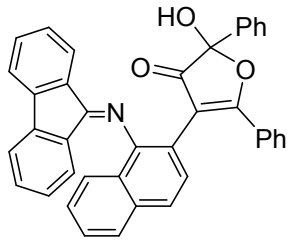
F2 - Processing parameters

SI	32768
SF	100.6138668 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

4-(1-(9H-fluoren-9-ylideneamino)naphthalen-2-yl)-2-hydroxy-2,5-diphenylfuran-3(2H)-one (28)

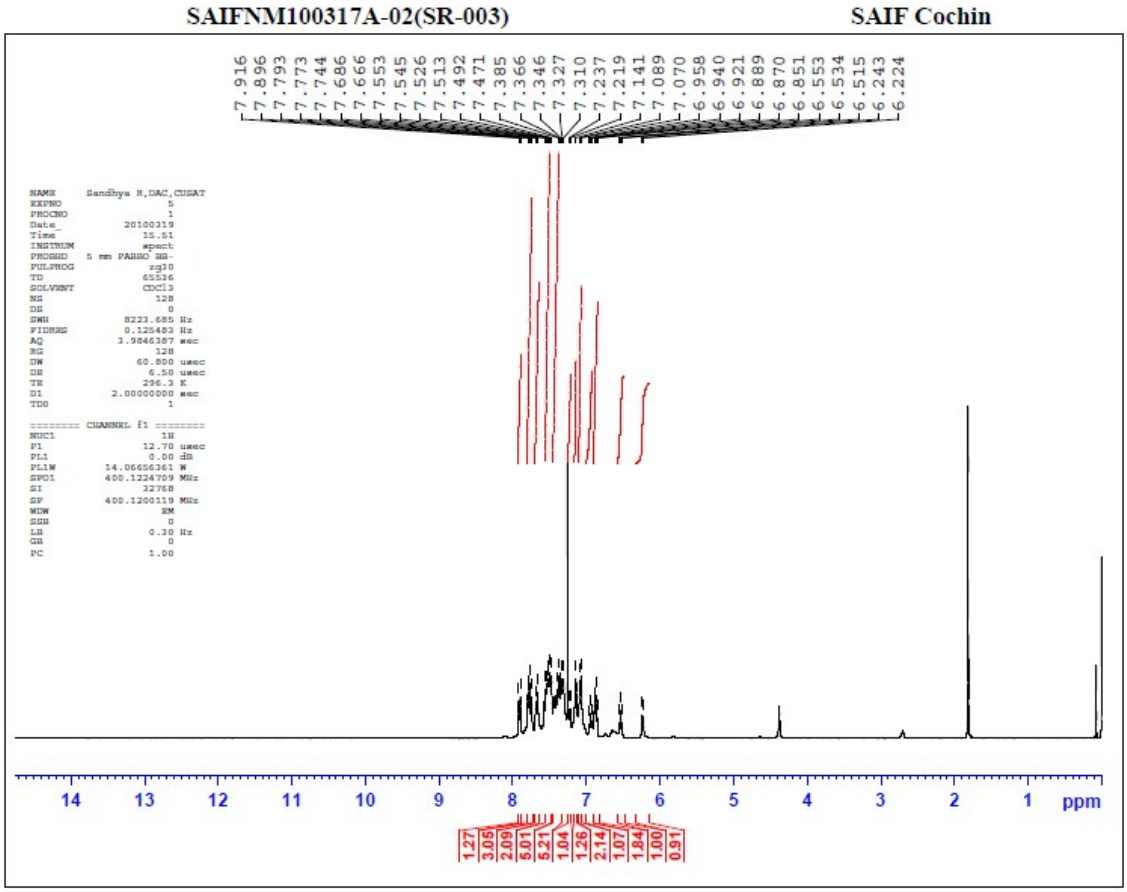
Yield = 87%

