Arylethynylacridines: Electrochemiluminescence and photophysical properties

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Electronic Supplementary Information

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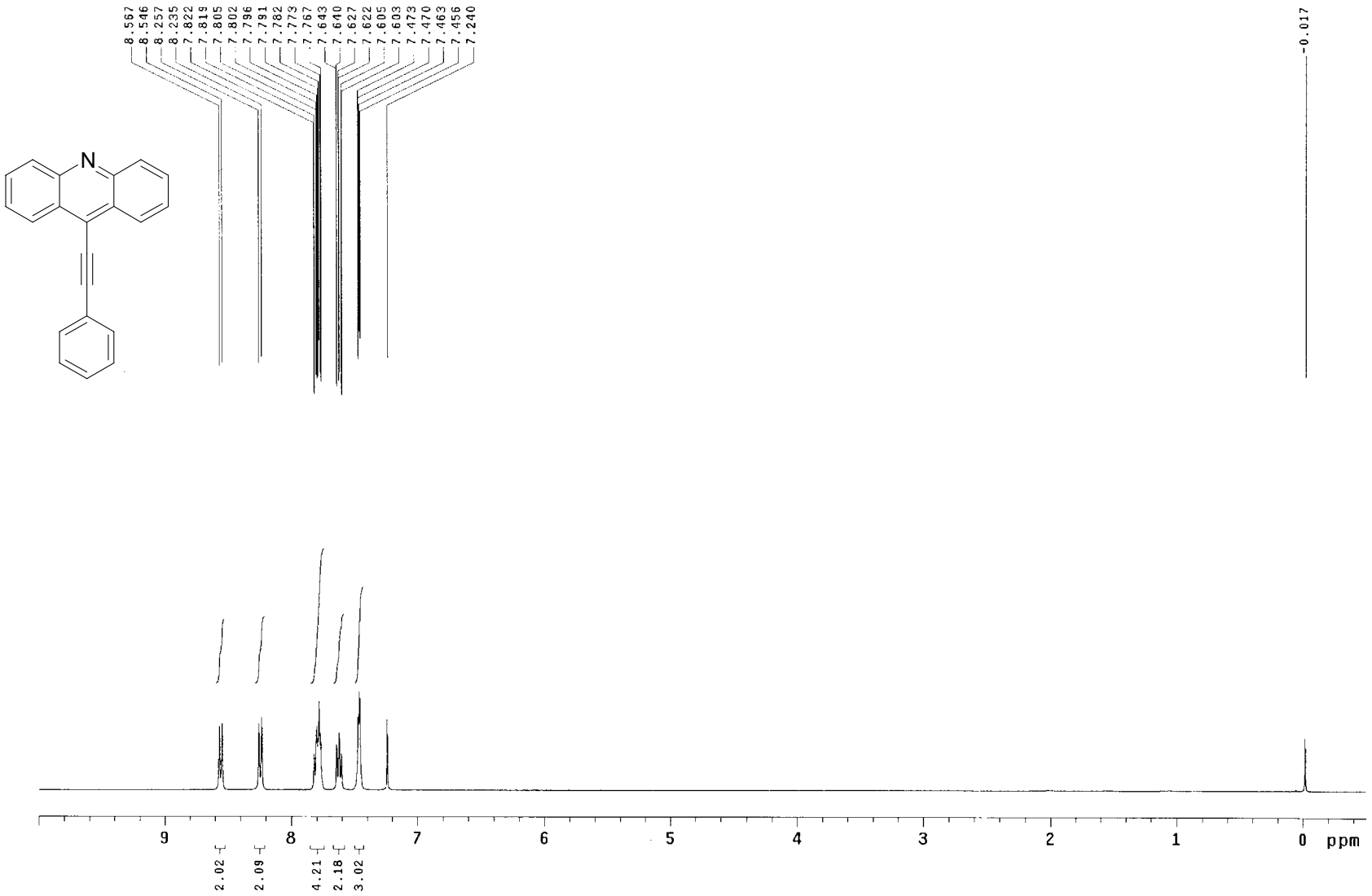
CH040318-phenyl

Pulse Sequence: s2pul



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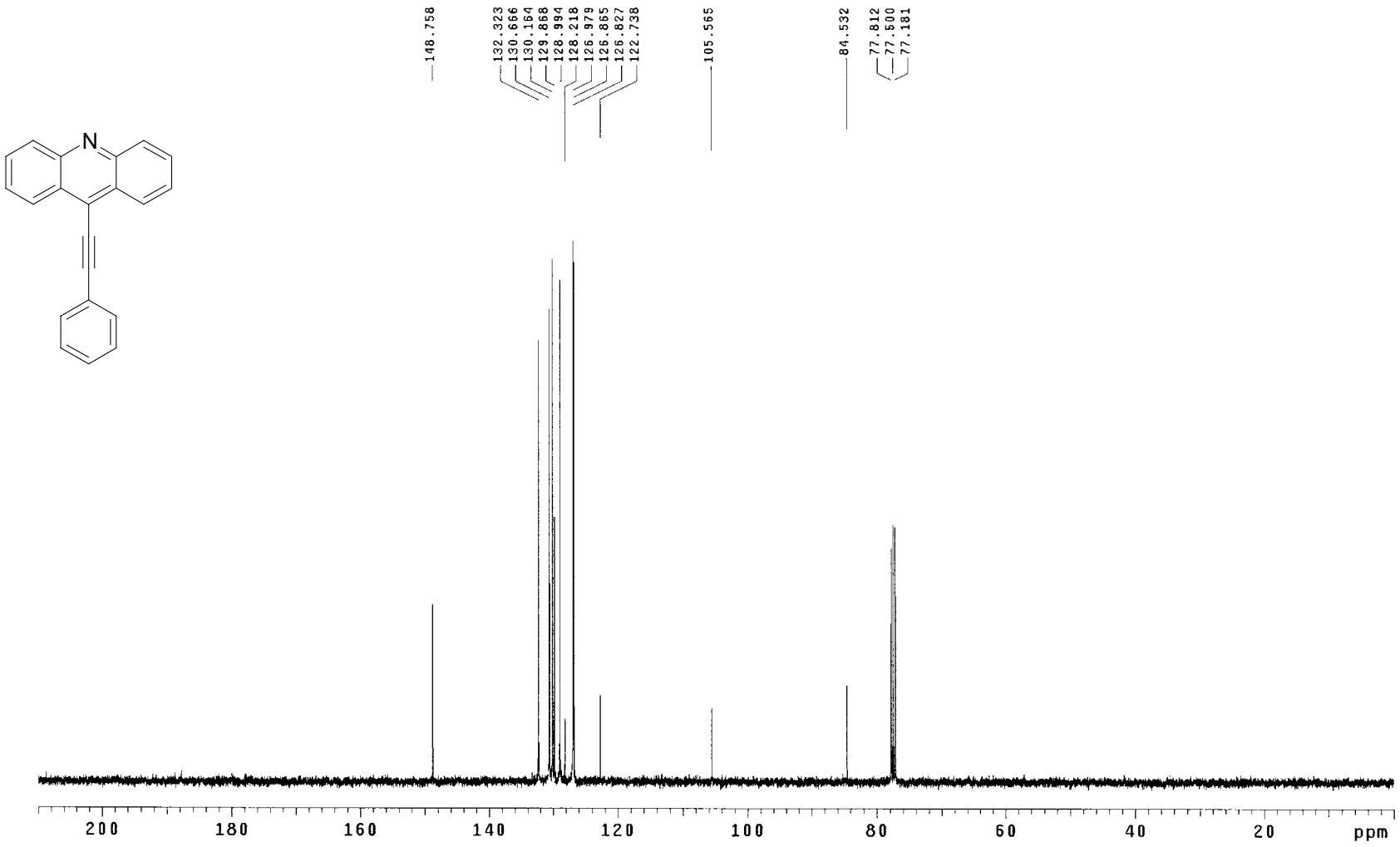

CH040220-Me

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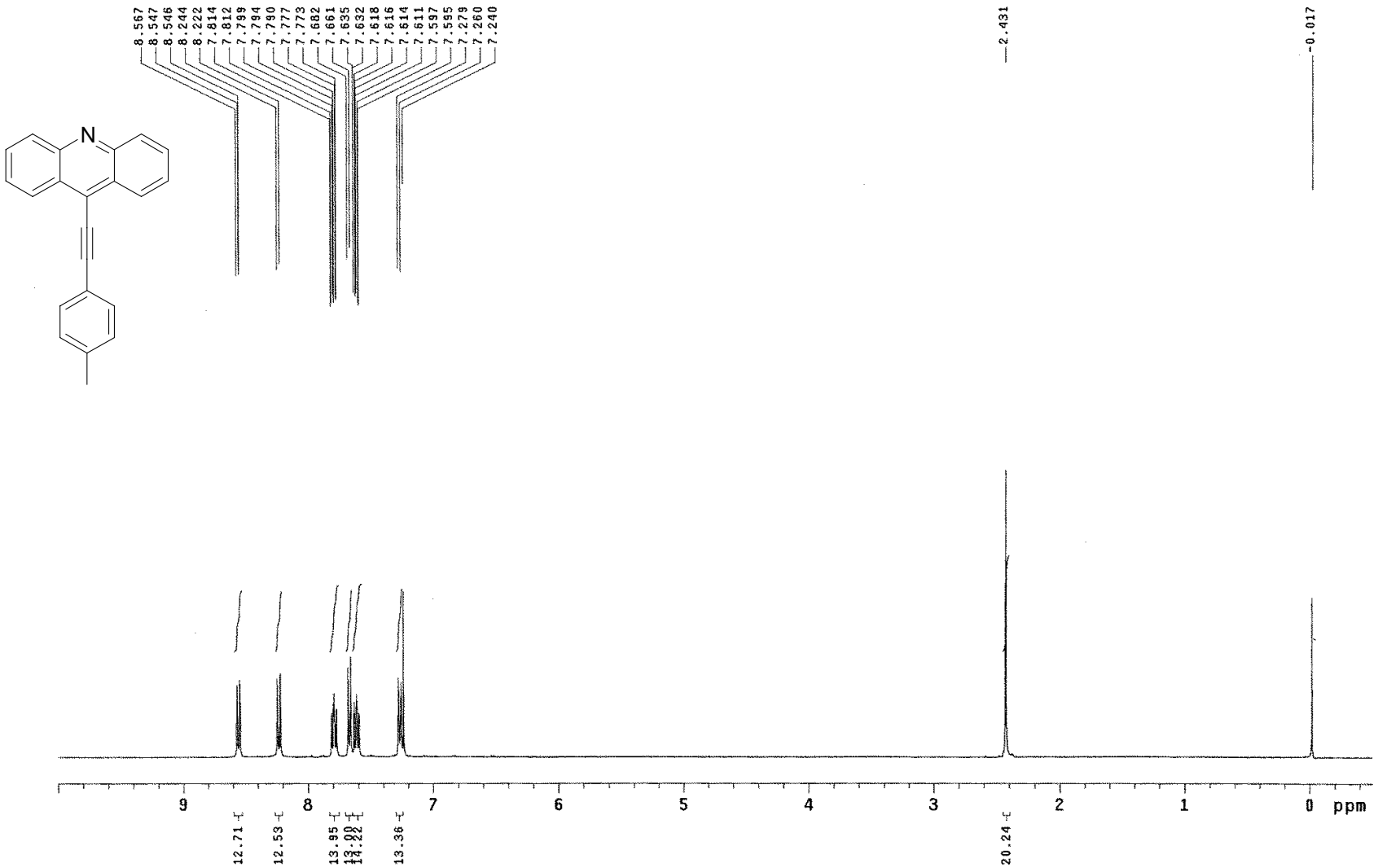

