Supporting Information

A Tandem Reaction of Benzyne with Functionalized Benzylidenephthalan to Afford Phenanthro[10,1-*bc*]furan

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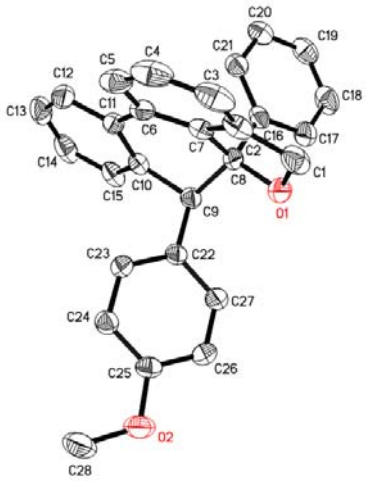
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1. Crystal data and structure refinement of product 3c.



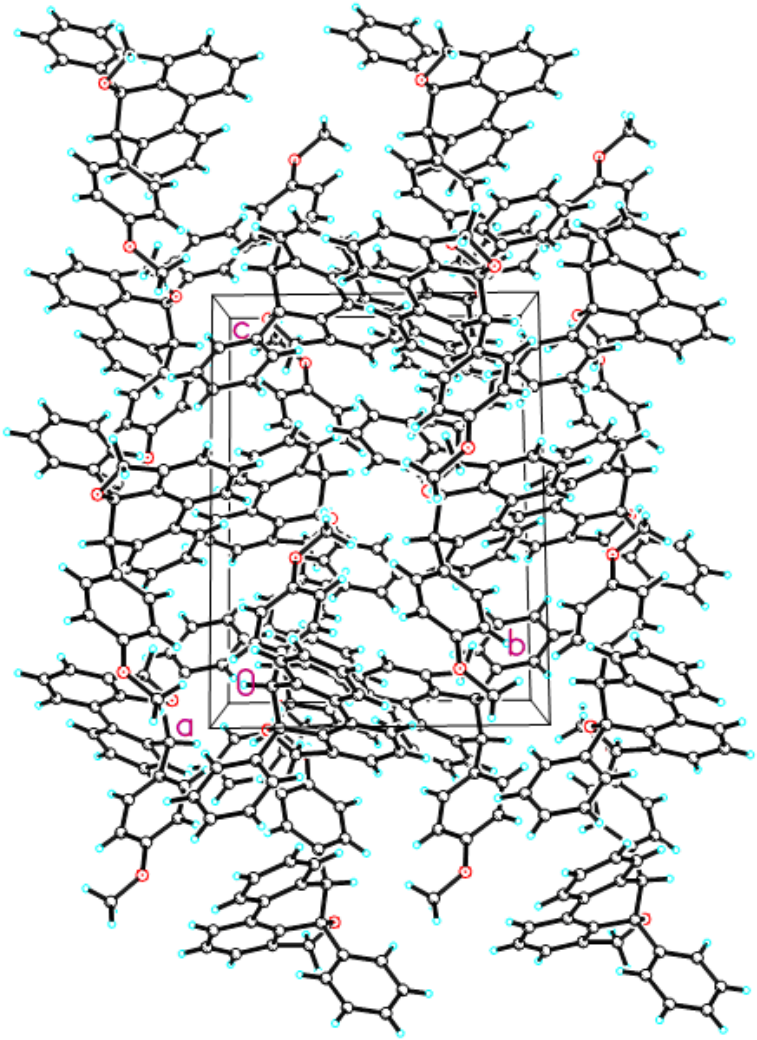


Table 1. Crystal data and structure refinement for **3c**.

Identification code	**3c**
CCDC number	CCDC 974317
Empirical formula	C28 H22 O2
Formula weight	390.46
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 13.0933(14) A alpha = 90 deg.
	b = 10.9512(11) A beta = 107.682(2) deg.
	c = 14.9276(15) A gamma = 90 deg.
Volume	2039.3(4) A^3
Z, Calculated density	4, 1.272 Mg/m^3
Absorption coefficient	0.079 mm^-1
F(000)	824
Crystal size	0.265 x 0.168 x 0.123 mm
Theta range for data collection	1.82 to 26.00 deg.
Limiting indices	-16<=h<=16, -8<=k<=13, -18<=l<=18
Reflections collected / unique	11693 / 4006 [R(int) = 0.0313]
Completeness to theta = 26.00	99.9 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.52232
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4006 / 0 / 272
Goodness-of-fit on F^2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0534, wR2 = 0.1339
R indices (all data)	R1 = 0.0749, wR2 = 0.1461
Largest diff. peak and hole	0.300 and -0.149 e.A^-3

Table 3. Bond lengths [A] and angles [deg] for **3c**.

O(1)-C(8)	1.437(2)
O(1)-C(1)	1.446(3)
O(2)-C(25)	1.372(2)
O(2)-C(28)	1.414(3)
C(1)-C(2)	1.484(3)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(3)	1.378(3)
C(2)-C(7)	1.379(3)
C(3)-C(4)	1.381(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.396(4)
C(4)-H(4)	0.9300

C(5)-C(6)	1.400(3)
C(5)-H(5)	0.9300
C(6)-C(7)	1.372(3)
C(6)-C(11)	1.477(3)
C(7)-C(8)	1.493(3)
C(8)-C(16)	1.542(3)
C(8)-C(9)	1.543(3)
C(9)-C(22)	1.521(3)
C(9)-C(10)	1.522(3)
C(9)-H(9)	0.9800
C(10)-C(15)	1.389(3)
C(10)-C(11)	1.410(3)
C(11)-C(12)	1.389(3)
C(12)-C(13)	1.377(4)
C(12)-H(12)	0.9300
C(13)-C(14)	1.360(4)
C(13)-H(13)	0.9300
C(14)-C(15)	1.376(3)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
C(16)-C(17)	1.380(3)
C(16)-C(21)	1.385(3)
C(17)-C(18)	1.391(3)
C(17)-H(17)	0.9300
C(18)-C(19)	1.363(4)
C(18)-H(18)	0.9300
C(19)-C(20)	1.365(3)
C(19)-H(19)	0.9300
C(20)-C(21)	1.390(3)
C(20)-H(20)	0.9300
C(21)-H(21)	0.9300
C(22)-C(23)	1.373(3)
C(22)-C(27)	1.389(3)
C(23)-C(24)	1.391(3)
C(23)-H(23)	0.9300
C(24)-C(25)	1.377(3)
C(24)-H(24)	0.9300
C(25)-C(26)	1.386(3)
C(26)-C(27)	1.371(3)
C(26)-H(26)	0.9300
C(27)-H(27)	0.9300
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600

C(8)-O(1)-C(1)	108.12(16)

C(25)-O(2)-C(28)	118.13(19)
O(1)-C(1)-C(2)	104.75(17)
O(1)-C(1)-H(1A)	110.8
C(2)-C(1)-H(1A)	110.8
O(1)-C(1)-H(1B)	110.8
C(2)-C(1)-H(1B)	110.8
H(1A)-C(1)-H(1B)	108.9
C(3)-C(2)-C(7)	118.8(2)
C(3)-C(2)-C(1)	133.7(2)
C(7)-C(2)-C(1)	107.38(19)
C(2)-C(3)-C(4)	118.2(2)
C(2)-C(3)-H(3)	120.9
C(4)-C(3)-H(3)	120.9
C(3)-C(4)-C(5)	122.3(2)
C(3)-C(4)-H(4)	118.8
C(5)-C(4)-H(4)	118.8
C(4)-C(5)-C(6)	119.5(3)
C(4)-C(5)-H(5)	120.2
C(6)-C(5)-H(5)	120.2
C(7)-C(6)-C(5)	116.3(2)
C(7)-C(6)-C(11)	116.39(17)
C(5)-C(6)-C(11)	127.2(2)
C(6)-C(7)-C(2)	124.61(19)
C(6)-C(7)-C(8)	125.25(17)
C(2)-C(7)-C(8)	109.97(19)
O(1)-C(8)-C(7)	102.62(16)
O(1)-C(8)-C(16)	109.34(15)
C(7)-C(8)-C(16)	114.13(16)
O(1)-C(8)-C(9)	112.95(15)
C(7)-C(8)-C(9)	108.35(15)
C(16)-C(8)-C(9)	109.41(15)
C(22)-C(9)-C(10)	112.35(15)
C(22)-C(9)-C(8)	114.41(16)
C(10)-C(9)-C(8)	107.97(15)
C(22)-C(9)-H(9)	107.3
C(10)-C(9)-H(9)	107.3
C(8)-C(9)-H(9)	107.3
C(15)-C(10)-C(11)	118.5(2)
C(15)-C(10)-C(9)	119.60(19)
C(11)-C(10)-C(9)	121.68(17)
C(12)-C(11)-C(10)	119.0(2)
C(12)-C(11)-C(6)	122.8(2)
C(10)-C(11)-C(6)	118.22(18)
C(13)-C(12)-C(11)	120.9(2)
C(13)-C(12)-H(12)	119.6
C(11)-C(12)-H(12)	119.6

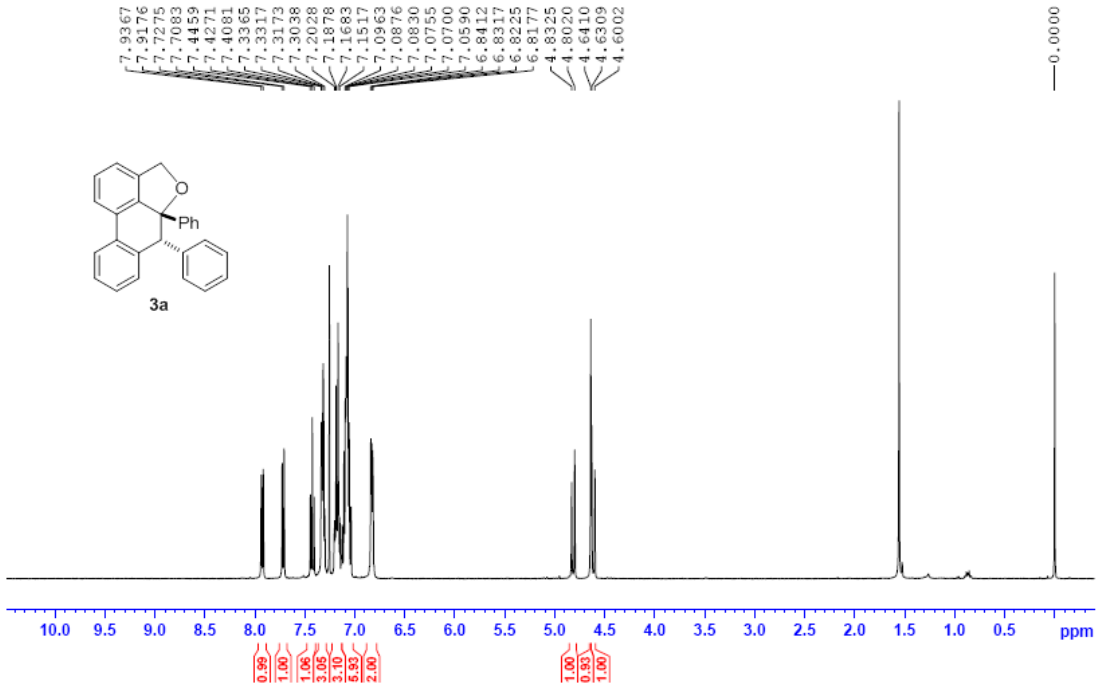
C(14)-C(13)-C(12)	120.1(2)
C(14)-C(13)-H(13)	119.9
C(12)-C(13)-H(13)	119.9
C(13)-C(14)-C(15)	120.4(2)
C(13)-C(14)-H(14)	119.8
C(15)-C(14)-H(14)	119.8
C(14)-C(15)-C(10)	121.0(2)
C(14)-C(15)-H(15)	119.5
C(10)-C(15)-H(15)	119.5
C(17)-C(16)-C(21)	117.8(2)
C(17)-C(16)-C(8)	119.02(19)
C(21)-C(16)-C(8)	123.15(18)
C(16)-C(17)-C(18)	120.6(2)
C(16)-C(17)-H(17)	119.7
C(18)-C(17)-H(17)	119.7
C(19)-C(18)-C(17)	120.8(2)
C(19)-C(18)-H(18)	119.6
C(17)-C(18)-H(18)	119.6
C(18)-C(19)-C(20)	119.5(2)
C(18)-C(19)-H(19)	120.3
C(20)-C(19)-H(19)	120.3
C(19)-C(20)-C(21)	120.2(2)
C(19)-C(20)-H(20)	119.9
C(21)-C(20)-H(20)	119.9
C(16)-C(21)-C(20)	121.1(2)
C(16)-C(21)-H(21)	119.4
C(20)-C(21)-H(21)	119.4
C(23)-C(22)-C(27)	117.02(19)
C(23)-C(22)-C(9)	123.22(17)
C(27)-C(22)-C(9)	119.69(18)
C(22)-C(23)-C(24)	122.14(19)
C(22)-C(23)-H(23)	118.9
C(24)-C(23)-H(23)	118.9
C(25)-C(24)-C(23)	119.69(19)
C(25)-C(24)-H(24)	120.2
C(23)-C(24)-H(24)	120.2
O(2)-C(25)-C(24)	125.2(2)
O(2)-C(25)-C(26)	115.80(19)
C(24)-C(25)-C(26)	119.0(2)
C(27)-C(26)-C(25)	120.3(2)
C(27)-C(26)-H(26)	119.9
C(25)-C(26)-H(26)	119.9
C(26)-C(27)-C(22)	121.9(2)
C(26)-C(27)-H(27)	119.1
C(22)-C(27)-H(27)	119.1
O(2)-C(28)-H(28A)	109.5