Orange red solid, mp: 132 °C

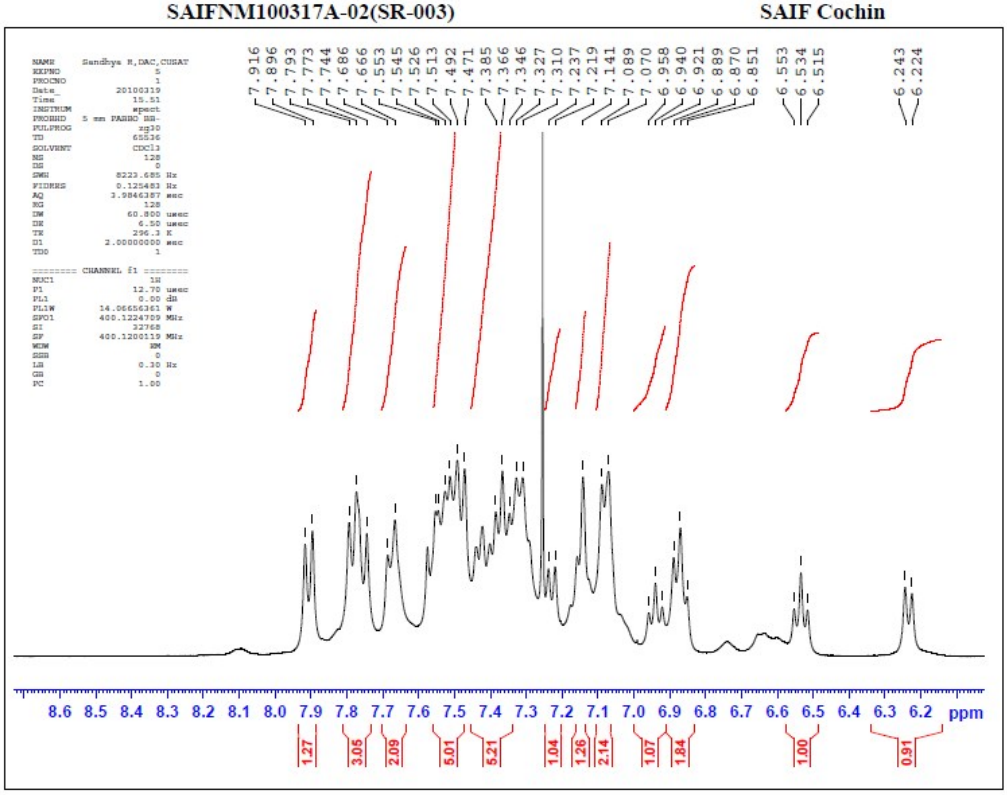


28

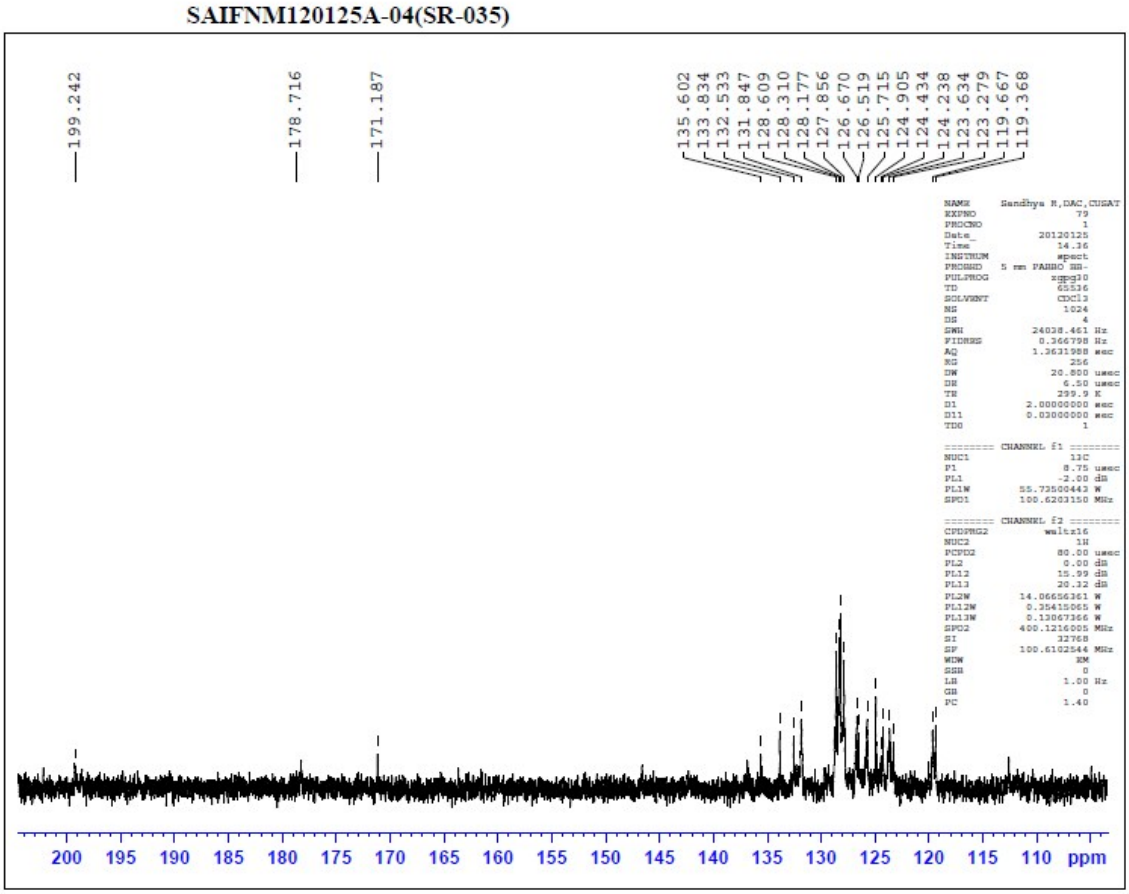
^{1}H NMR Spectrum of Compound 28 (full and expanded)

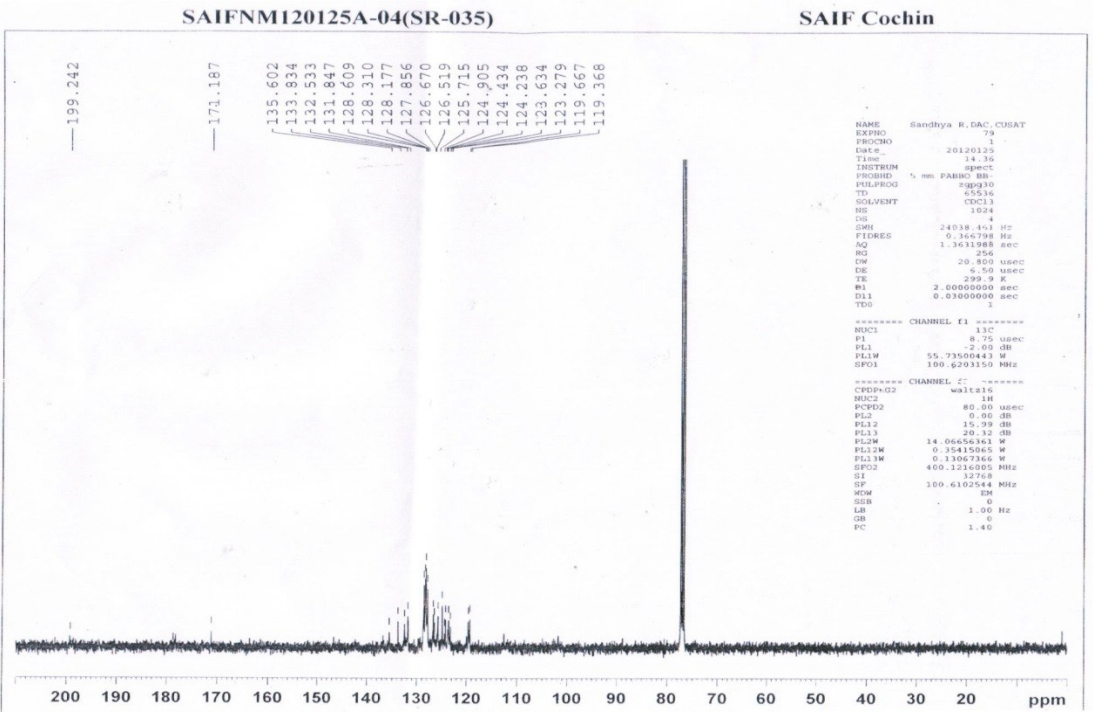


SAIFNM100317A-02(SR-003) SAIF Cochin



^{13}C NMR Spectrum of Compound 28 (expanded and full)