CH040414-acri-Me

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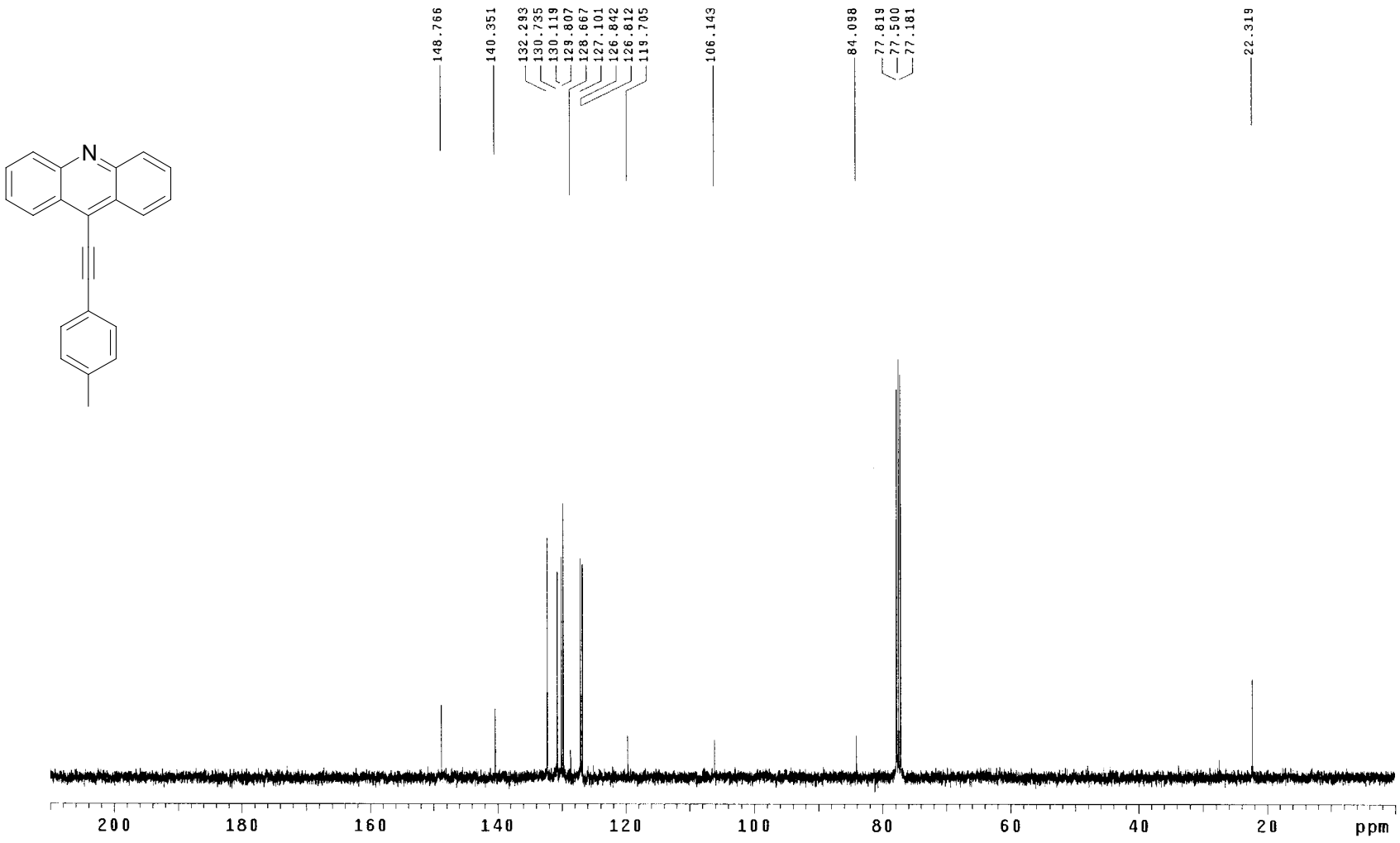

CH040220-OMe

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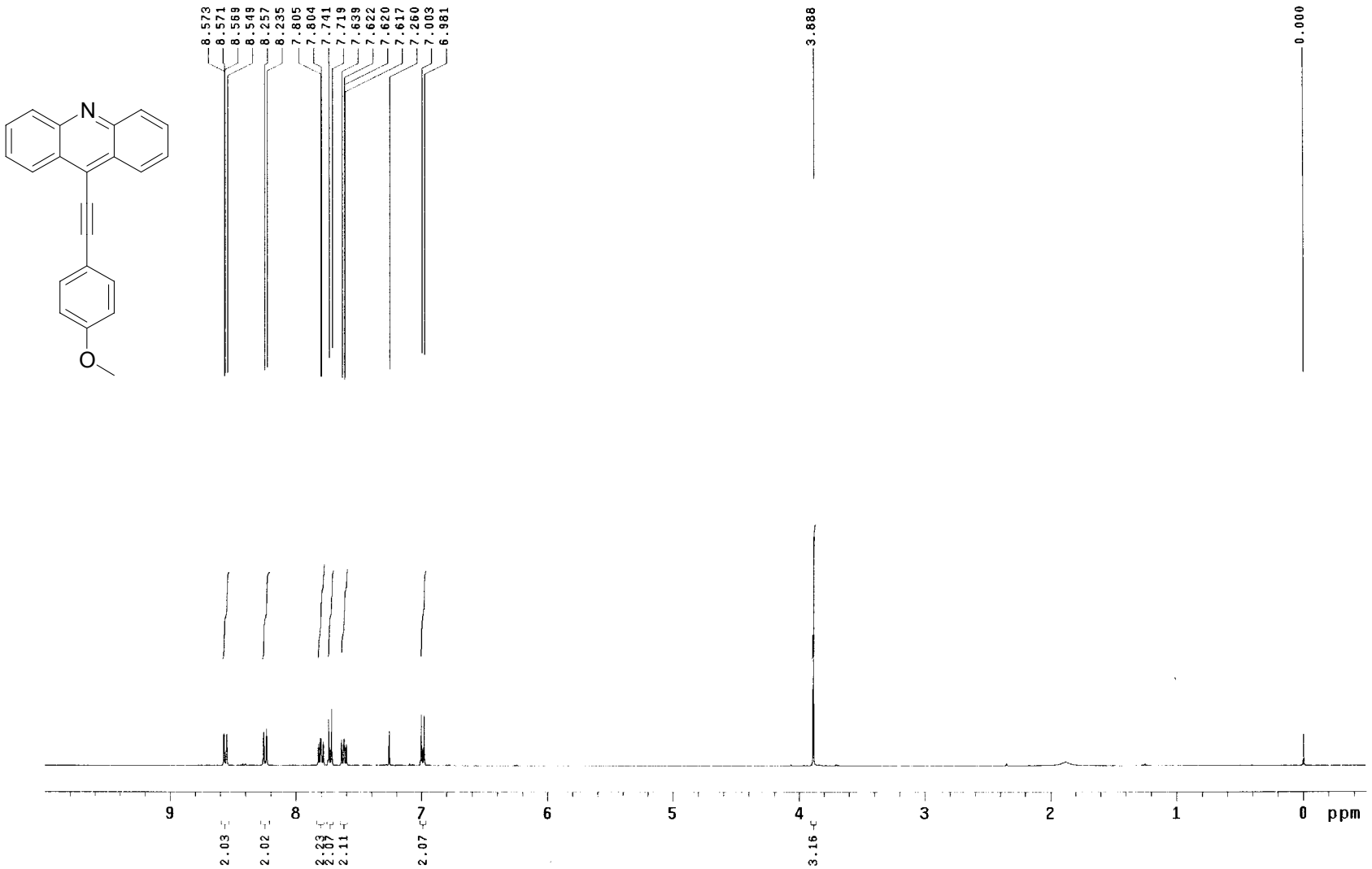