O(2)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
O(2)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5

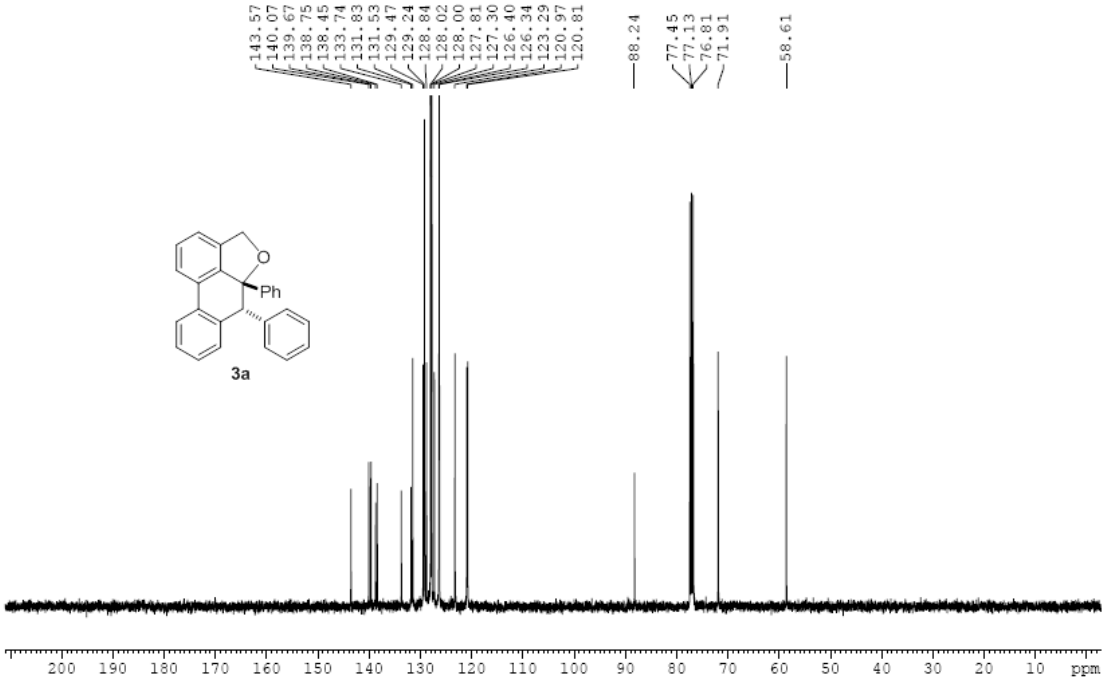
Symmetry transformations used to generate equivalent atoms:

2. Copies of ^{1}H and ^{13}C NMR spectra

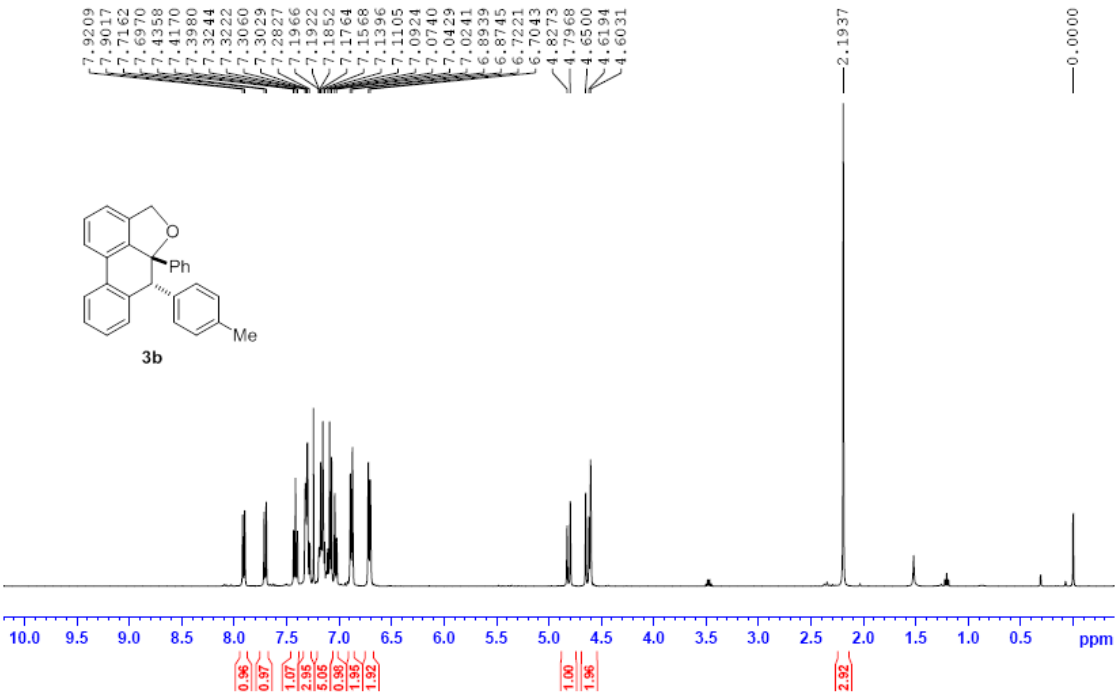
^{1}H NMR of 5a,6-diphenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3a)**



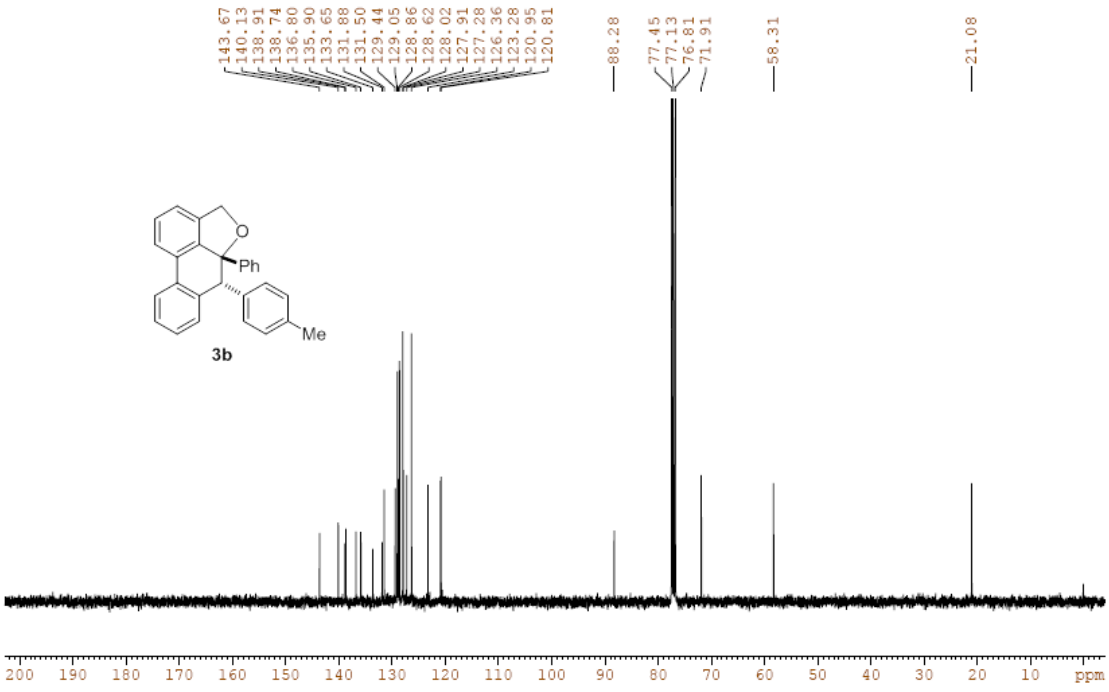
^{13}C NMR of 5a,6-diphenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3a)**



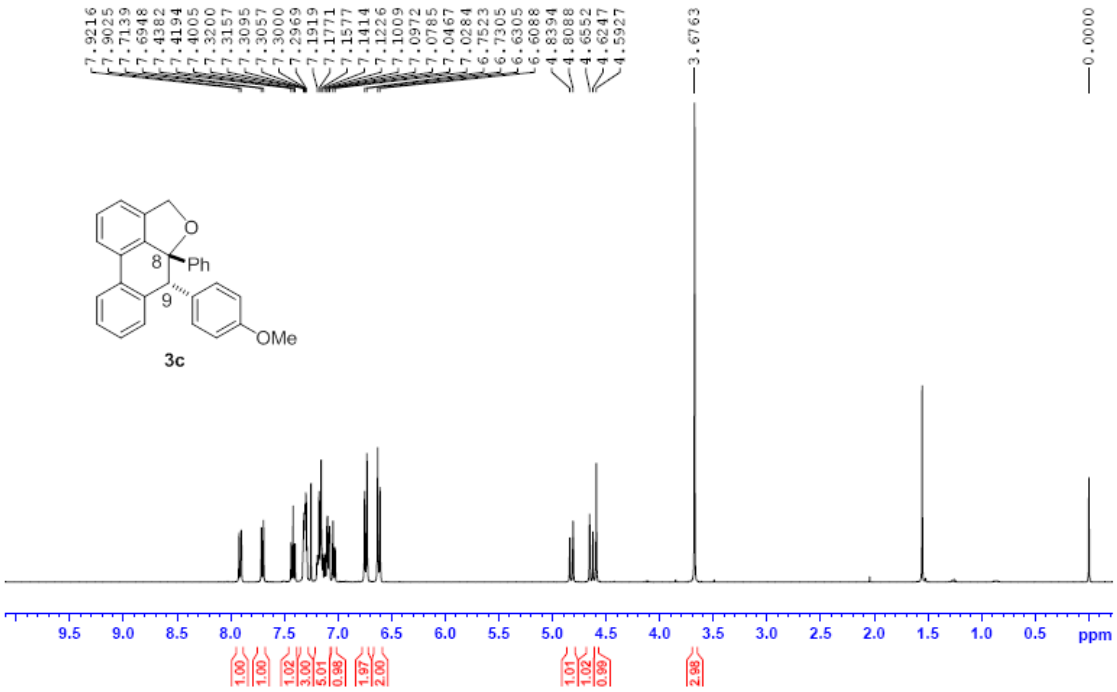
^{1}H NMR of 5a-phenyl-6-(*p*-tolyl)-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3b)**