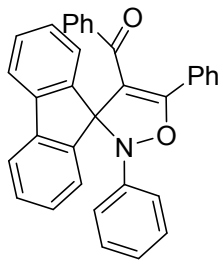




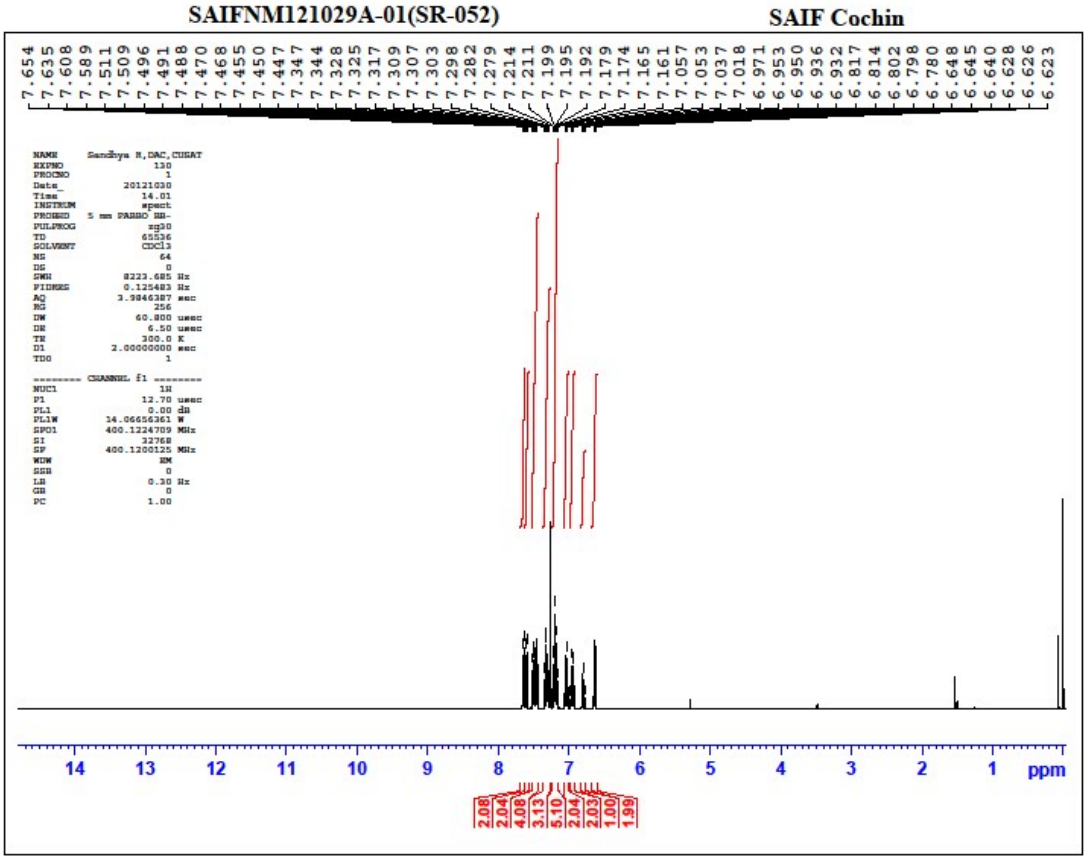
***2',5'-diphenyl-2'H-spiro[fluorene-9,3'-isoxazole]-4'-yl)(phenyl)methanone* (32)**