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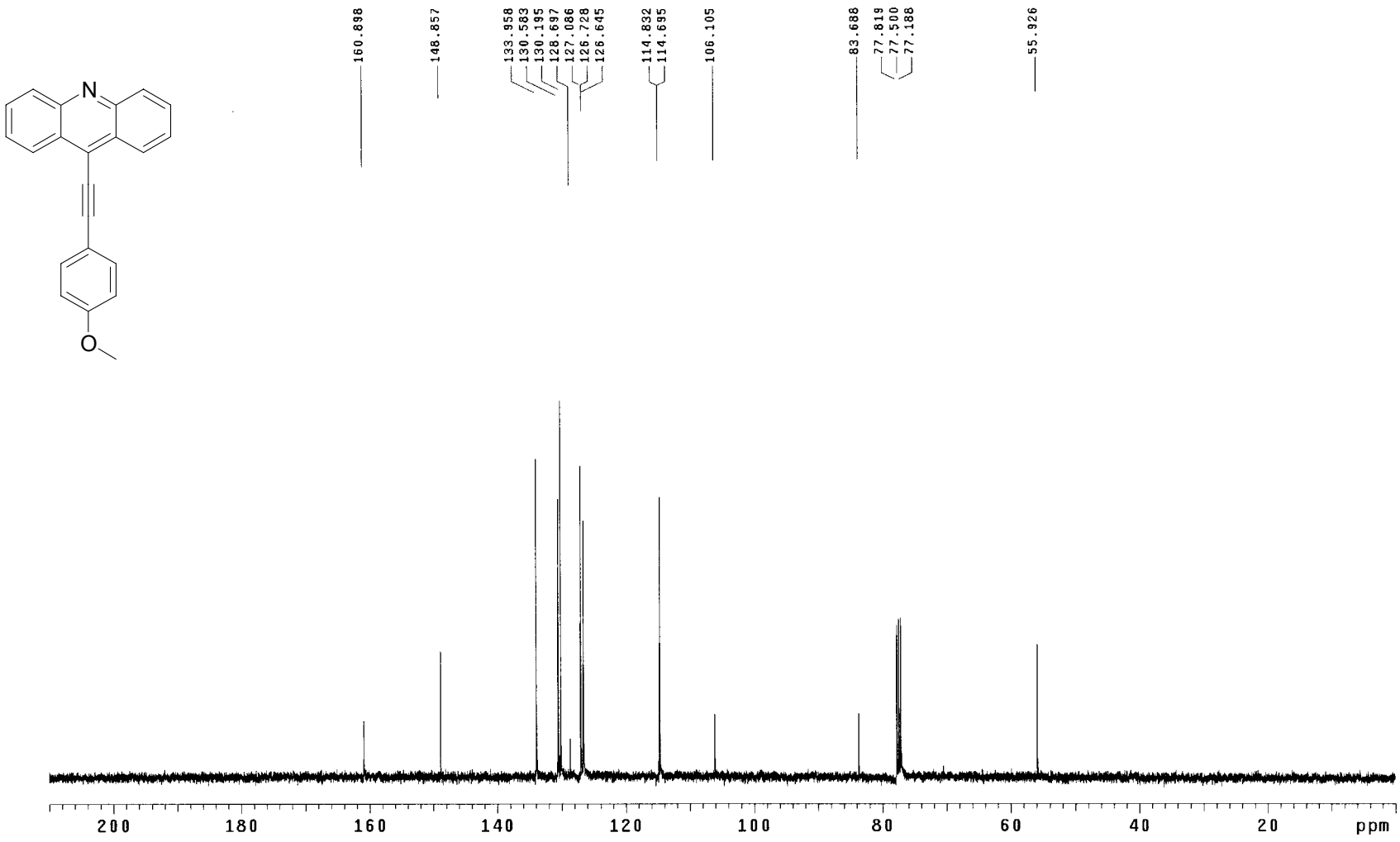

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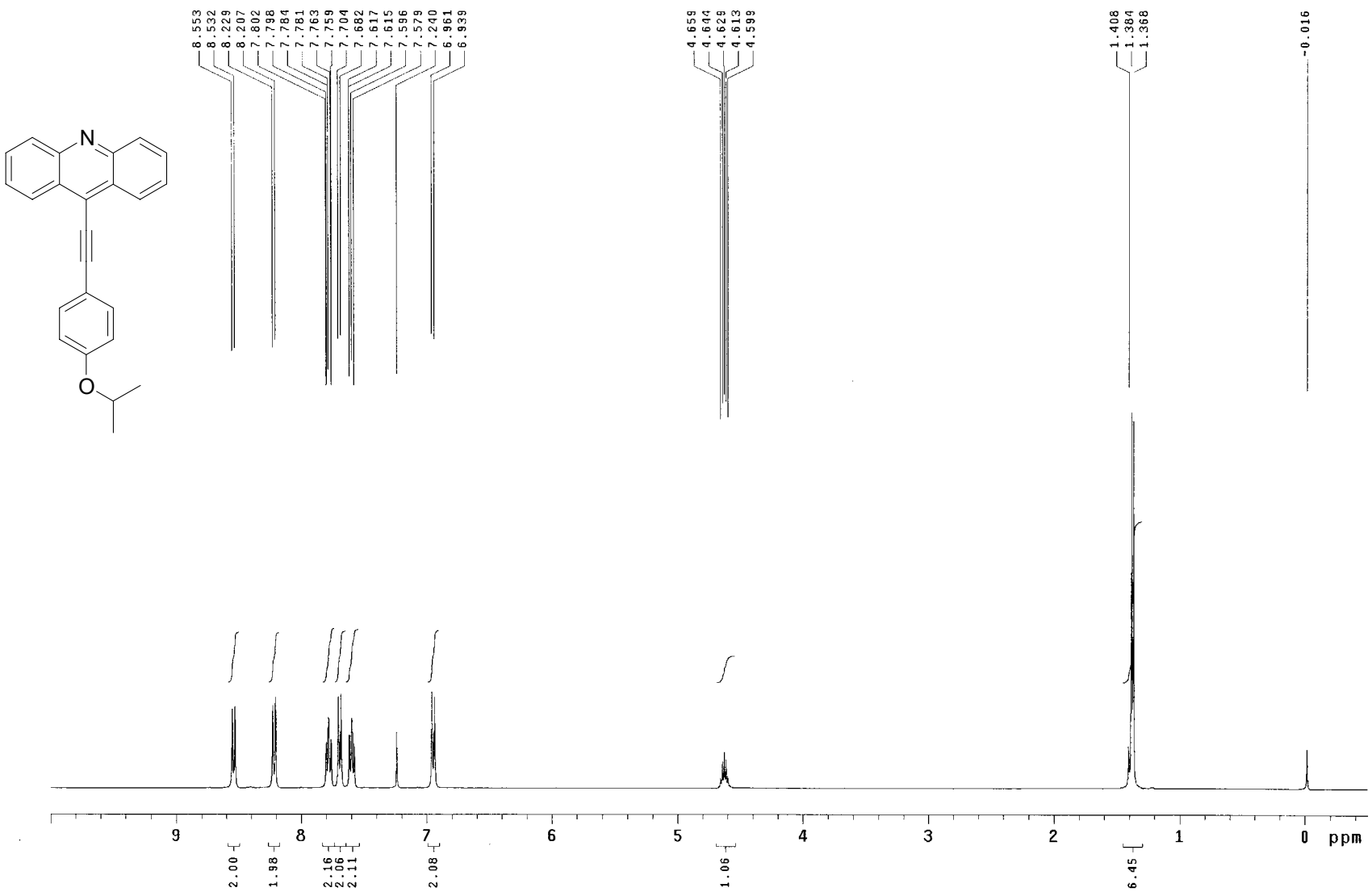
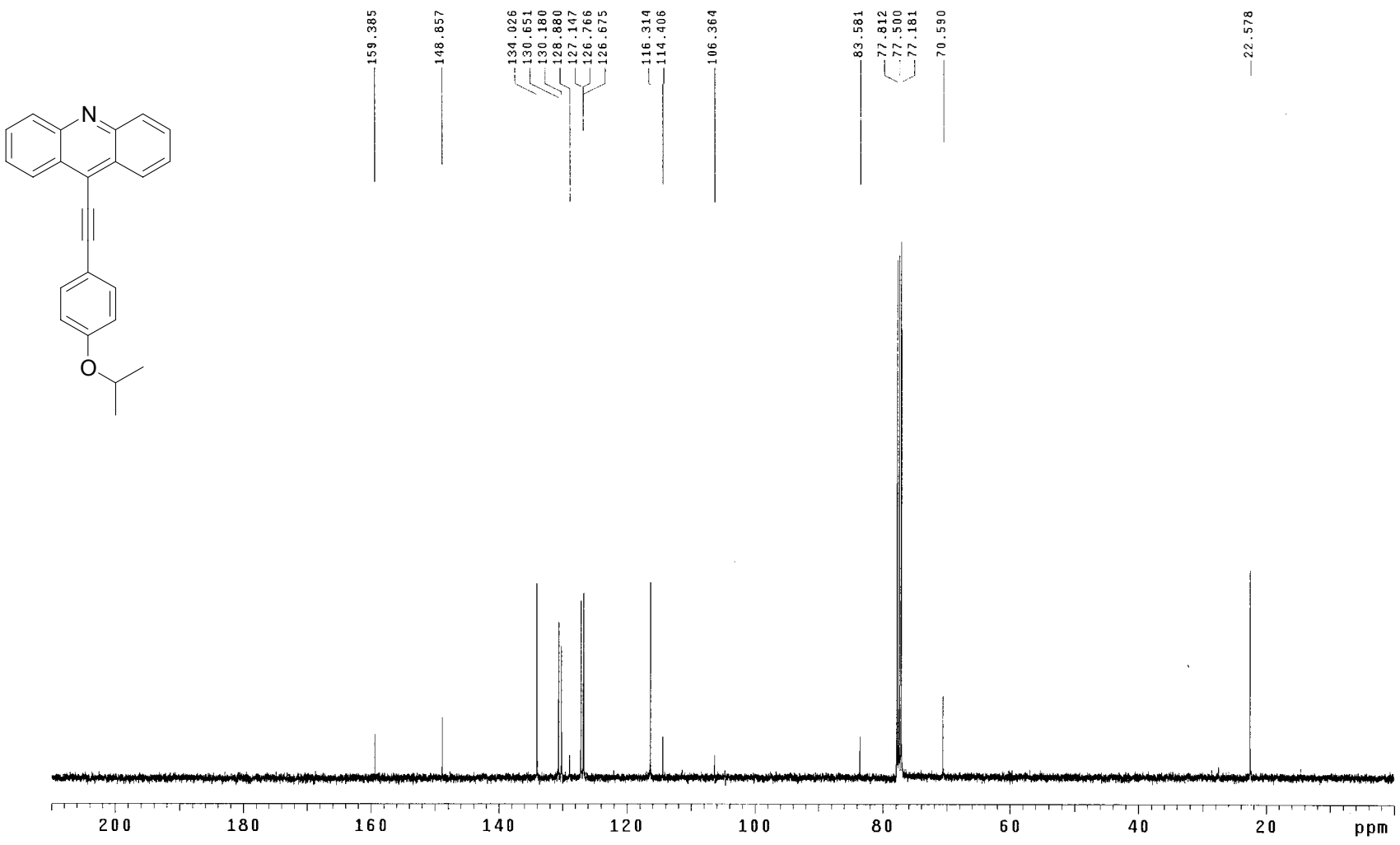