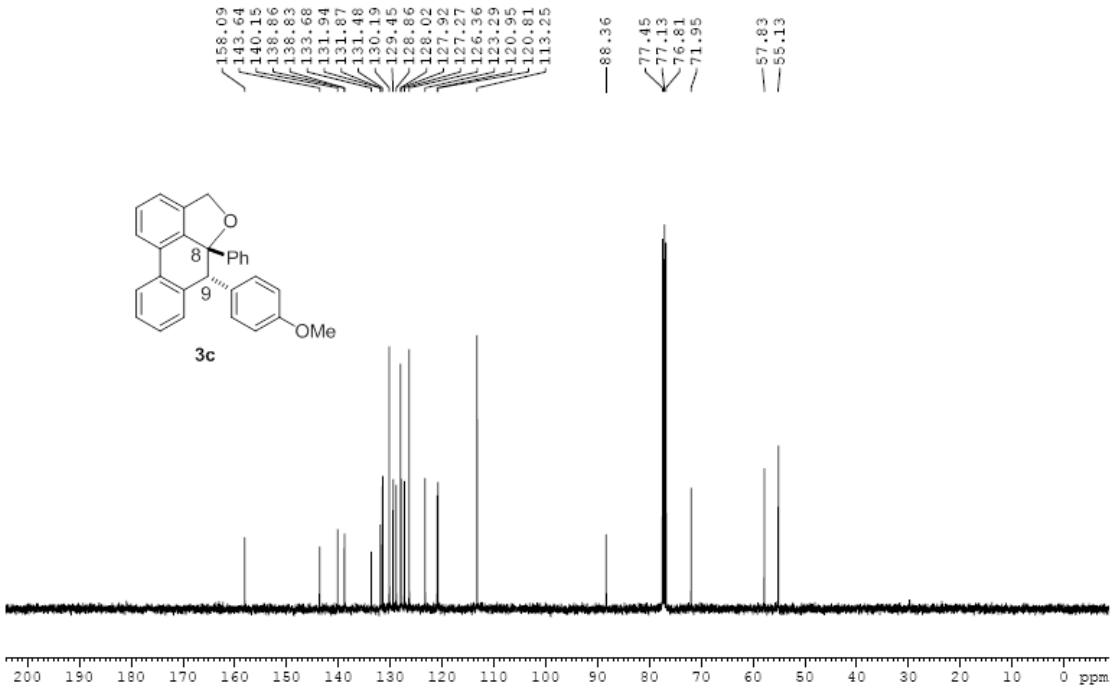
^{13}C NMR of 5a-phenyl-6-(*p*-tolyl)-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3b)**



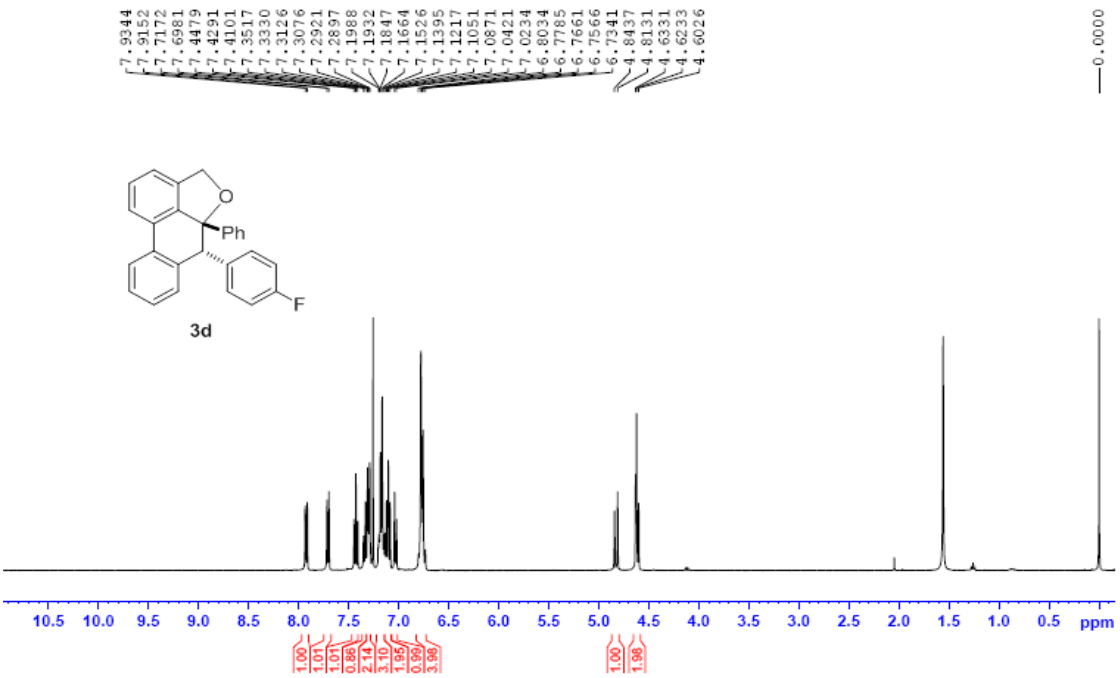
^{1}H NMR of 6-(4-methoxyphenyl)-5a-phenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3c)**



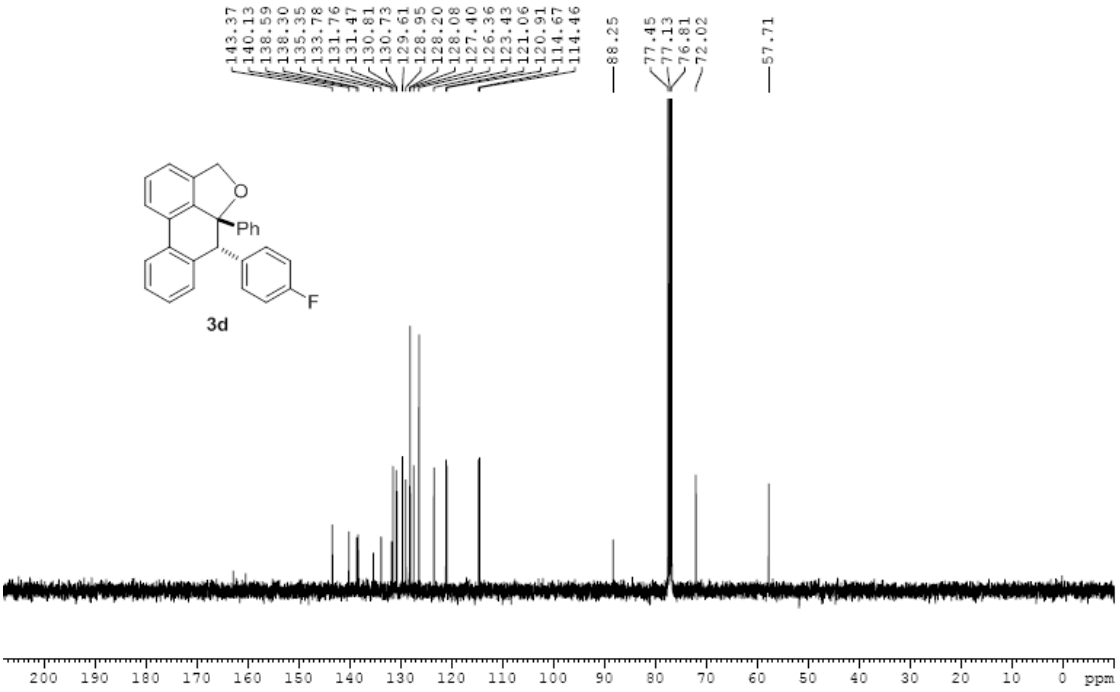
^{13}C NMR of 6-(4-methoxyphenyl)-5a-phenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3c)**



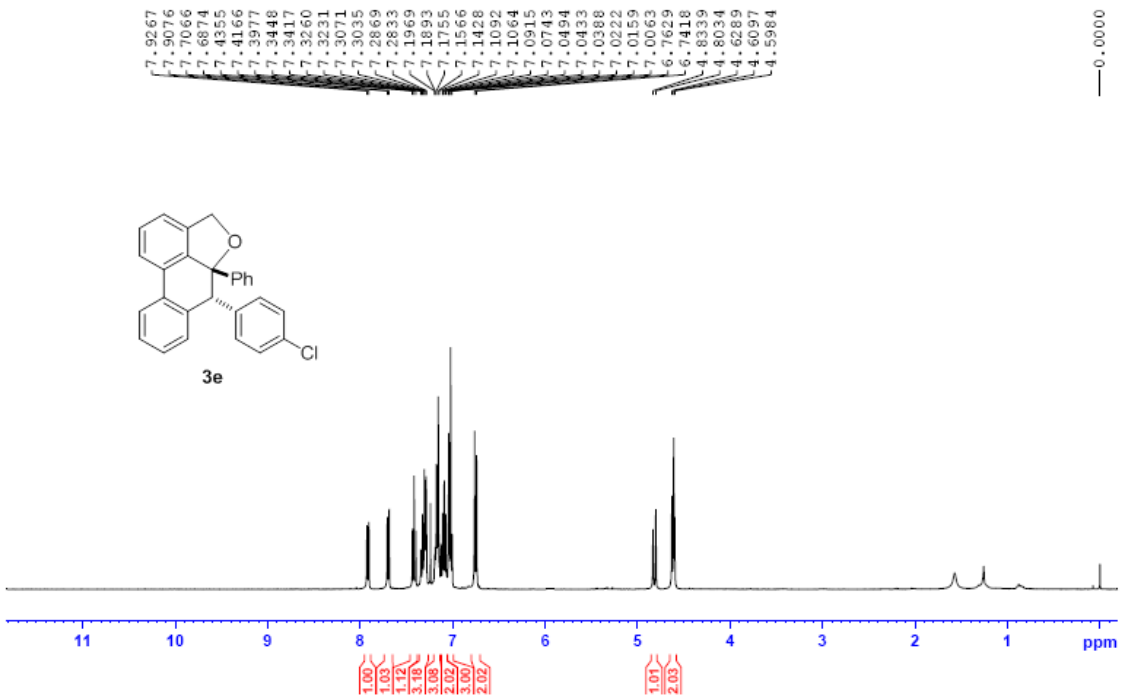
^{1}H NMR of 6-(4-fluorophenyl)-5a-phenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3d)**