Yield = 3%

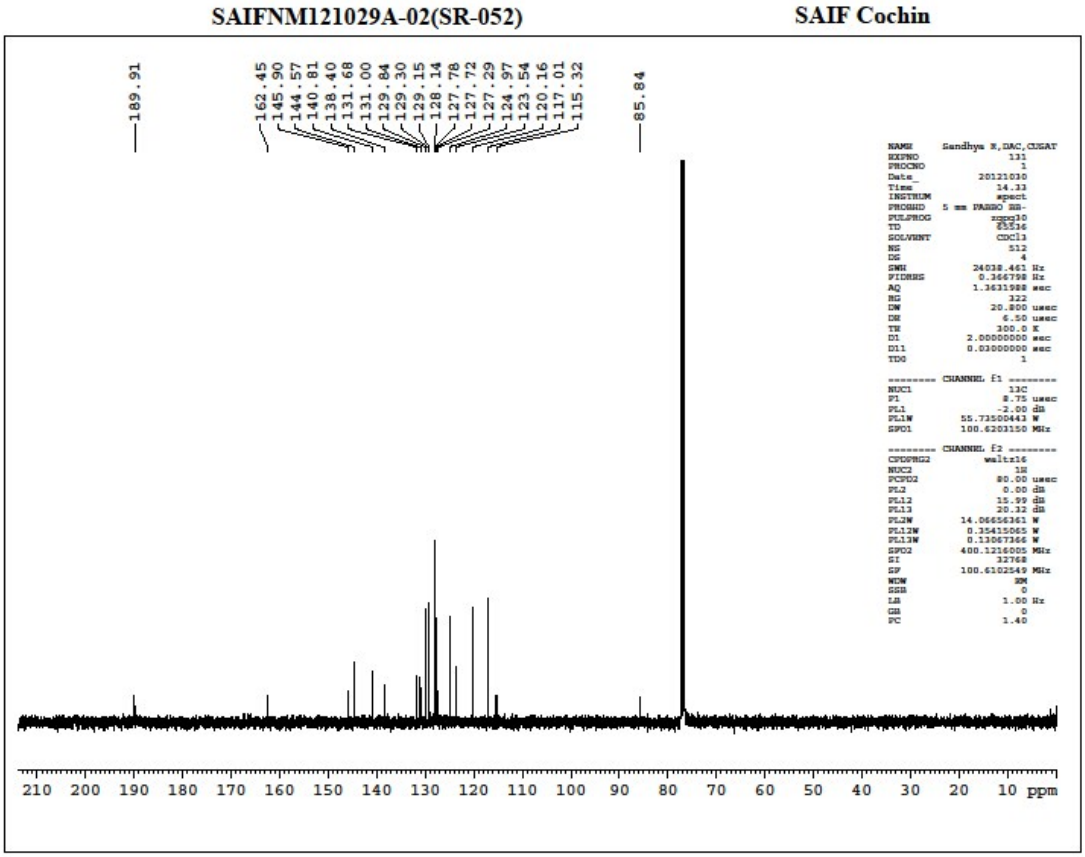
Yellow solid, mp: 142°C



^{1}H NMR Spectrum of Compound 32



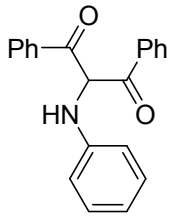
^{13}C NMR Spectrum of Compound 32



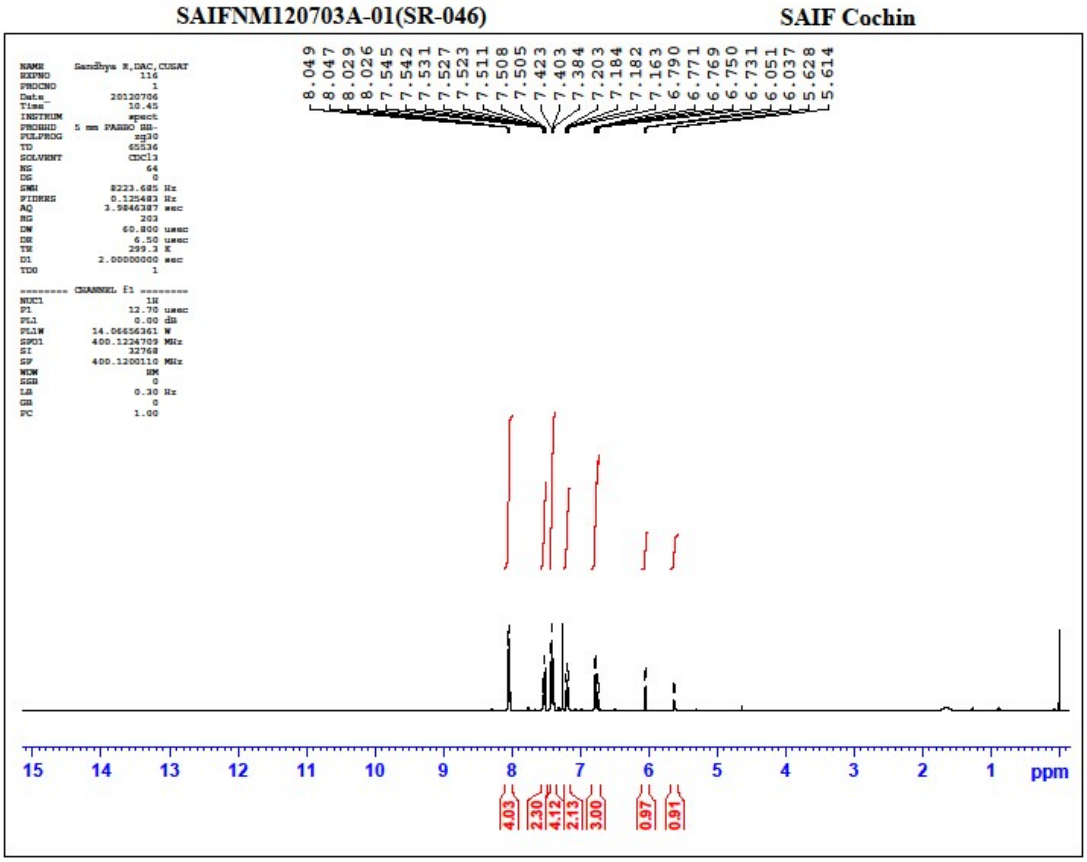
1,3-diphenyl-2-(phenylamino)propane-1,3-dione **(35)**