CH040318-isopropyl

Pulse Sequence: s2pul



CH040412-alkyl

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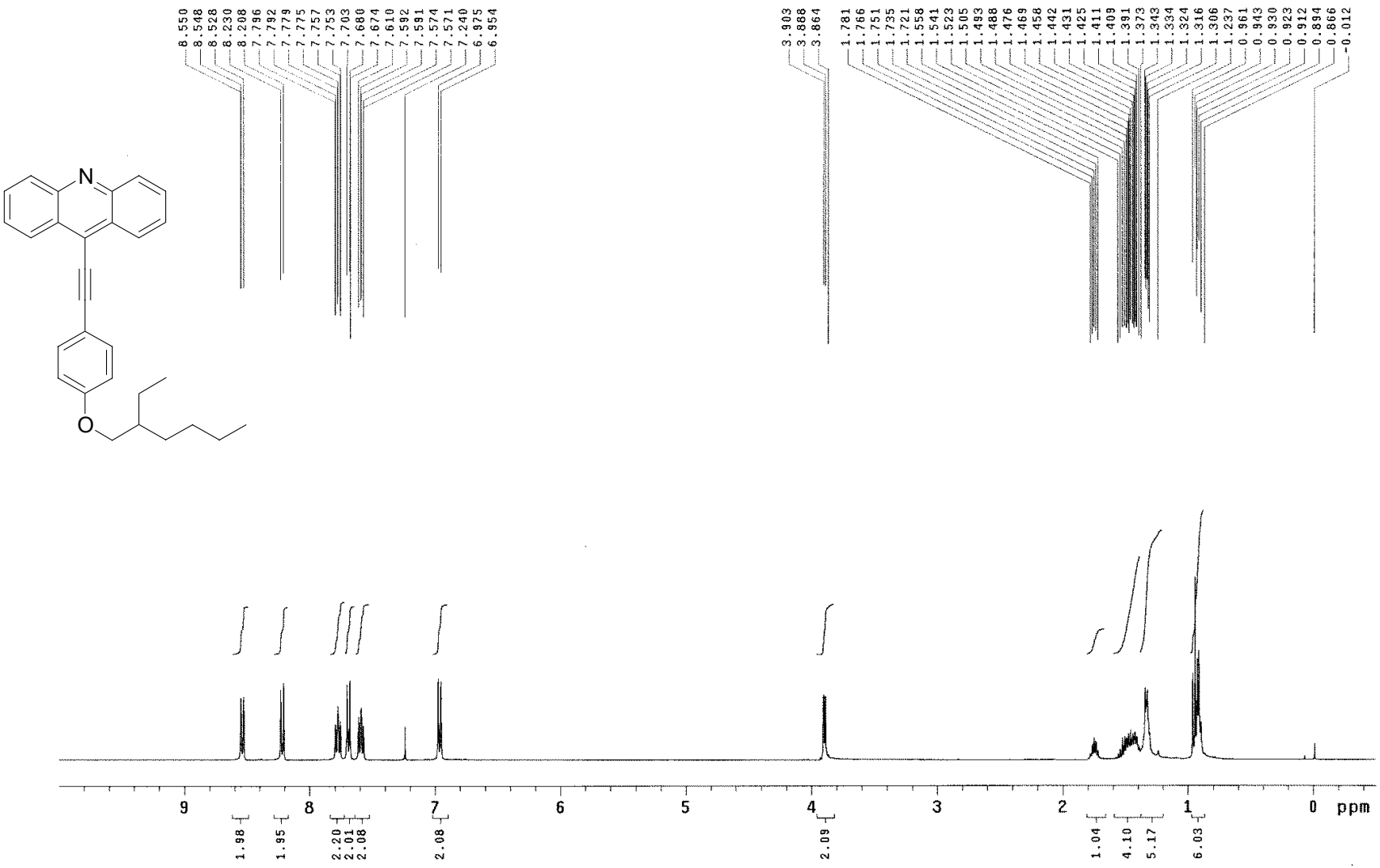
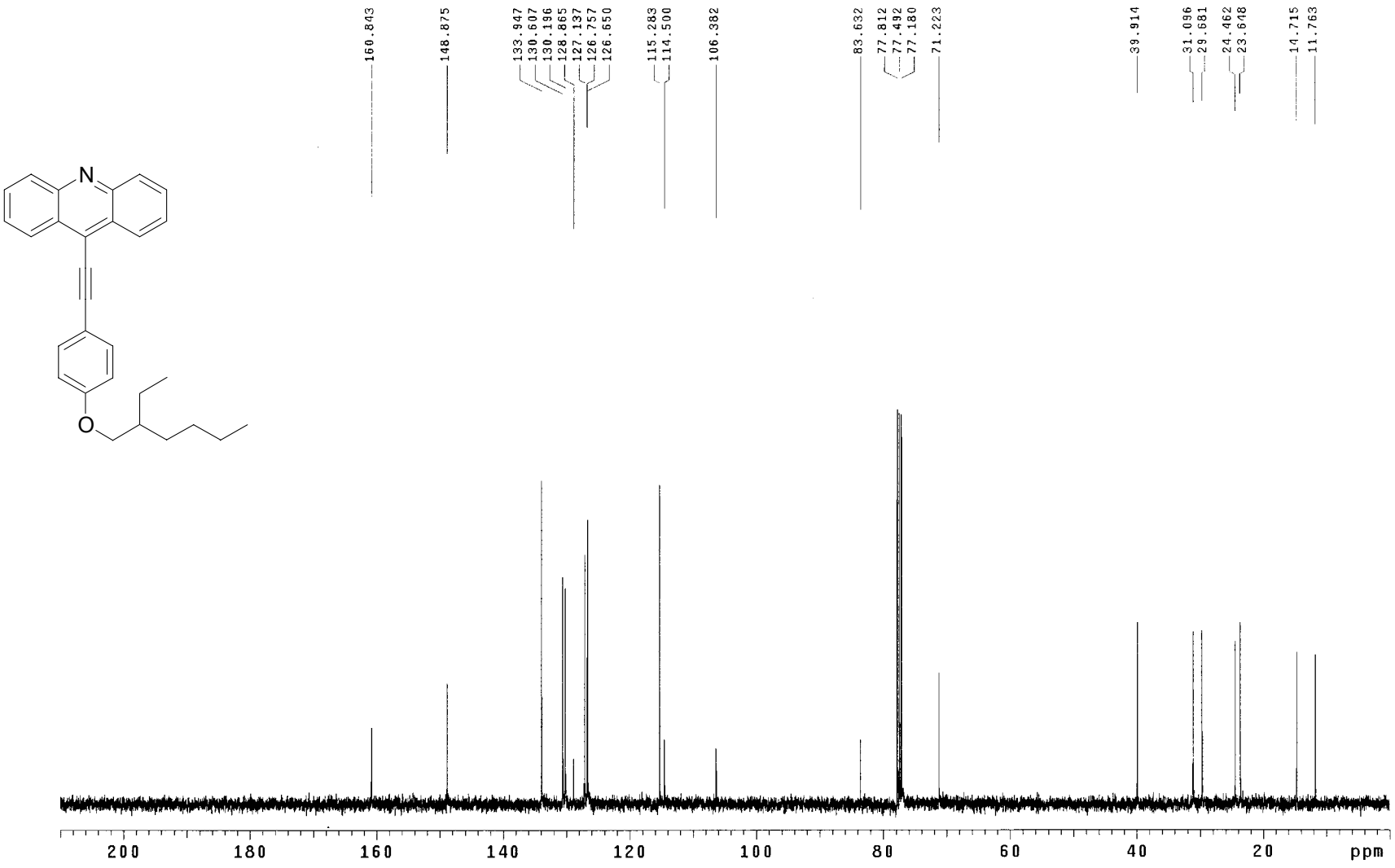