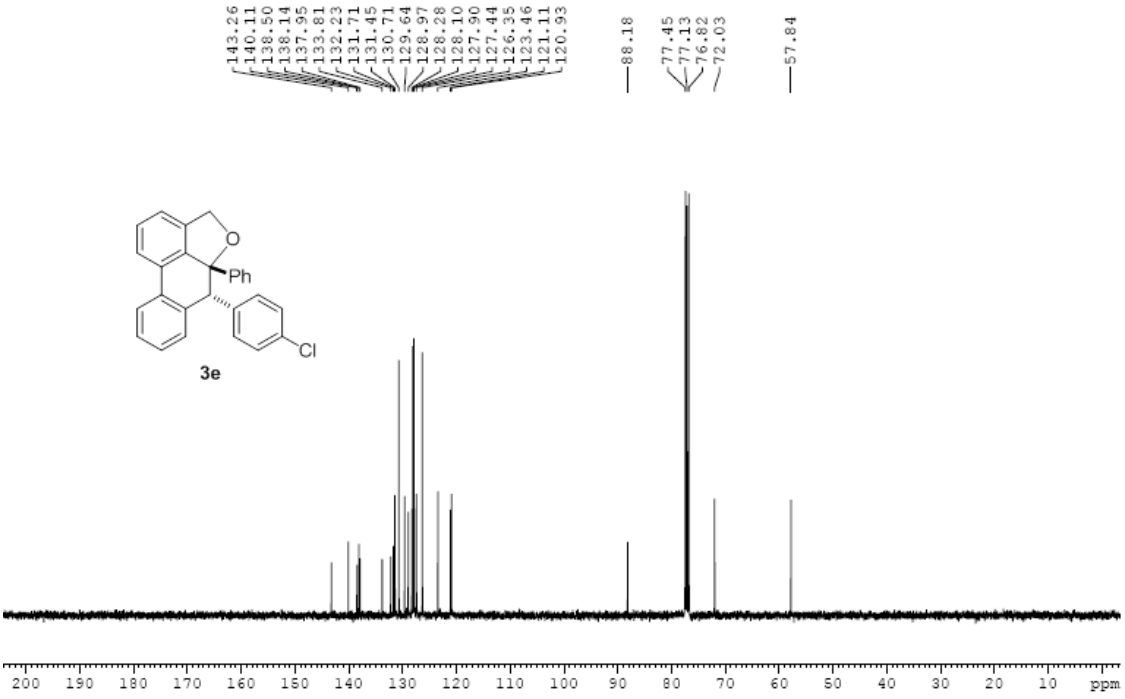
^{13}C NMR of 6-(4-fluorophenyl)-5a-phenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3d)**



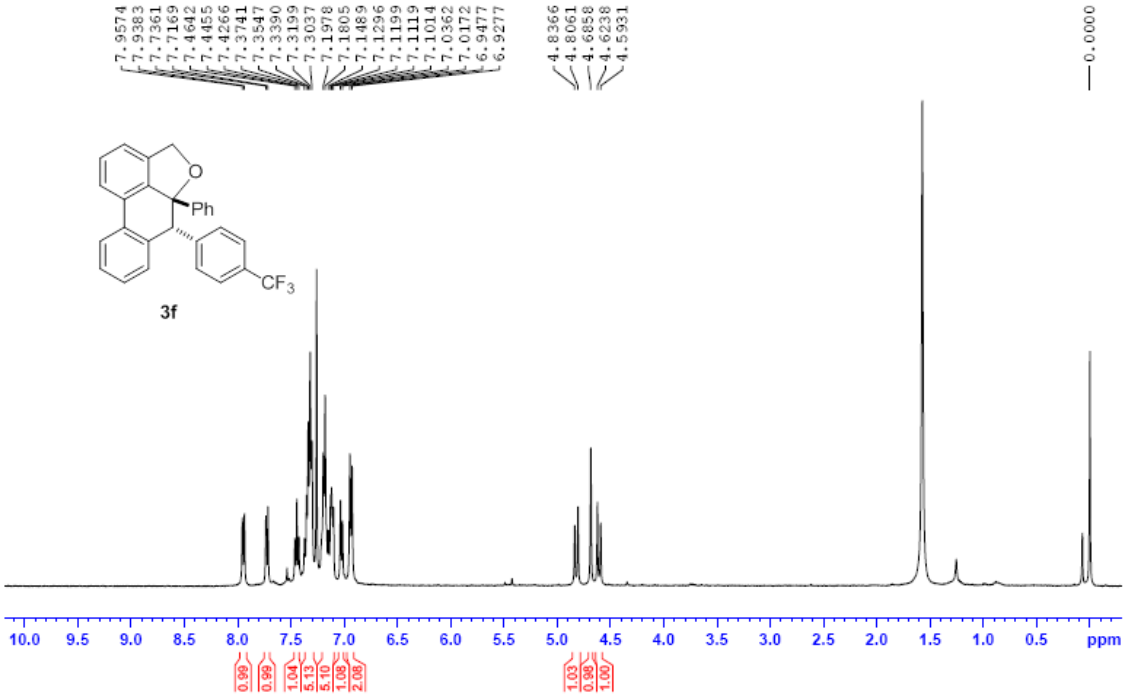
^{1}H NMR of 6-(4-chlorophenyl)-5a-phenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3e)**



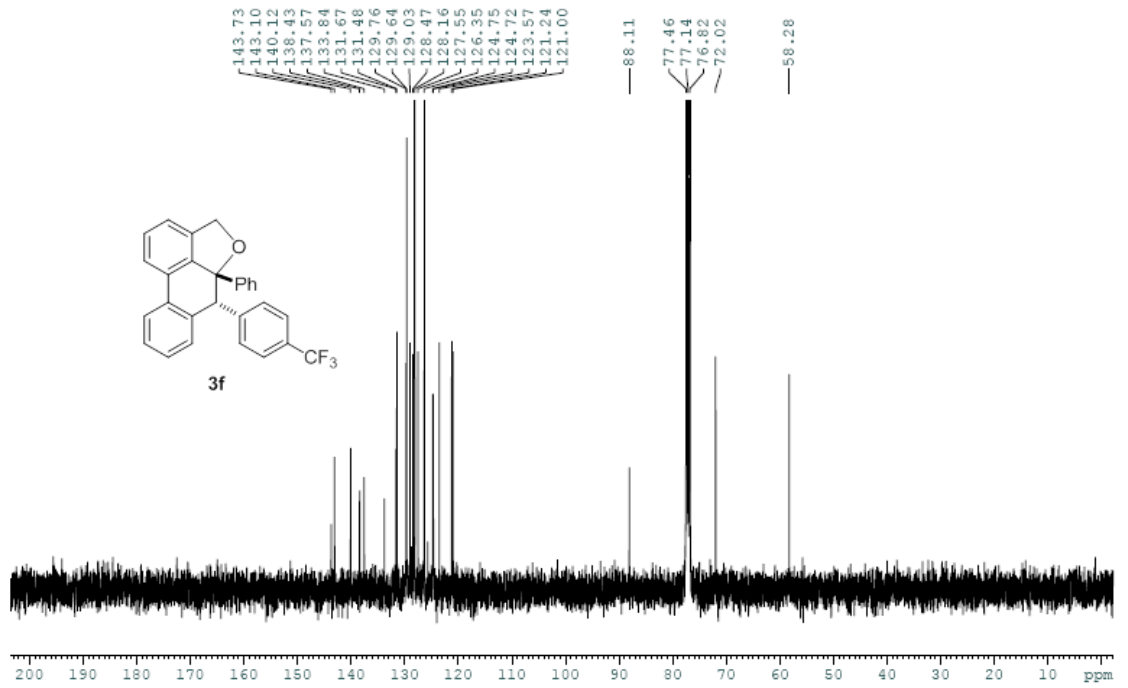
^{13}C NMR of 6-(4-chlorophenyl)-5a-phenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3e)**



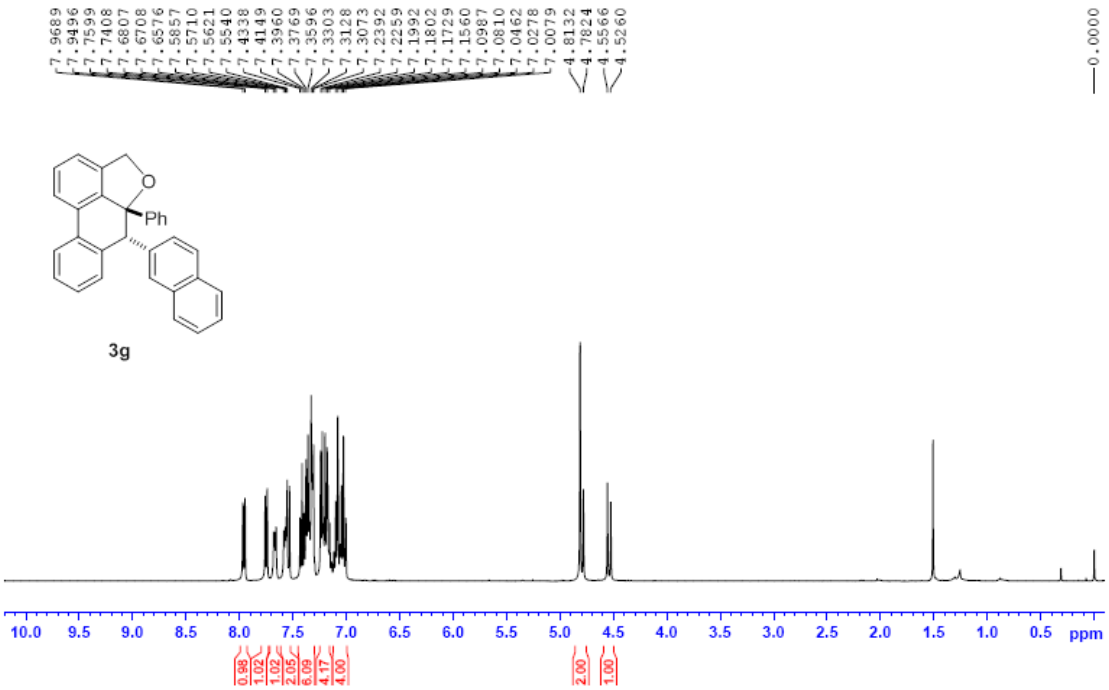
^{1}H NMR of 5a-phenyl-6-(4-(trifluoromethyl)phenyl)-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3f)**



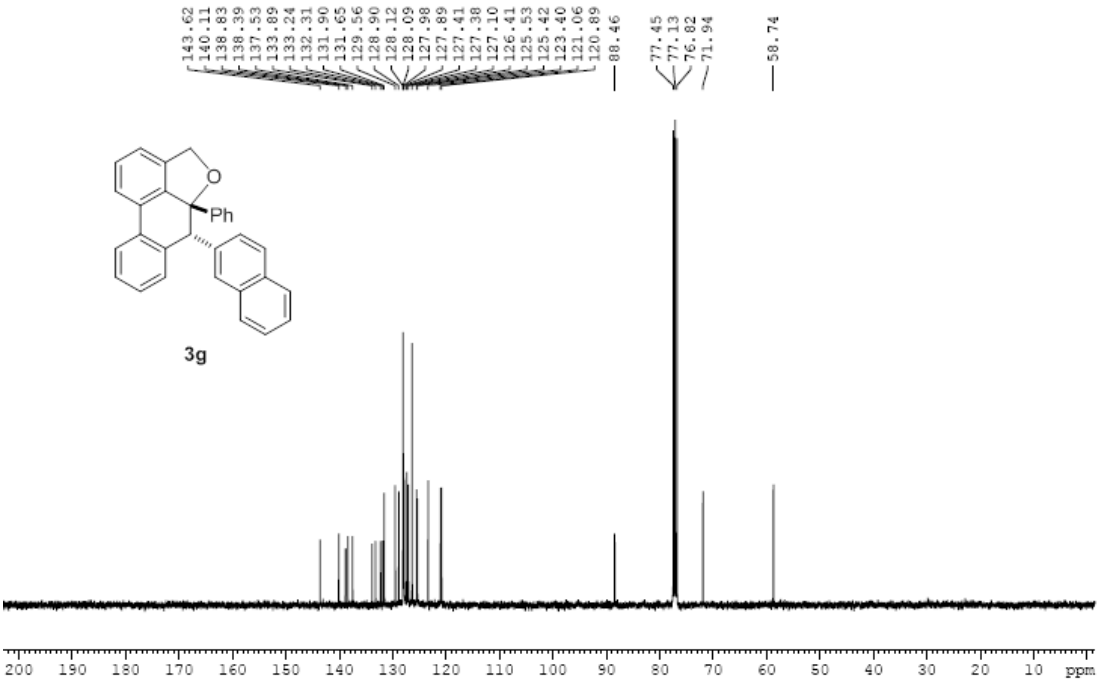
^{13}C NMR of 5a-phenyl-6-(4-(trifluoromethyl)phenyl)-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3f)**