Yield = 16%

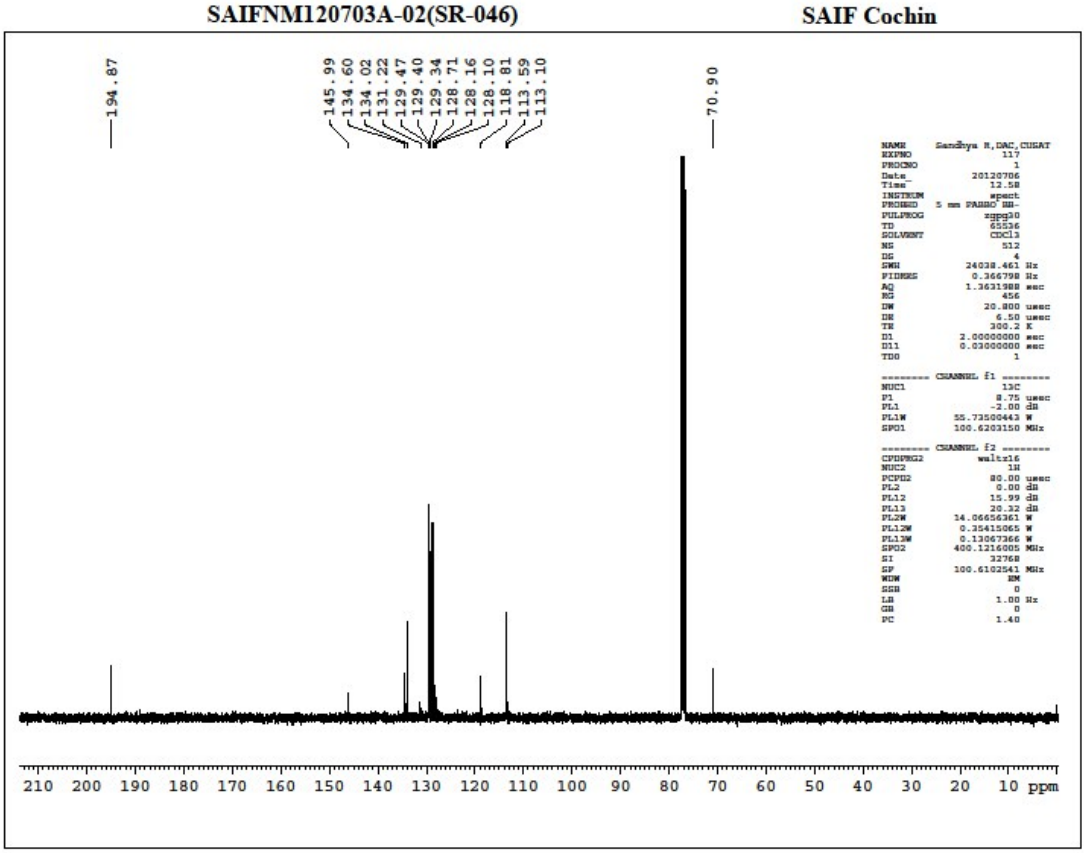
Yellow solid, mp: 70°C



[1]H NMR Spectrum of Compound 35



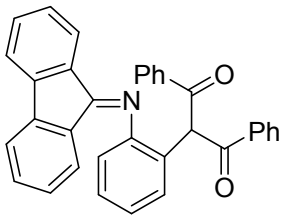
[13]C NMR Spectrum of Compound 35



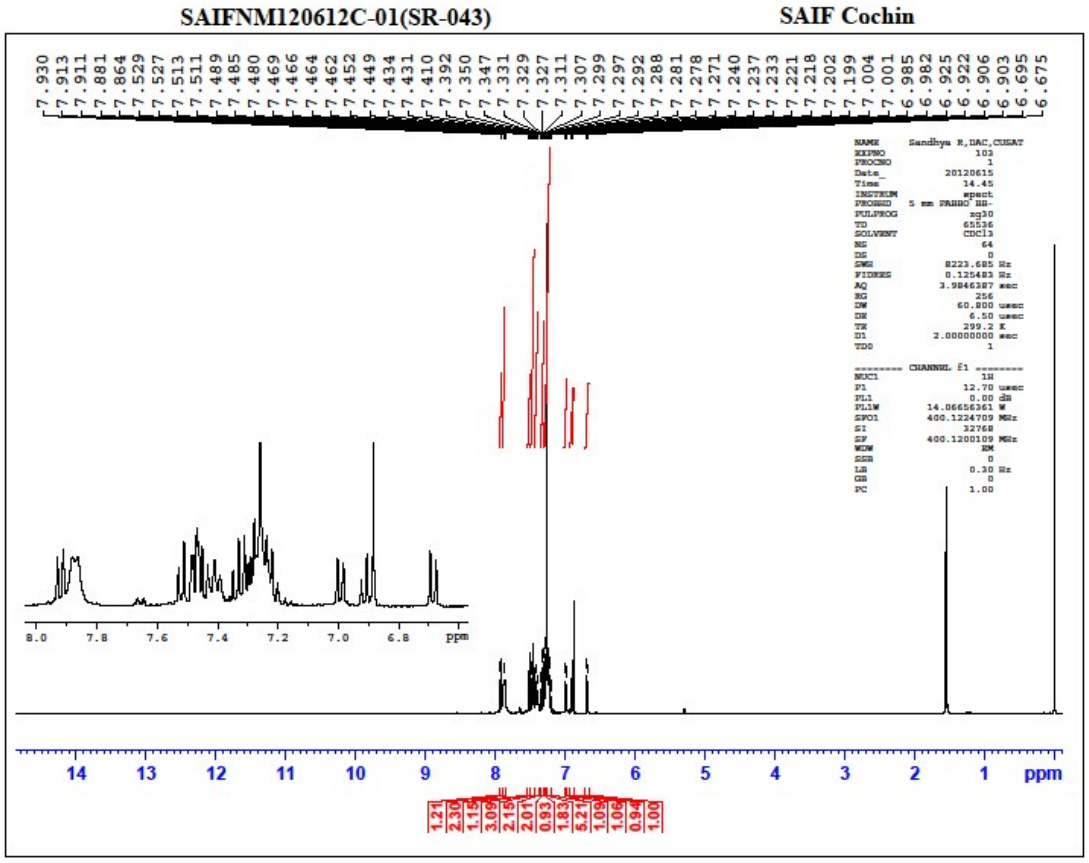
2-(2-(9H-fluoren-9-ylideneamino)phenyl)-1,3-diphenylpropane-1,3-dione **(36)**