CH040412-alkyl

Pulse Sequence: s2pul



CH040309-cry-NMe2

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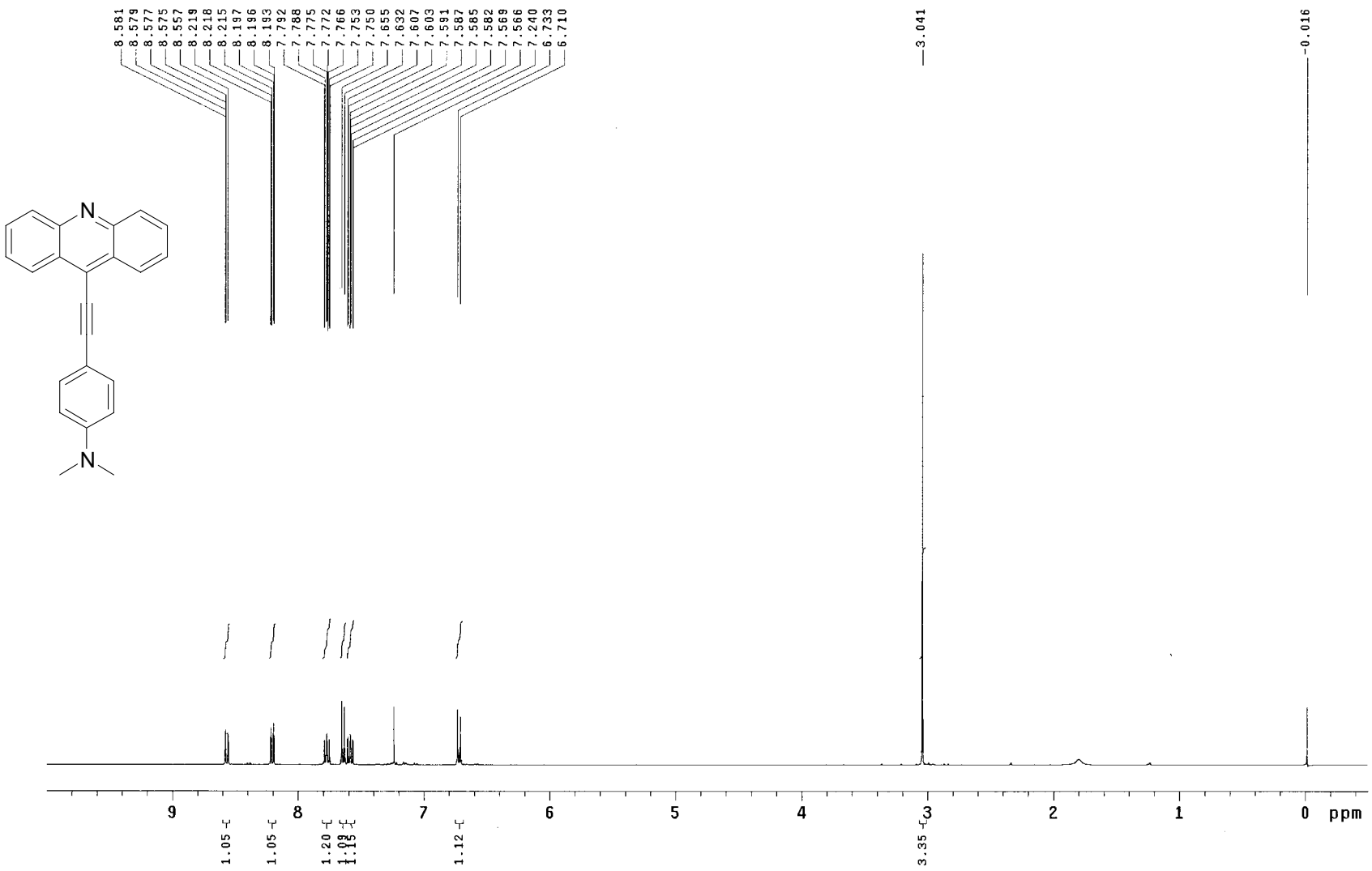
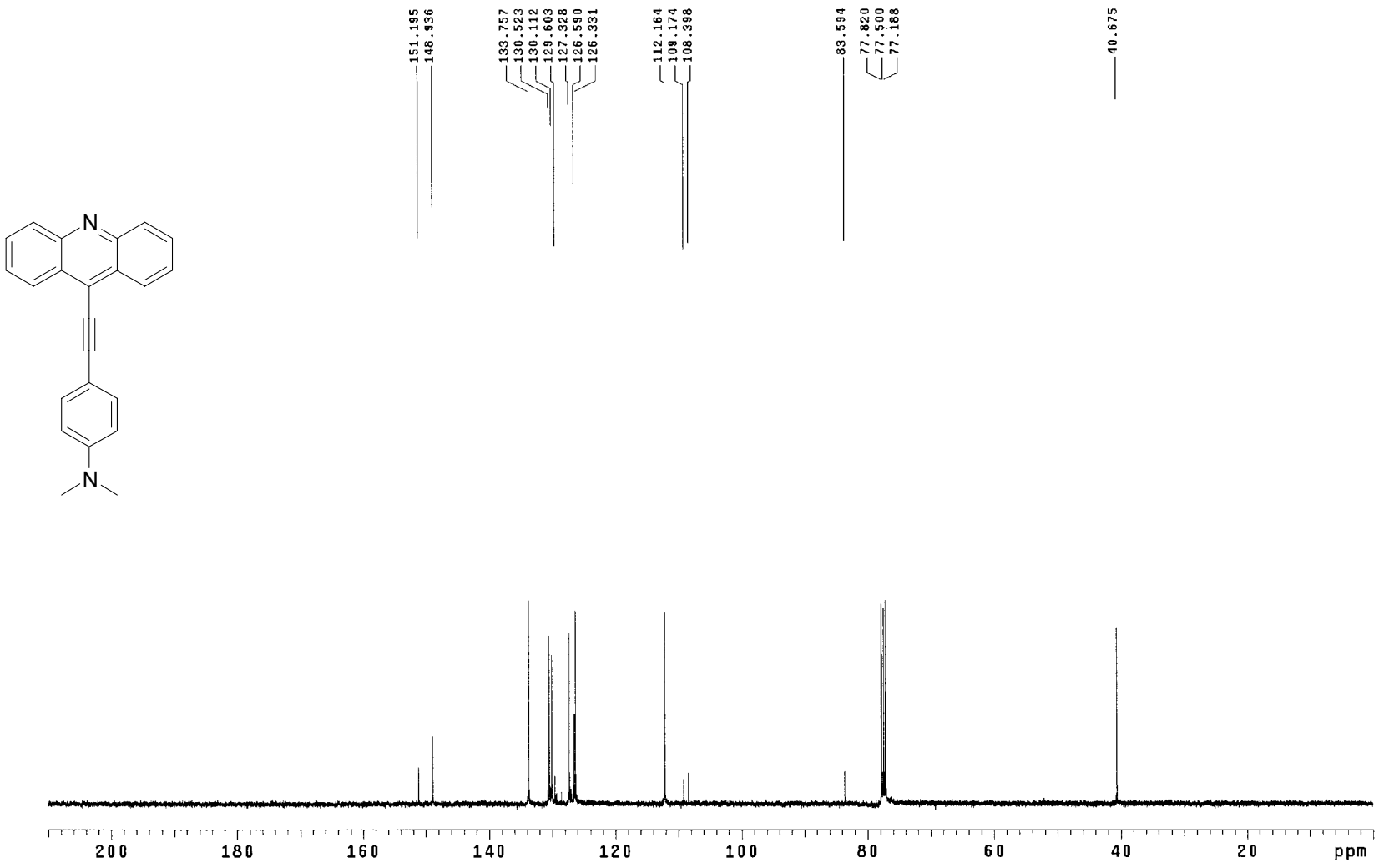
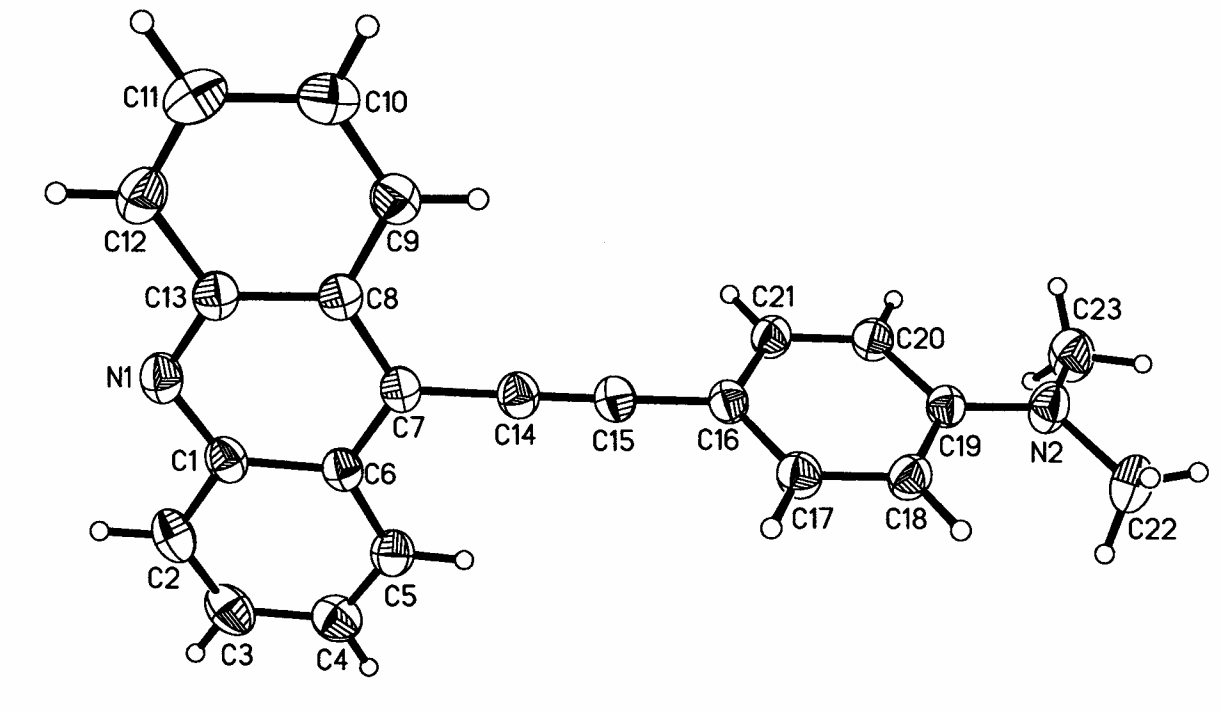


CH040506-acri-NMe2

Pulse Sequence: s2pul





Crystal structure of **6** (ORTEP) showing twist between the donor-substituted phenyl group and acridinyl moiety (thermal ellipsoid drawn at 50% probability)

Table 1. Crystal data and structure refinement for IC10594 (Compound 6).