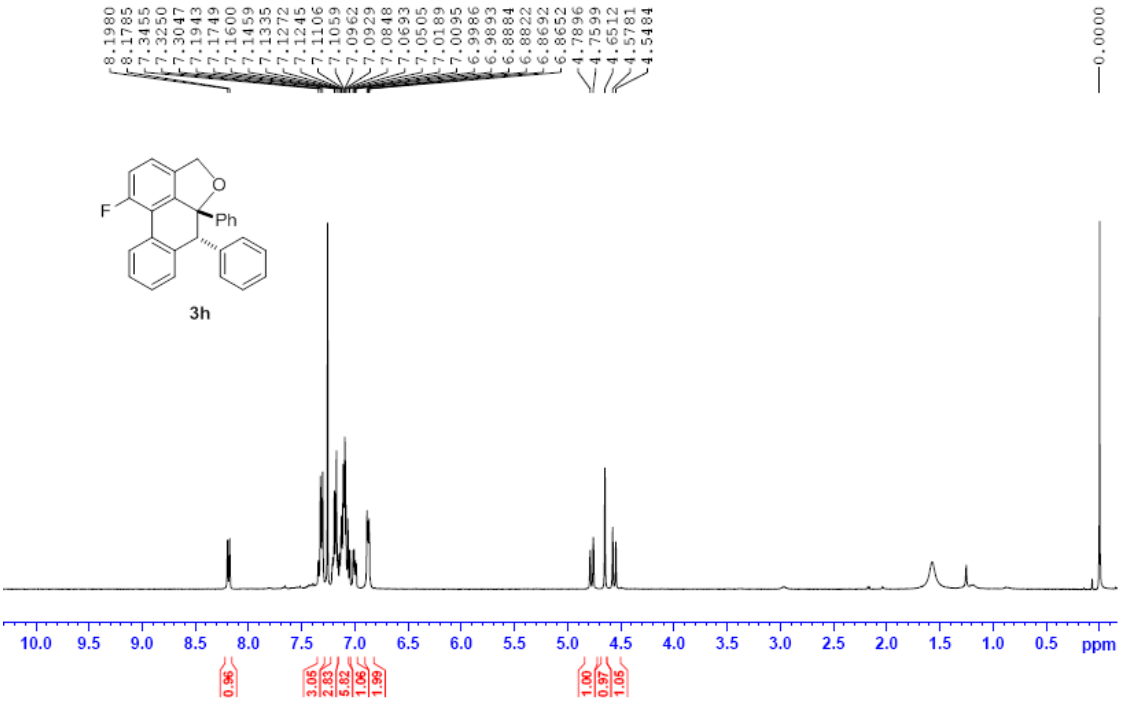
^{1}H NMR of 6-(naphthalen-2-yl)-5a-phenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3g)**



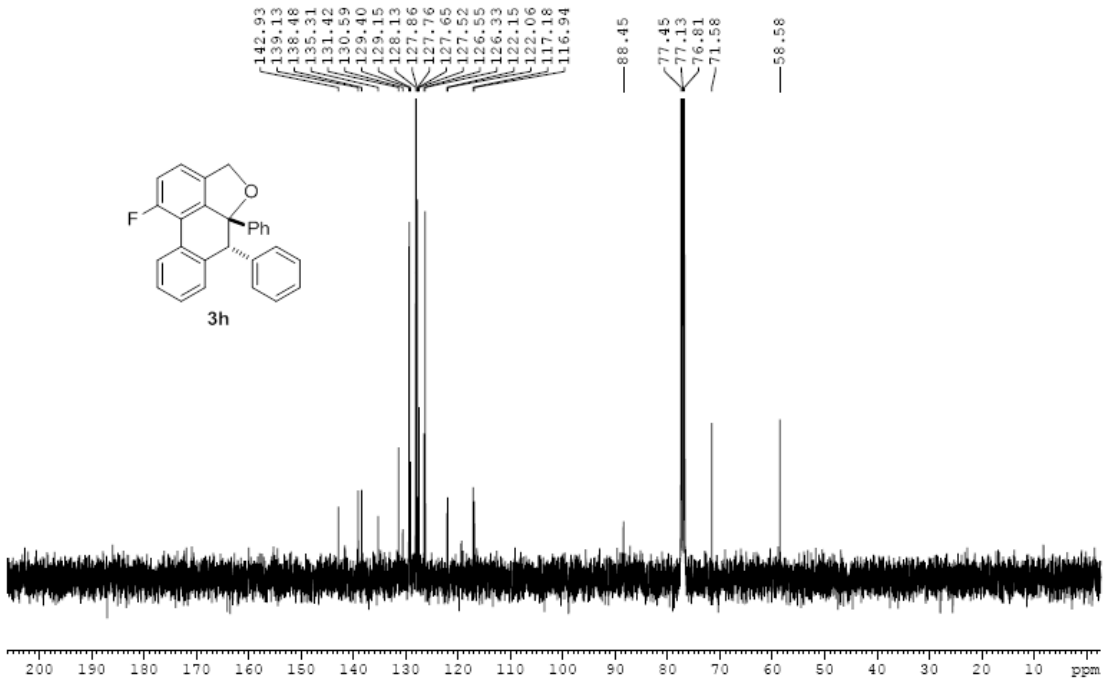
^{13}C NMR of 6-(naphthalen-2-yl)-5a-phenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3g)**



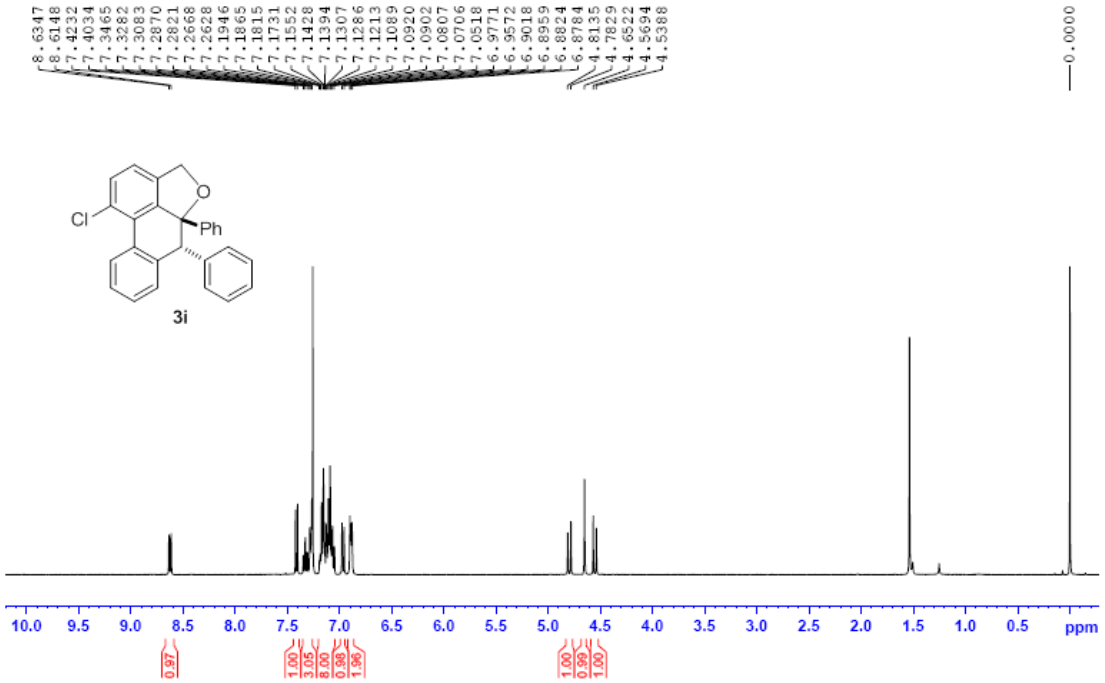
^{1}H NMR of 1-fluoro-5a,6-diphenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3h)**



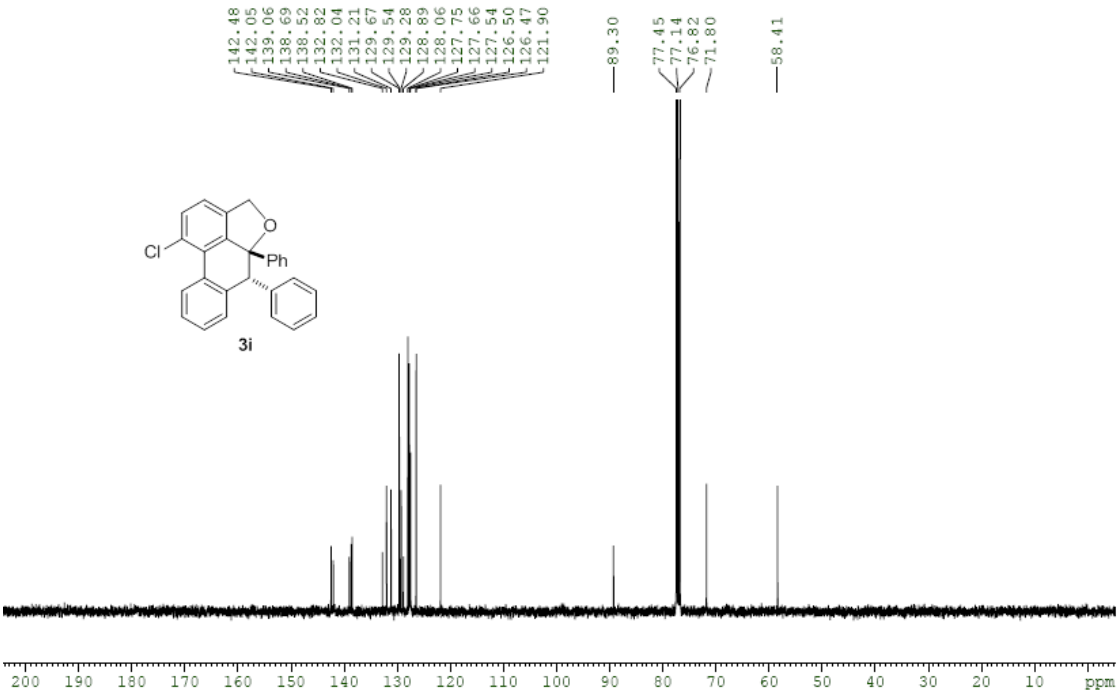
^{13}C NMR of 1-fluoro-5a,6-diphenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3h)**