Yield = 64%

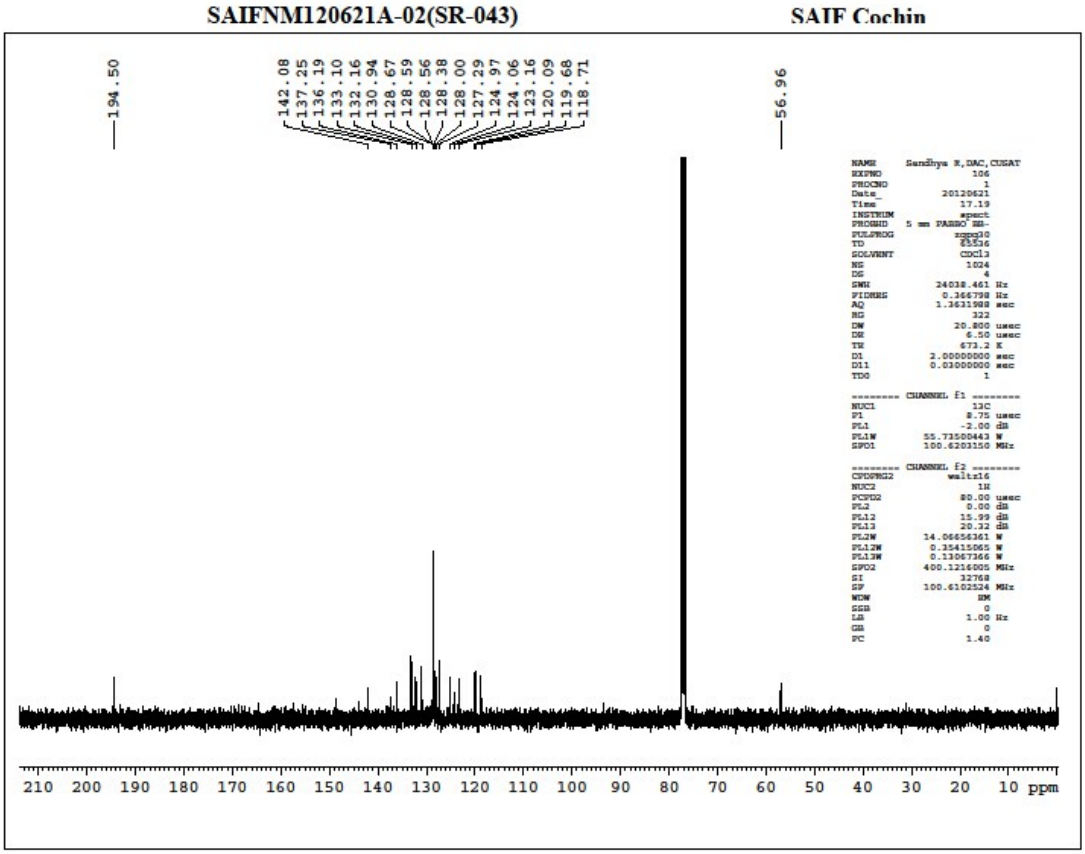
Yellow solid, mp: 174°C



^{1}H NMR Spectrum of Compound 36



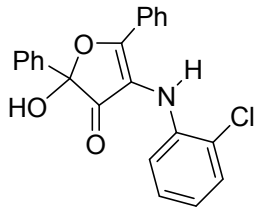
^{13}C NMR Spectrum of Compound 36



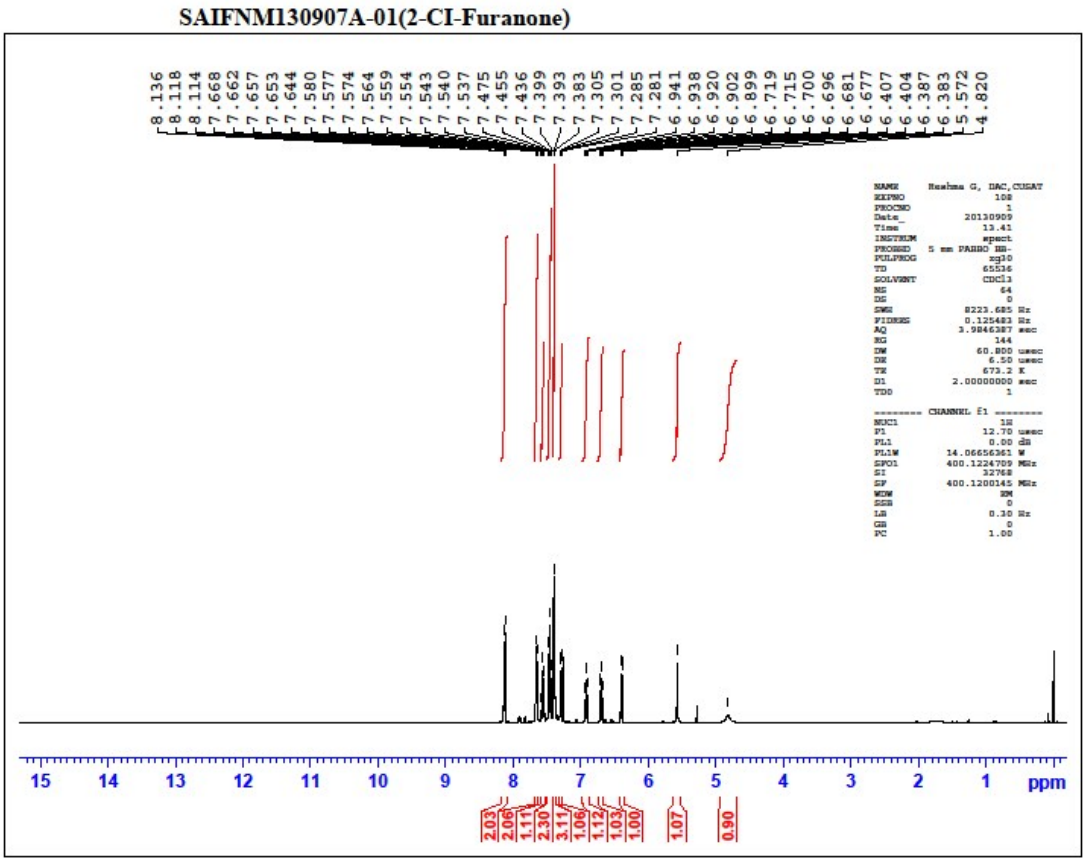
4-(2-chlorophenylamino)-2-hydroxy-2,5-diphenylfuran-3(2H)-one (39)