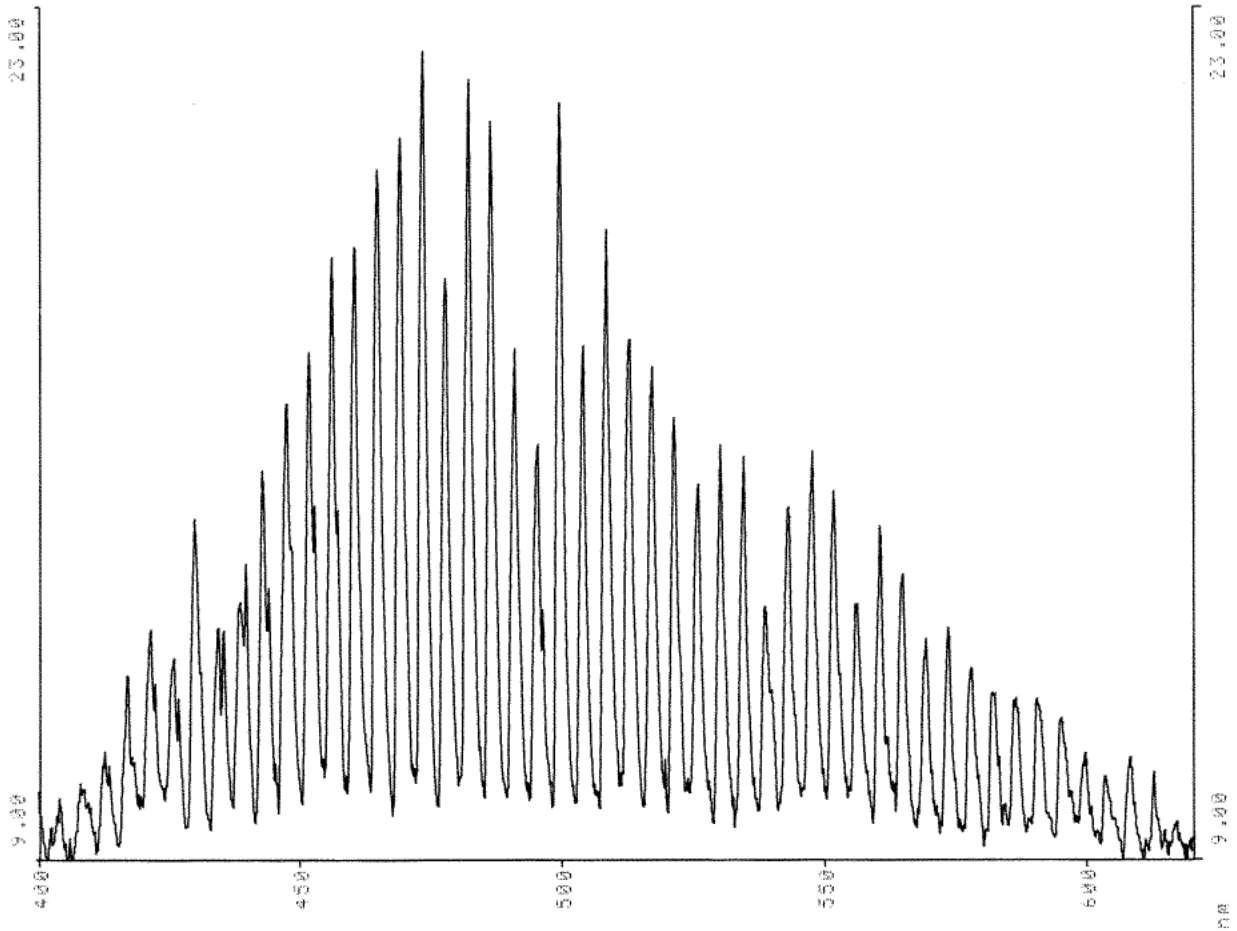
Identification code	ic10594
Diffractometer used	Nonius KappaCCD
Empirical formula	$C_{23}H_{18}N_2$
Formula weight	322.39
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 9.2870(2) Å alpha = 81.7260(10)° b = 9.3930(2) Å beta = 72.9830(10)° c = 10.7350(3) Å gamma = 71.805(2)°
Volume, Z	849.25(3) $Å^3$, 2
Density (calculated)	1.261 Mg/m^3
Absorption coefficient	0.074 mm^{-1}
F(000)	340
Crystal size	0.30 x 0.25 x 0.15 mm
θ range for data collection	1.99 to 27.45°
Limiting indices	$-11 \le h \le 11$, $-11 \le k \le 12$, $-13 \le l \le 13$
Reflections collected	5997
Independent reflections	3827 (R_{int} = 0.0192)
Absorption correction	Multi-scan
Max. and min. transmission	0.988 and 0.945
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3799 / 0 / 227
Goodness-of-fit on F^2	1.023
Final R indices [I>2σ(I)]	R1 = 0.0483, wR2 = 0.1278
R indices (all data)	R1 = 0.0671, wR2 = 0.1449
Extinction coefficient	0.02(2)
Largest diff. peak and hole	0.179 and -0.129 $eÅ^{-3}$

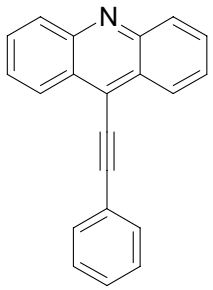
Table 2. Bond lengths [Å] and angles [°] for 10594(Compound 6).

N(1)-C(1)	1.342(2)	N(1)-C(13)	1.345(2)
N(2)-C(19)	1.374(2)	N(2)-C(22)	1.440(2)
N(2)-C(23)	1.440(2)	C(1)-C(2)	1.428(2)
C(1)-C(6)	1.430(2)	C(2)-C(3)	1.345(2)
C(3)-C(4)	1.409(2)	C(4)-C(5)	1.357(2)
C(5)-C(6)	1.421(2)	C(6)-C(7)	1.407(2)
C(7)-C(8)	1.406(2)	C(7)-C(14)	1.432(2)
C(8)-C(9)	1.421(2)	C(8)-C(13)	1.432(2)
C(9)-C(10)	1.352(2)	C(10)-C(11)	1.411(2)
C(11)-C(12)	1.348(2)	C(12)-C(13)	1.424(2)
C(14)-C(15)	1.197(2)	C(15)-C(16)	1.433(2)
C(16)-C(17)	1.390(2)	C(16)-C(21)	1.391(2)
C(17)-C(18)	1.372(2)	C(18)-C(19)	1.401(2)
C(19)-C(20)	1.404(2)	C(20)-C(21)	1.374(2)

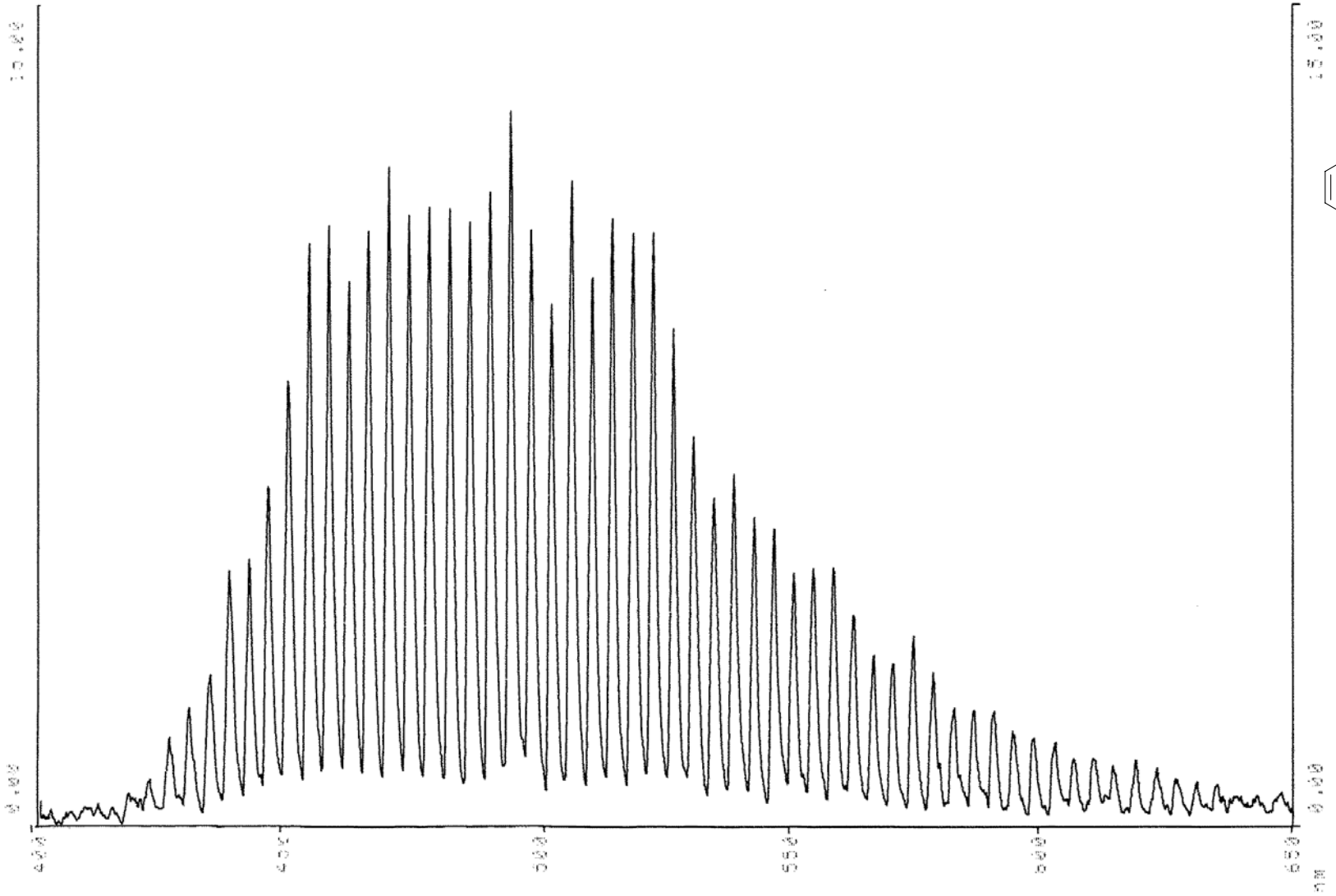
C(1)-N(1)-C(13)	117.99(11)	C(19)-N(2)-C(22)	120.94(13)
C(19)-N(2)-C(23)	120.85(13)	C(22)-N(2)-C(23)	116.78(13)
N(1)-C(1)-C(2)	118.47(13)	N(1)-C(1)-C(6)	123.54(12)
C(2)-C(1)-C(6)	117.99(13)	C(3)-C(2)-C(1)	121.11(14)
C(2)-C(3)-C(4)	120.87(14)	C(5)-C(4)-C(3)	120.4(2)
C(4)-C(5)-C(6)	120.74(14)	C(7)-C(6)-C(5)	123.18(12)
C(7)-C(6)-C(1)	117.95(12)	C(5)-C(6)-C(1)	118.87(12)
C(6)-C(7)-C(8)	119.11(11)	C(6)-C(7)-C(14)	120.48(12)
C(8)-C(7)-C(14)	120.41(12)	C(7)-C(8)-C(9)	123.29(12)
C(7)-C(8)-C(13)	118.01(12)	C(9)-C(8)-C(13)	118.70(12)
C(10)-C(9)-C(8)	120.73(14)	C(9)-C(10)-C(11)	120.46(14)
C(12)-C(11)-C(10)	121.07(14)	C(11)-C(12)-C(13)	120.60(14)
N(1)-C(13)-C(12)	118.22(12)	N(1)-C(13)-C(8)	123.36(12)
C(12)-C(13)-C(8)	118.42(13)	C(15)-C(14)-C(7)	178.88(14)
C(14)-C(15)-C(16)	178.54(14)	C(17)-C(16)-C(21)	117.57(12)
C(17)-C(16)-C(15)	121.56(12)	C(21)-C(16)-C(15)	120.87(12)
C(18)-C(17)-C(16)	121.62(13)	C(17)-C(18)-C(19)	121.22(12)
N(2)-C(19)-C(18)	121.41(12)	N(2)-C(19)-C(20)	121.66(12)
C(18)-C(19)-C(20)	116.93(12)	C(21)-C(20)-C(19)	121.30(13)
C(20)-C(21)-C(16)	121.35(12)		