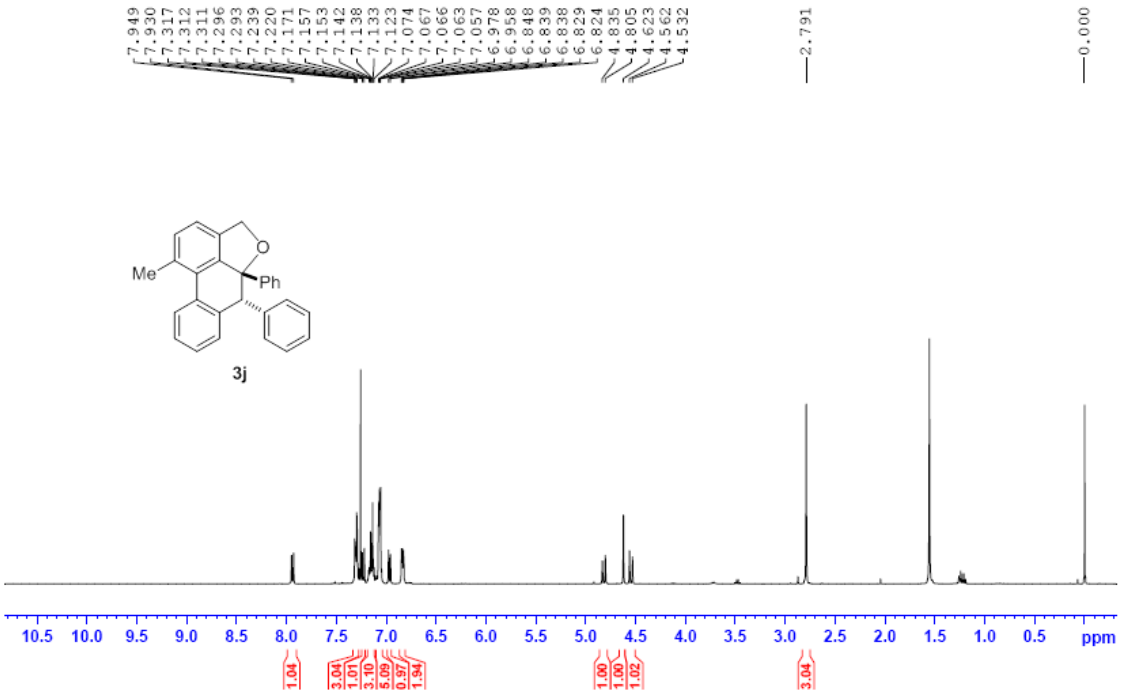
^{1}H NMR of 1-chloro-5a,6-diphenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3i)**



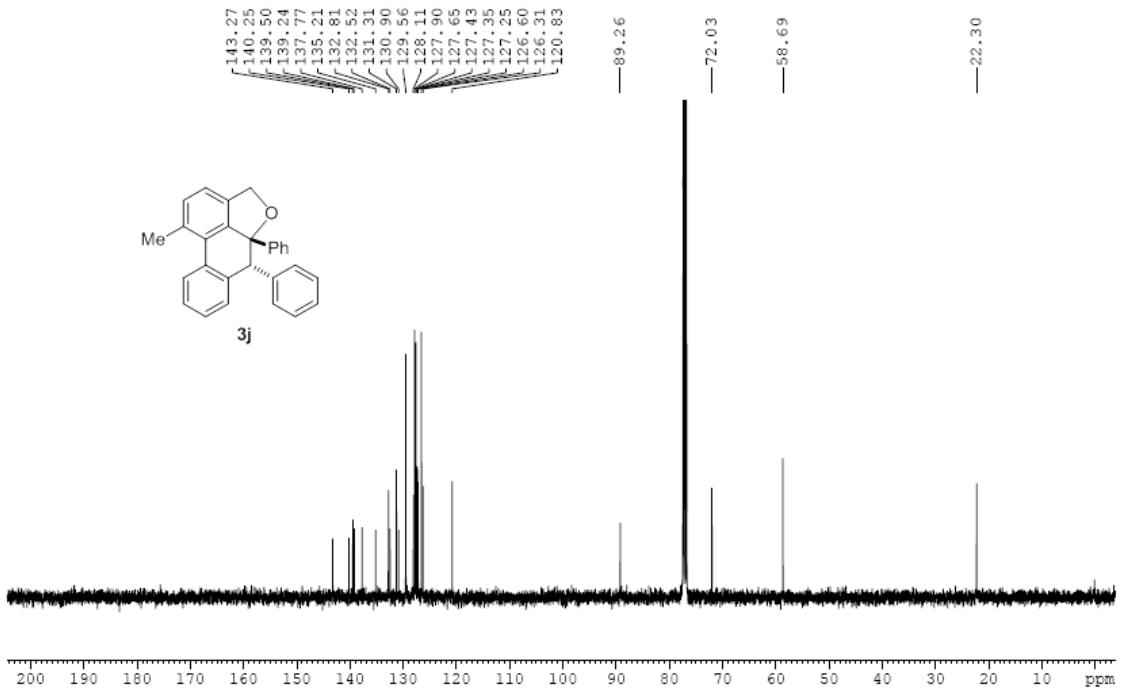
^{13}C NMR of 1-chloro-5a,6-diphenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3i)**



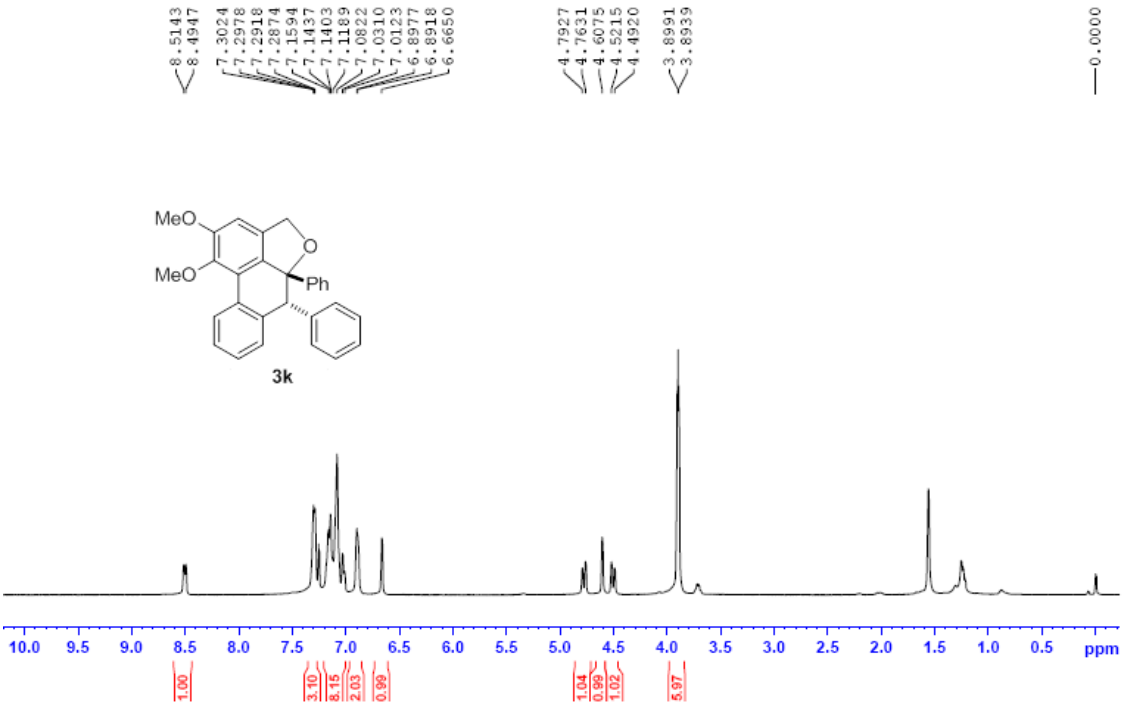
^{1}H NMR of 1-methyl-5a,6-diphenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3j)**



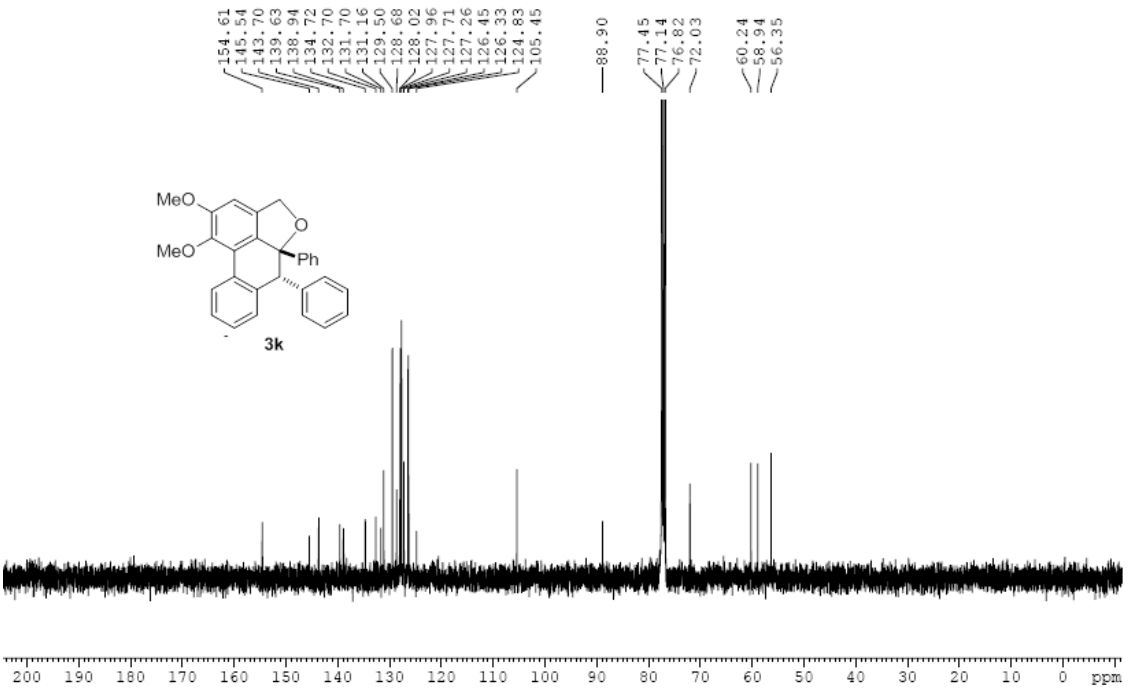
^{13}C NMR of 1-methyl-5a,6-diphenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3j)**



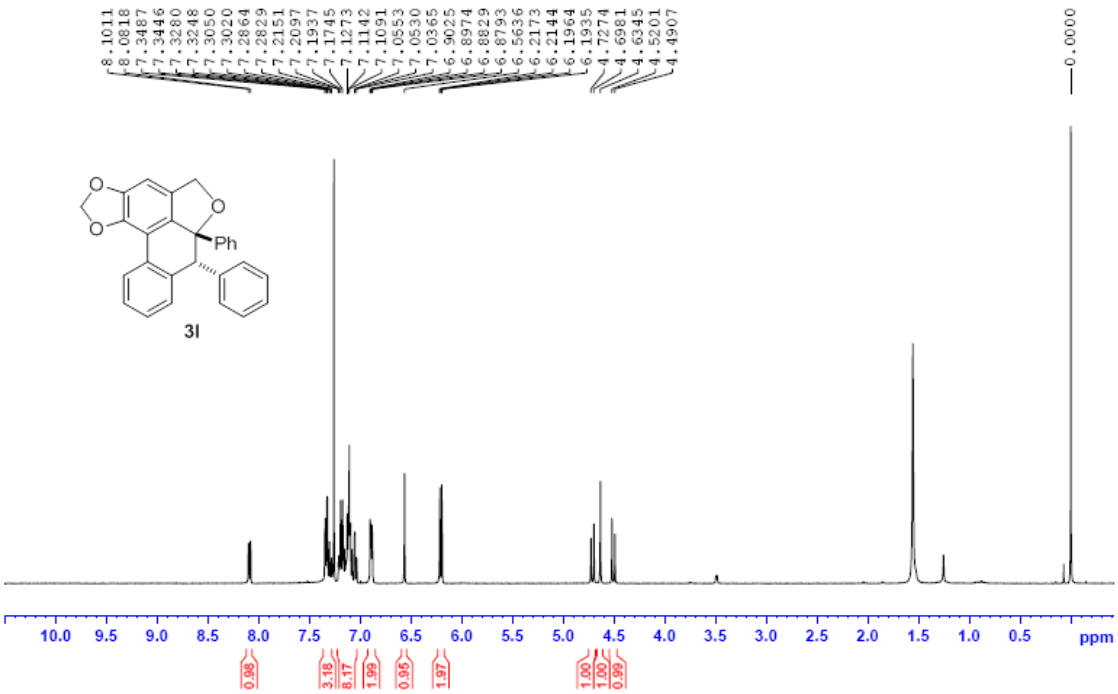
^{1}H NMR of 1,2-dimethoxy-5a,6-diphenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3k)**