Yield = 87%

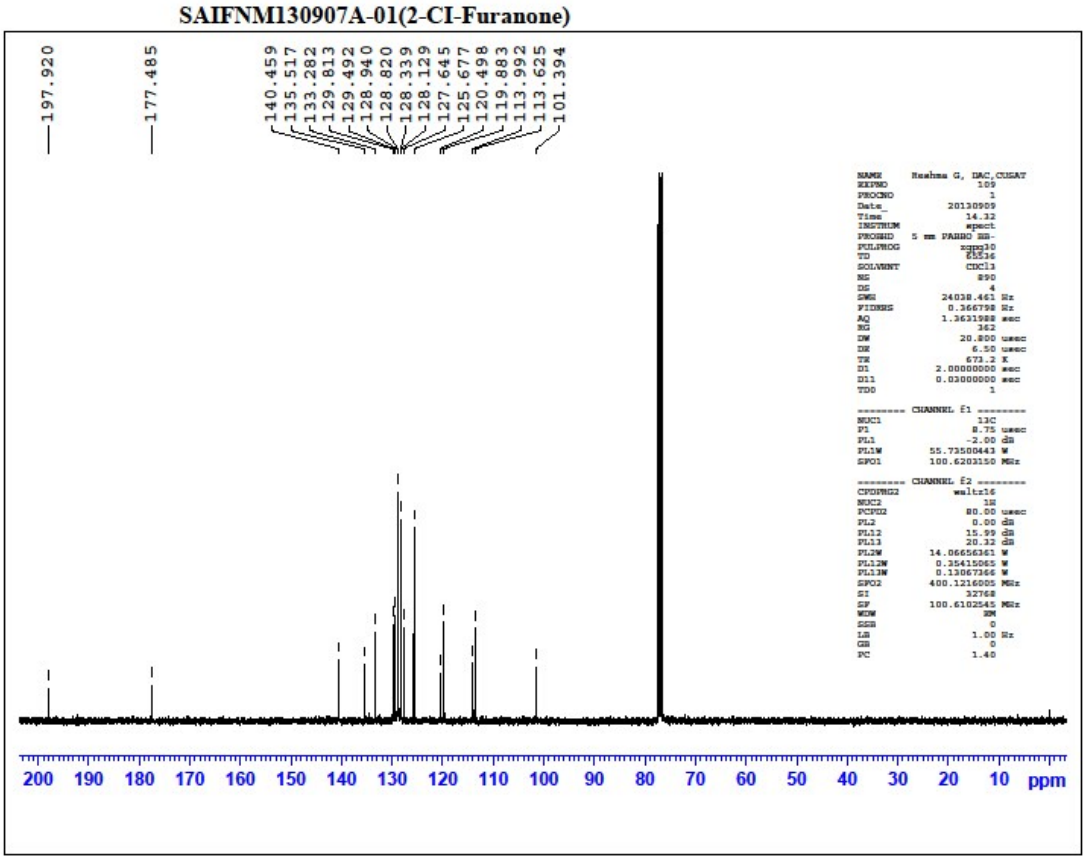
Orange solid, mp: 142 °C



^{1}H NMR Spectrum of Compound 39

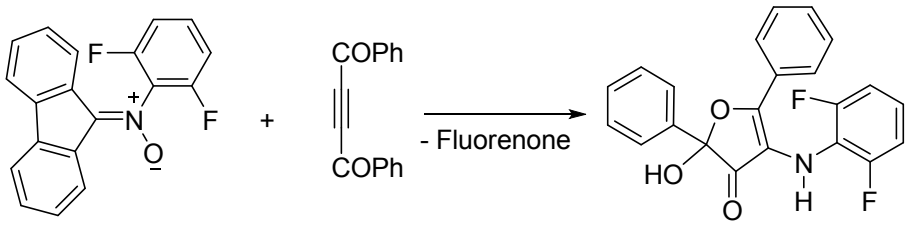


^{13}C NMR Spectrum of Compound 39

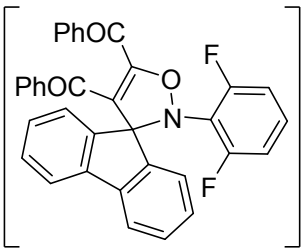


Additional Experiment (not included in the manuscript

1. **Reaction between *N-(9H-fluoren-9-ylidene)-2,6-difluoroaniline oxide* (*C*) and DBA**