Symmetry transformations used to generate equivalent atoms:

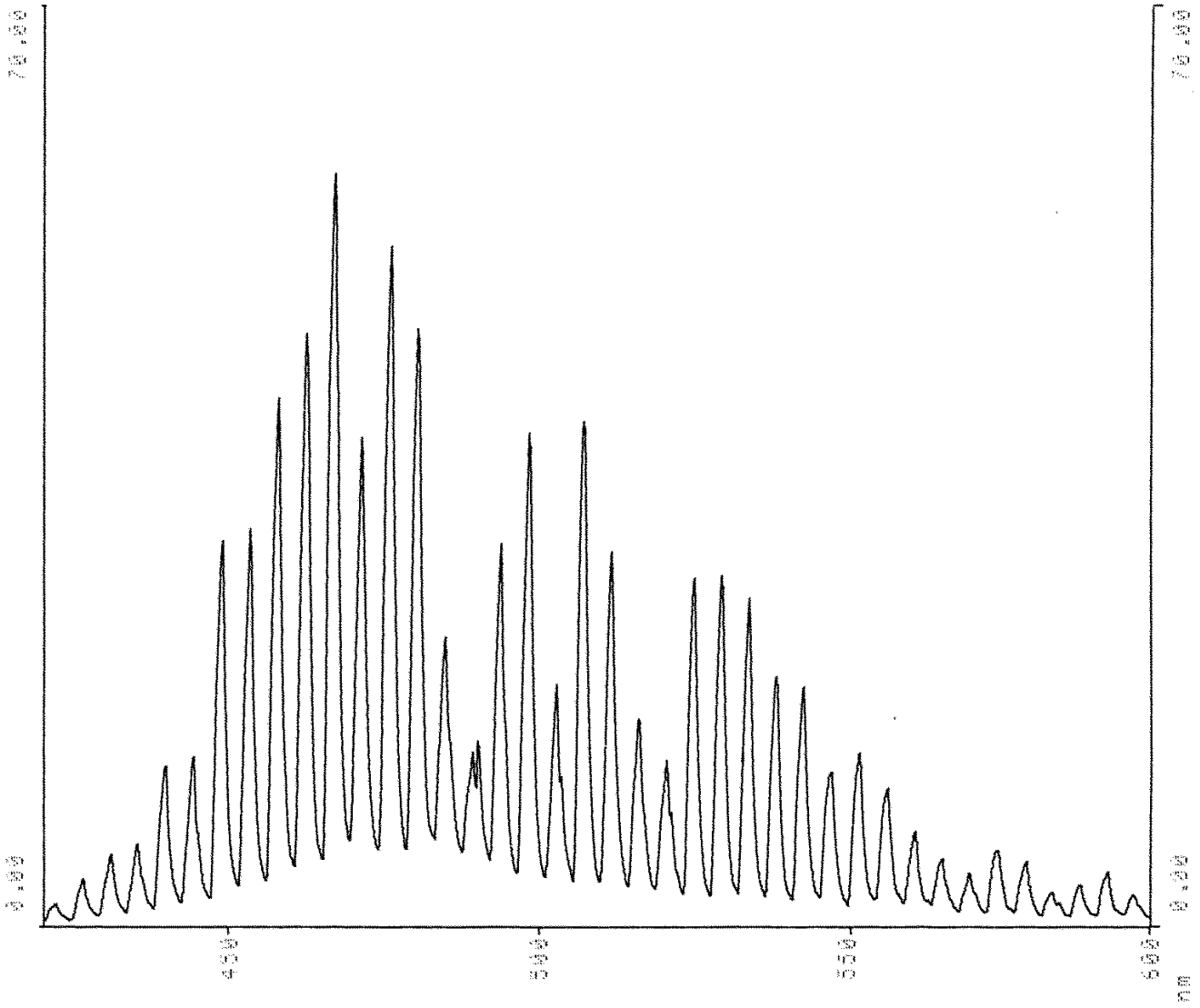


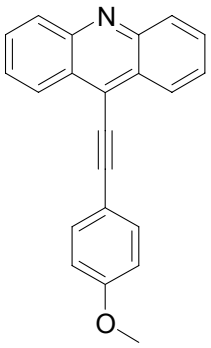


ECL spectrum of **1**. Pulse rates: anode: 0.2s; cathode: 0.2s; hold: 1s

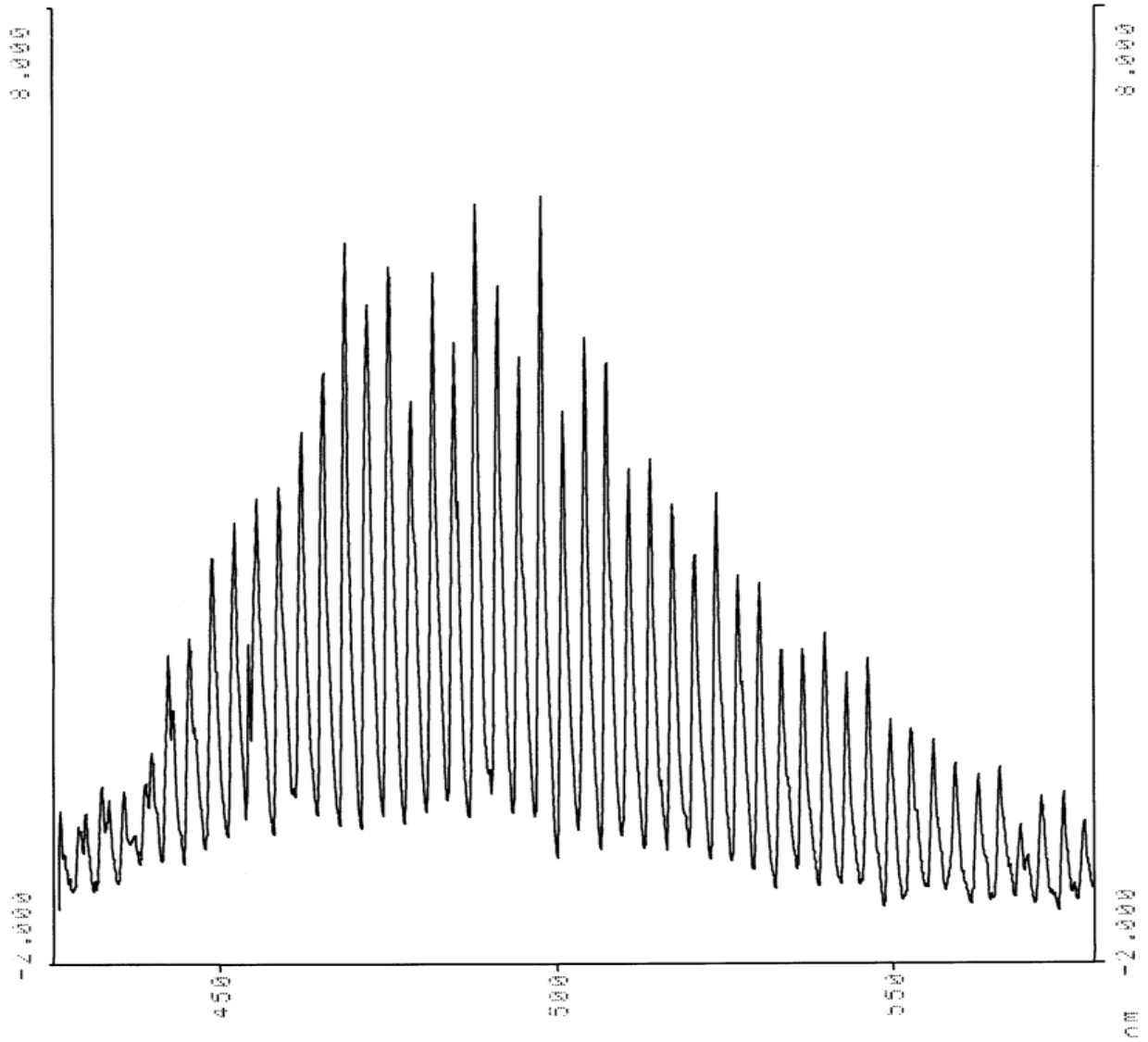


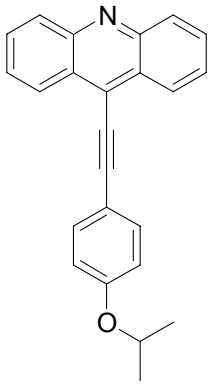
ECL spectrum of **2**. Pulse rates: anode: 0.25s; cathode: 0.25s; hold: 1.5s