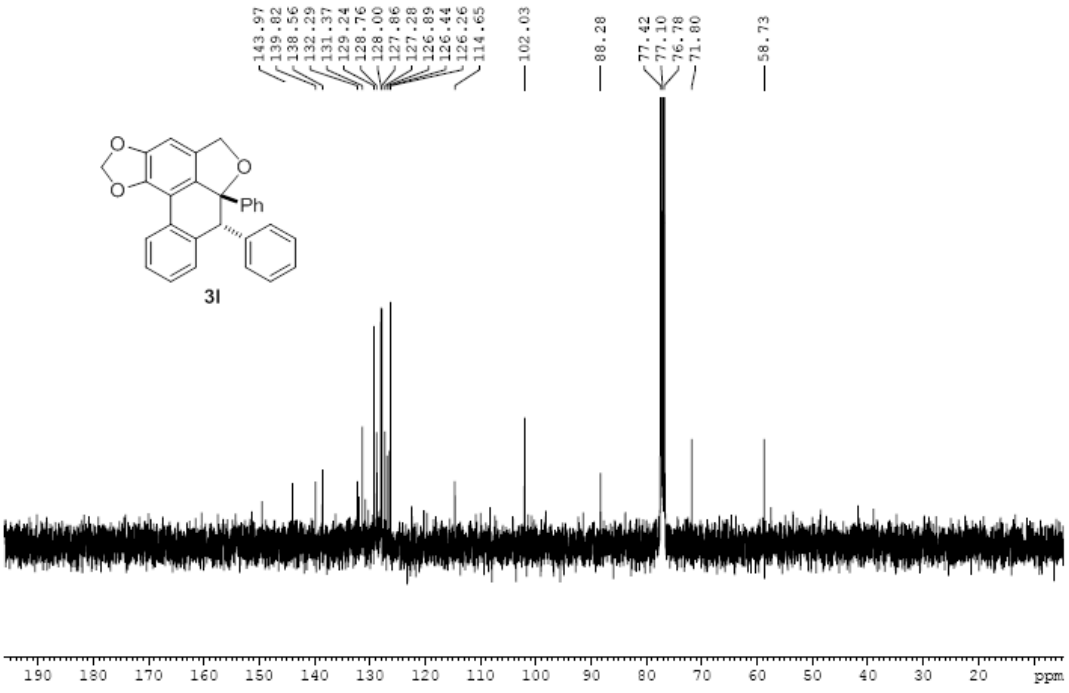
^{13}C NMR of 1,2-dimethoxy-5a,6-diphenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3k)**



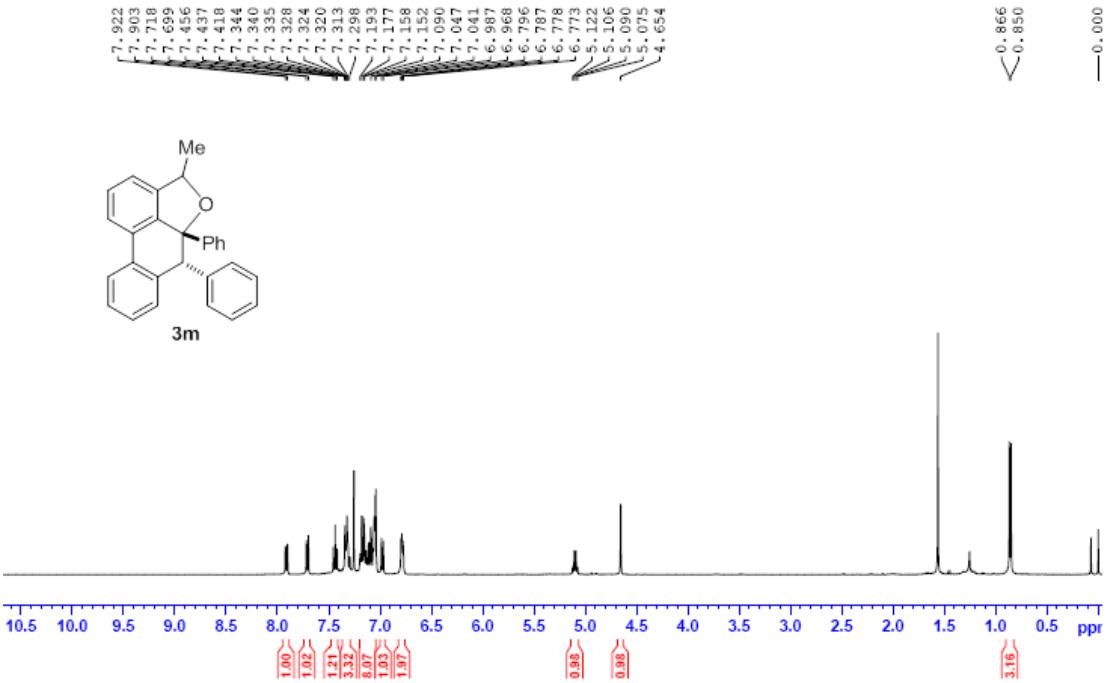
^{1}H NMR of 6a,7-diphenyl-6a,7-dihydro-5*H*-furo[2',3',4':10,1]phenanthro[3,4-*d*][1,3]dioxole **(3l)**



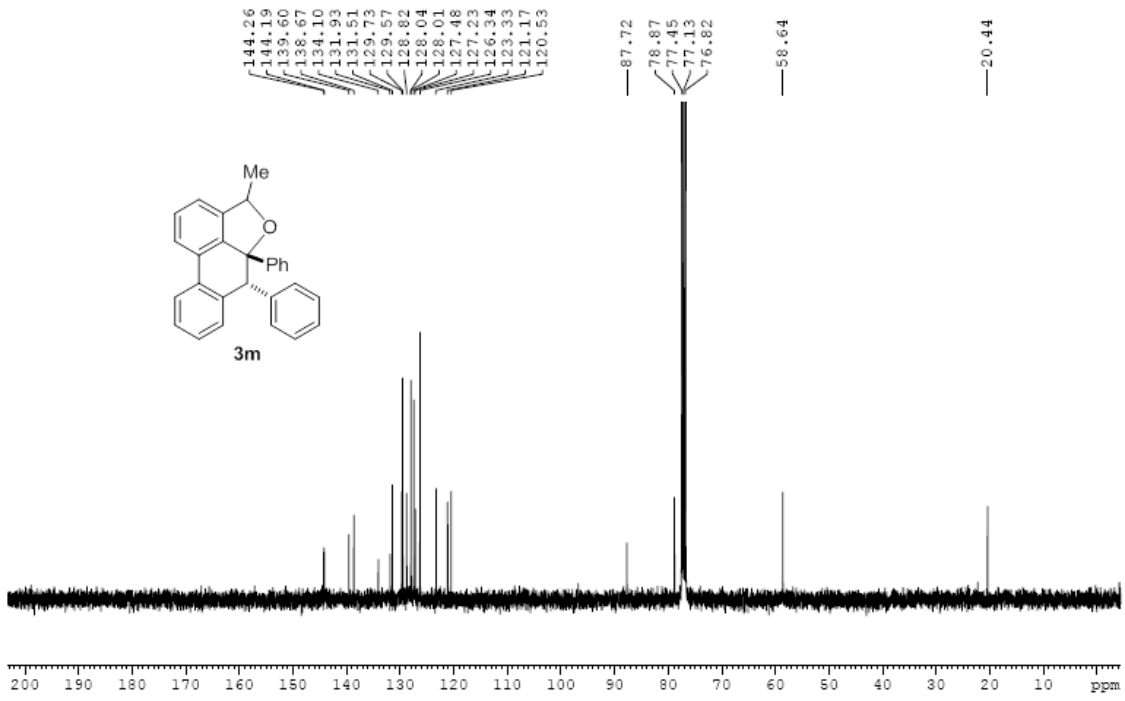
^{13}C NMR of 6a,7-diphenyl-6a,7-dihydro-5*H*-furo[2',3',4':10,1]phenanthro[3,4-*d*][1,3]dioxole **(3l)**



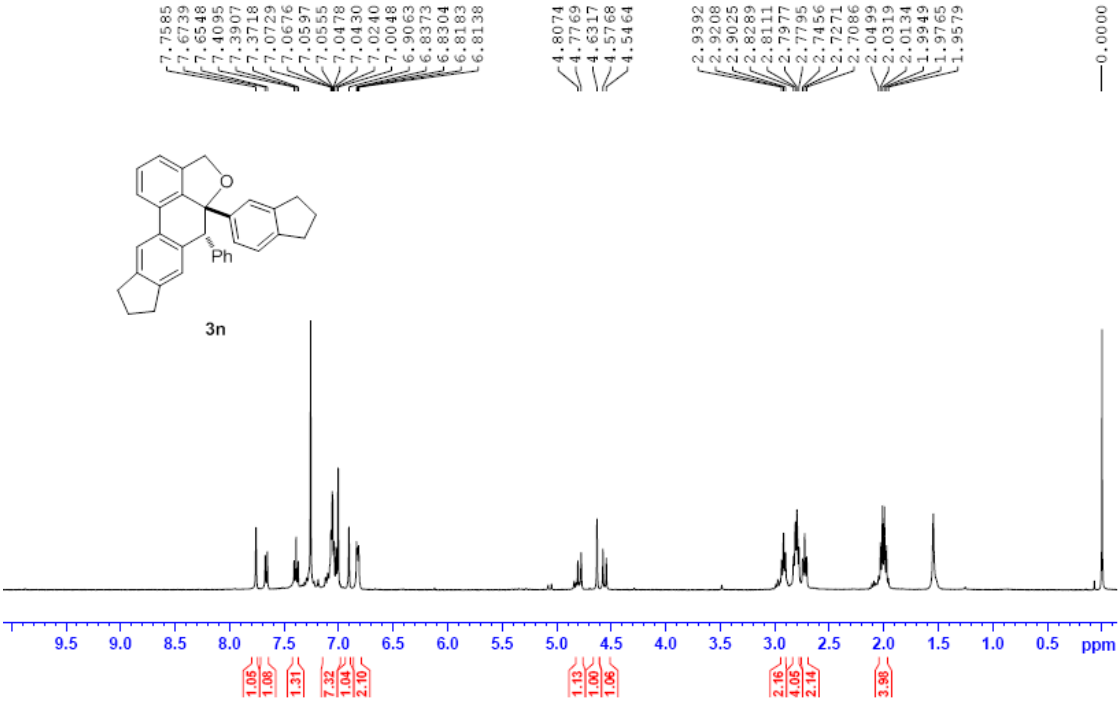
^{1}H NMR of 4-methyl-5a,6-diphenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3m)**