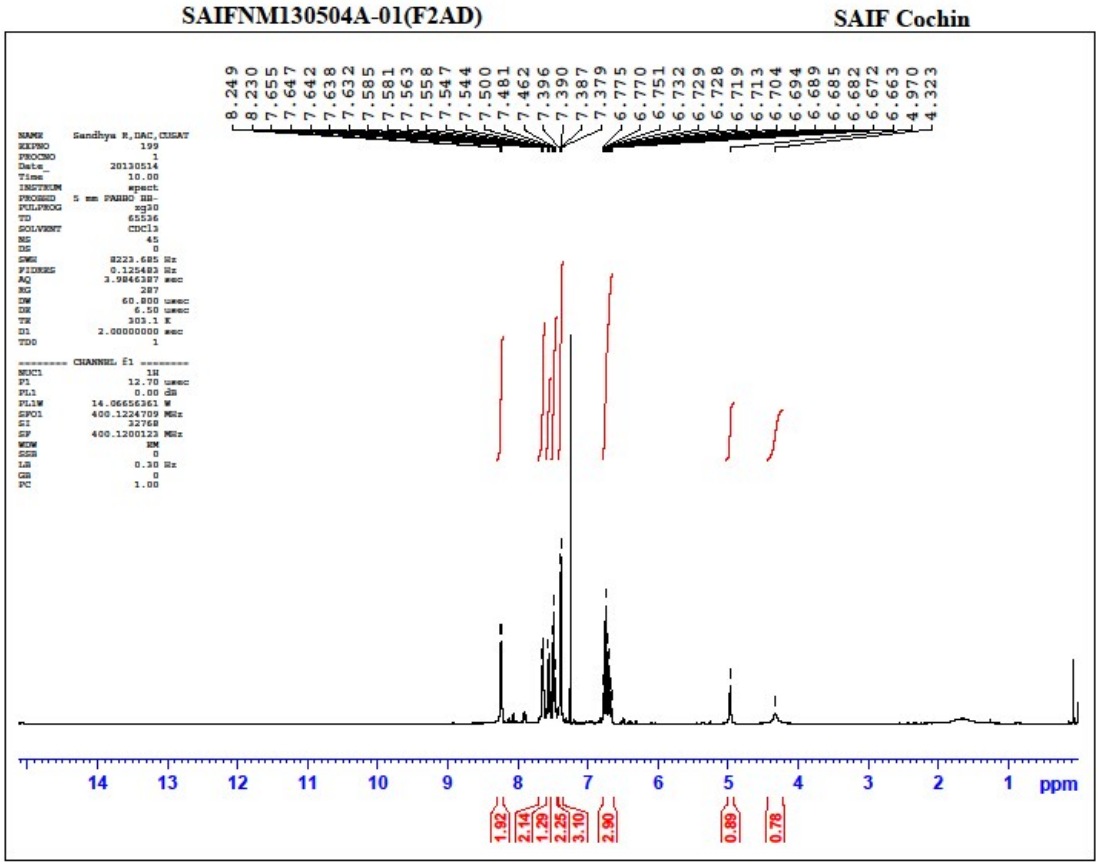
C **D**



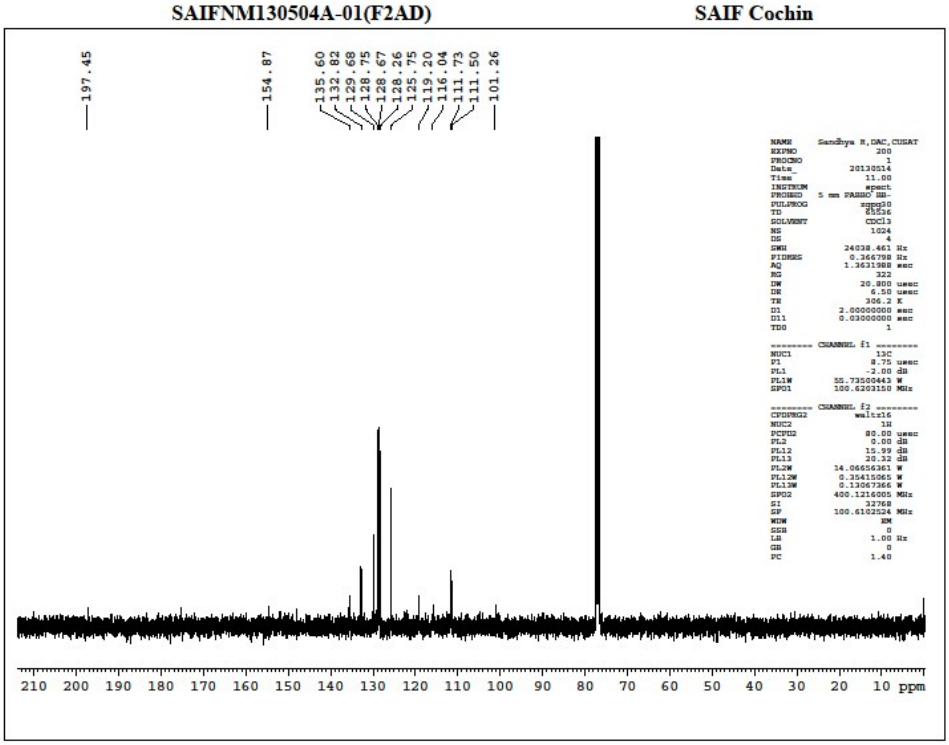
F

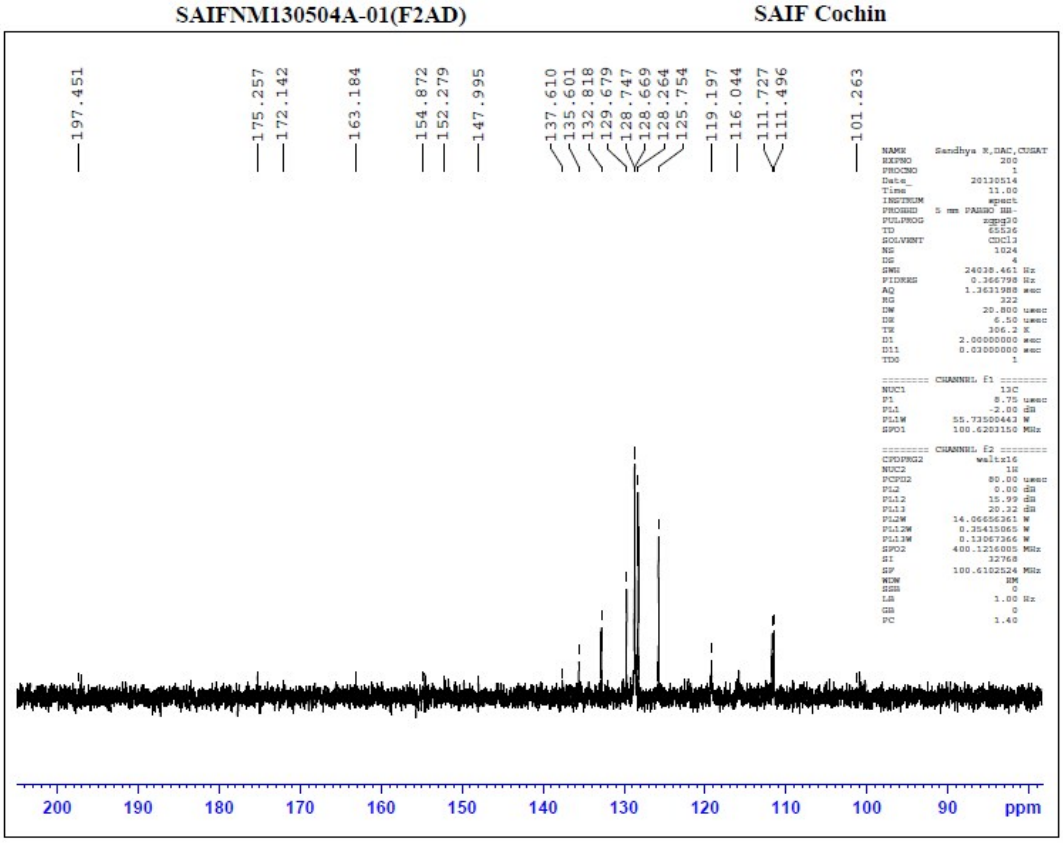
A mixture of nitrone **C** (307 mg, 1 mmol) and DBA (234 mg, 1 mmol) in 10 mL of acetonitrile was stirred at RT for 2h. Since the reaction proceeded extremely slowly, the mixture was refluxed overnight. TLC analysis indicated that substantial amount of **C** and DBA remained unchanged even after refluxing overnight. Solvent was removed under reduced pressure and the residue was chromatographed over silica gel to yield 368 mg (66%) of unchanged nitrone **C**, 53 mg (14%) of furanone **D** and 22 mg (12%) of fluorenone. In this case also, isoxazoline **F** could not be isolated in the pure form. *This experiment was conducted to establish that blocking 2,6-positions of N-aryl substituent on nitrone will suppress [3,3]-sigmatropic shift paving way to exclusive generation of isoxazoline derived products..*

^{1}H NMR spectrum of *4-(2,6-difluorophenylamino)-2-hydroxy-2,5-diphenylfuran-3(2H)-one (D)*



^{13}C NMR spectrum of *4-(2,6-difluorophenylamino)-2-hydroxy-2,5-diphenylfuran-3(2H)-one (D)* (full and expanded)

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SAIF Cochin
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175.257
172.142
163.184
154.872
152.279
147.995
137.610
135.601
132.818
129.679
128.747
128.669
128.264
125.754
119.197
116.044
111.727
111.496
101.263
200
190
180
170
160
150
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130
120
110
100
90
ppm