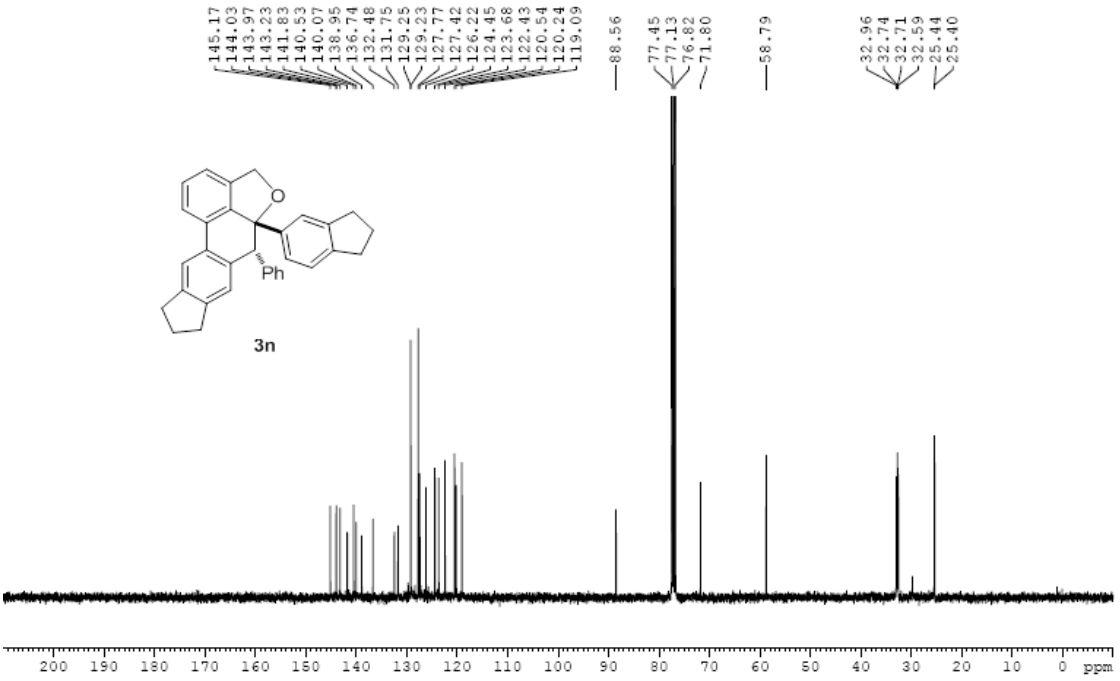
^{13}C NMR of 4-methyl-5a,6-diphenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3m)**



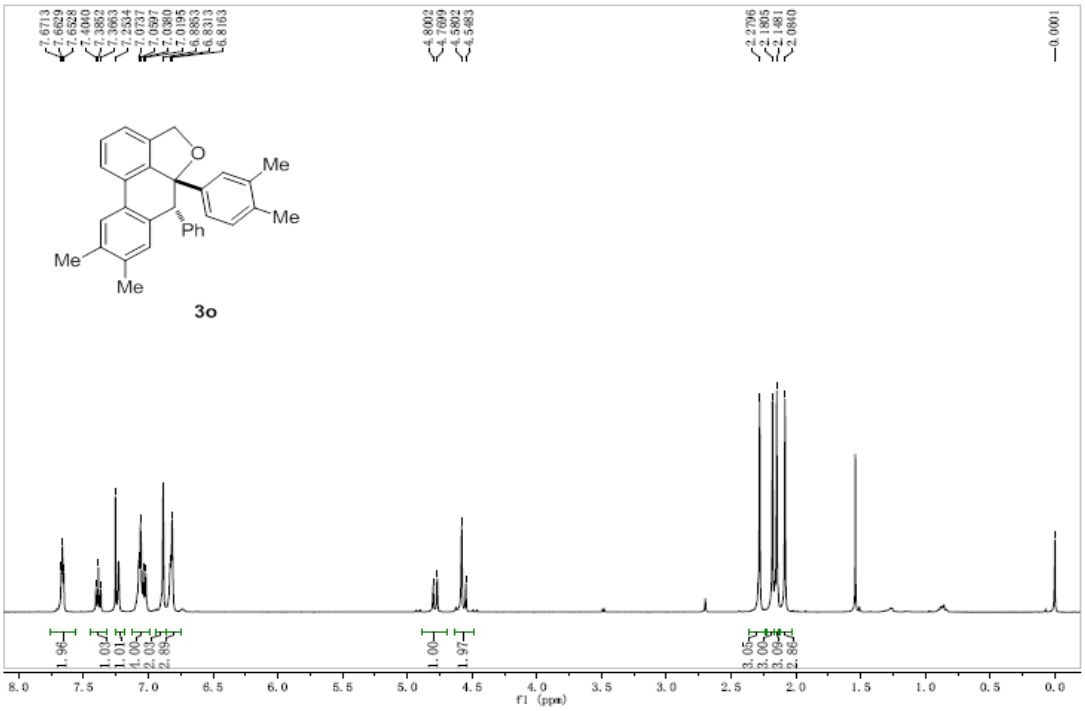
^{1}H NMR of 5a-(2,3-dihydro-1*H*-inden-5-yl)-6-phenyl-4,5a,6,8,9,10-hexahydrocyclopenta[6,7]phenanthro[10,1-*bc*]furan **(3n)**



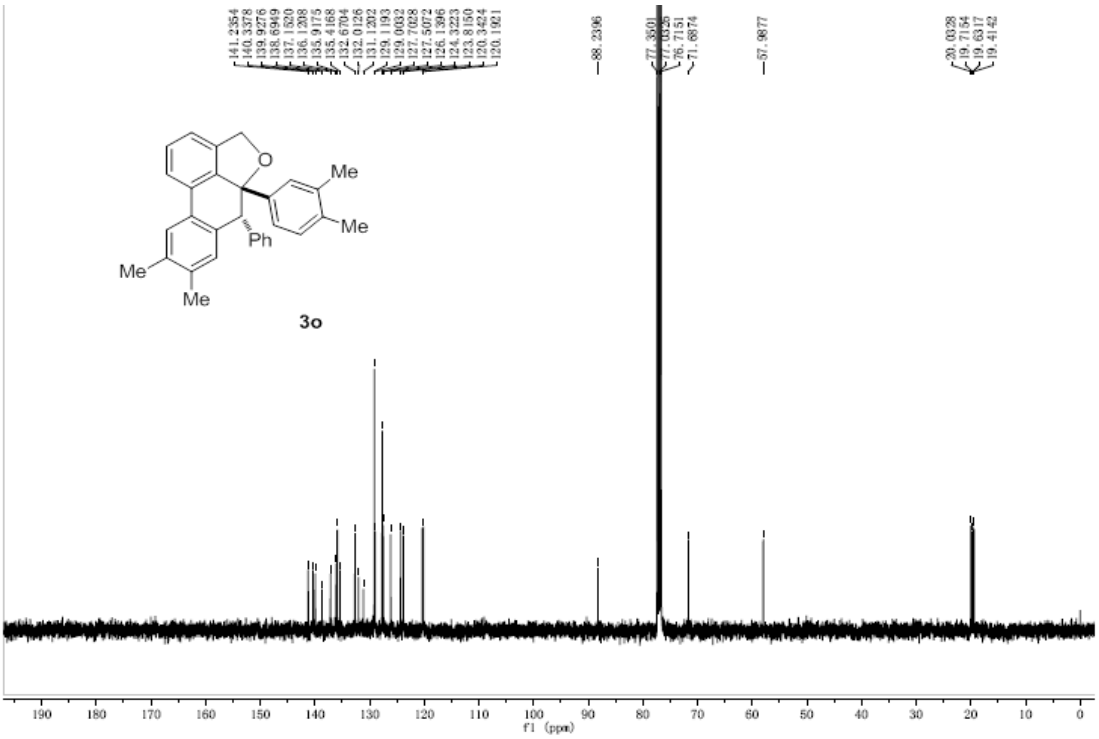
^{13}C NMR of 5a-(2,3-dihydro-1*H*-inden-5-yl)-6-phenyl-4,5a,6,8,9,10-hexahydrocyclopenta[6,7]phenanthro[10,1-*bc*]furan **(3n)**



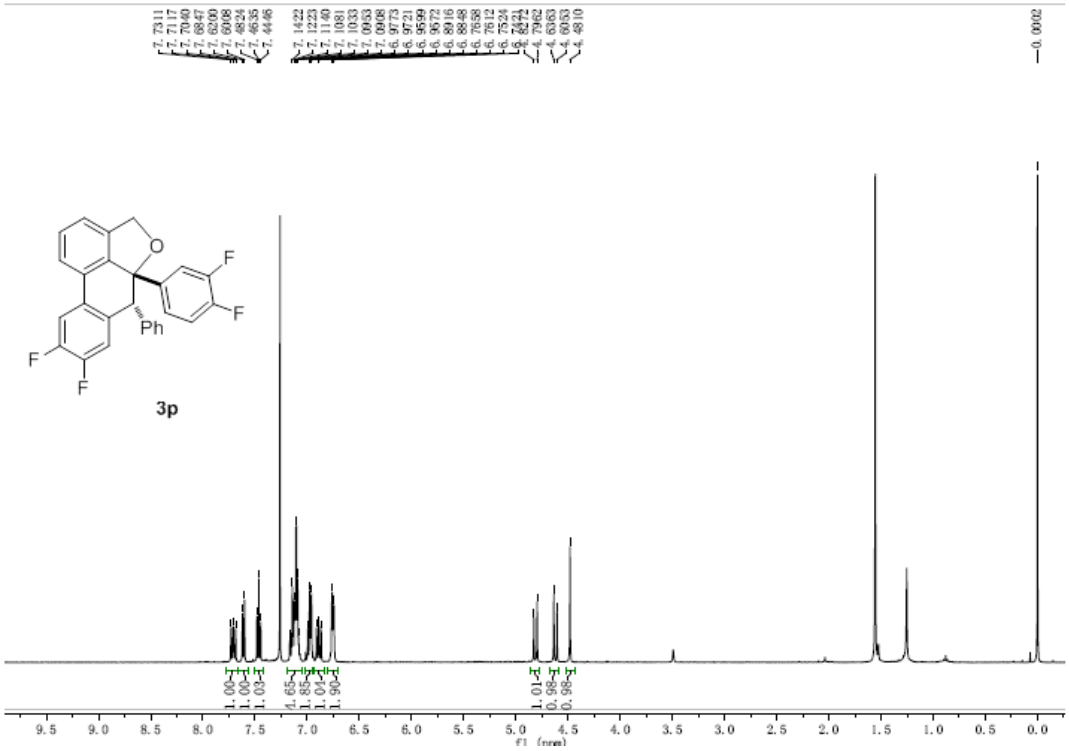
^{1}H NMR of 5a-(3,4-dimethylphenyl)-8,9-dimethyl-6-phenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3o)**



^{13}C NMR of 5a-(3,4-dimethylphenyl)-8,9-dimethyl-6-phenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3o)**



^{1}H NMR of 5a-(3,4-difluorophenyl)-8,9-difluoro-6-phenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3p)**



^{13}C NMR of 5a-(3,4-difluorophenyl)-8,9-difluoro-6-phenyl-5a,6-dihydro-4*H*-phenanthro[10,1-*bc*]furan **(3p)**