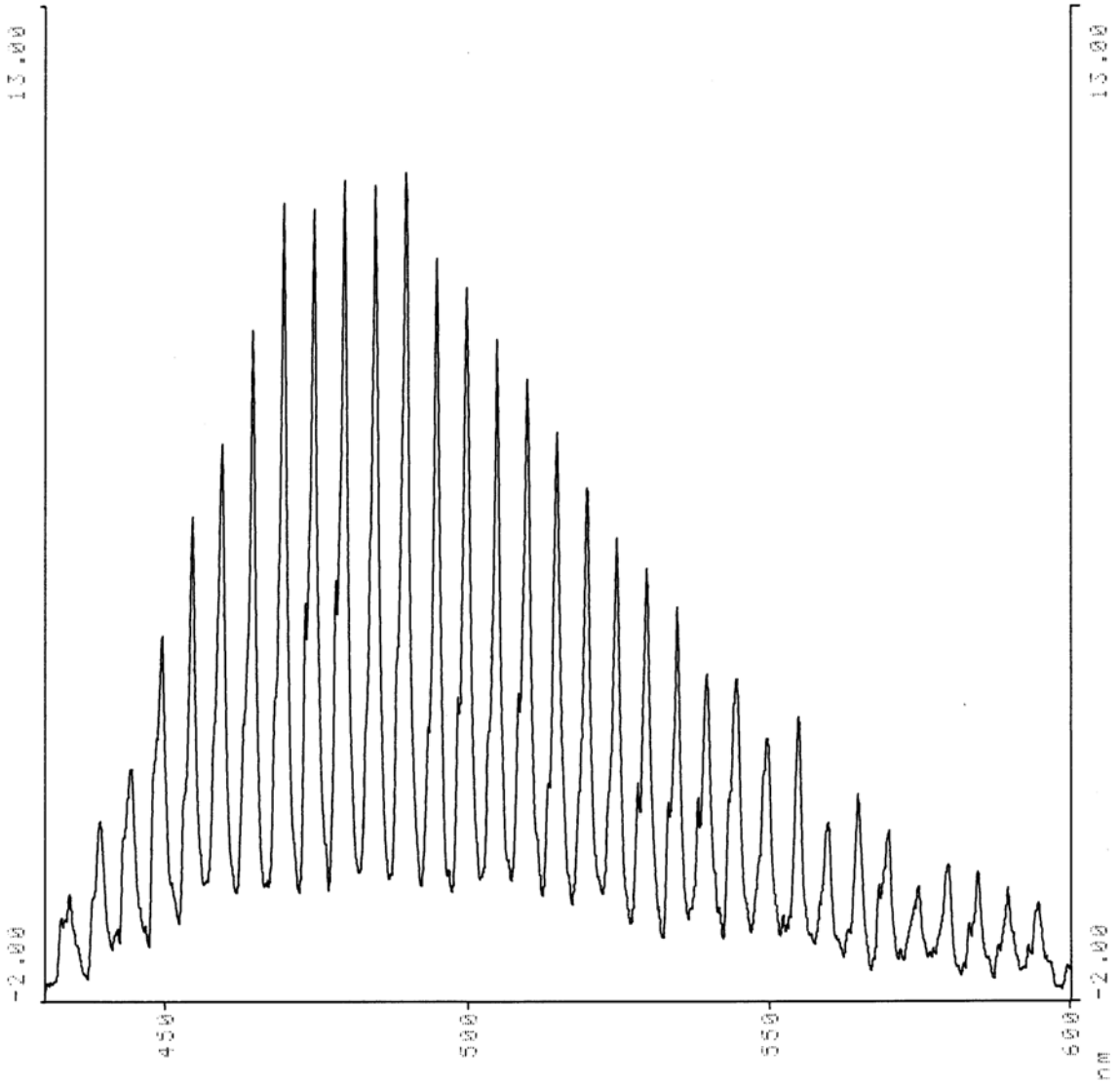


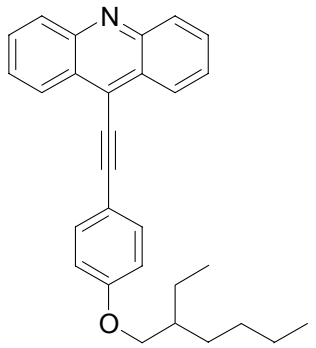
ECL spectrum of **3**. Pulse rates: anode = 0.5s; cathode: 0.5s; hold: 3s



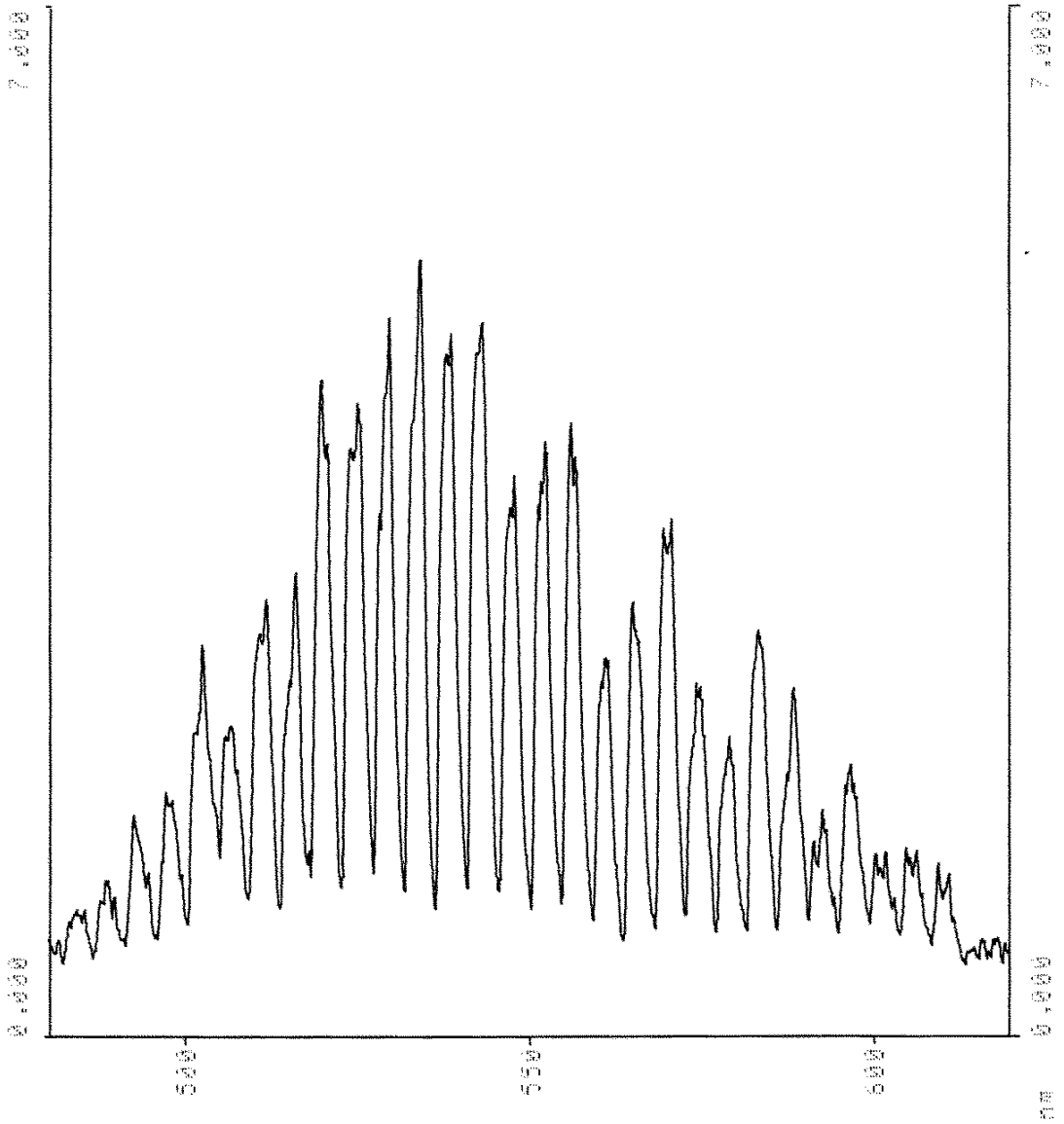


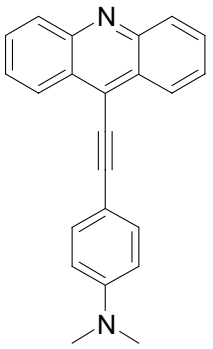
ECL spectrum of **4**. Pulse rates: anode 0.3s; cathode: 0.3s; hold: 2s





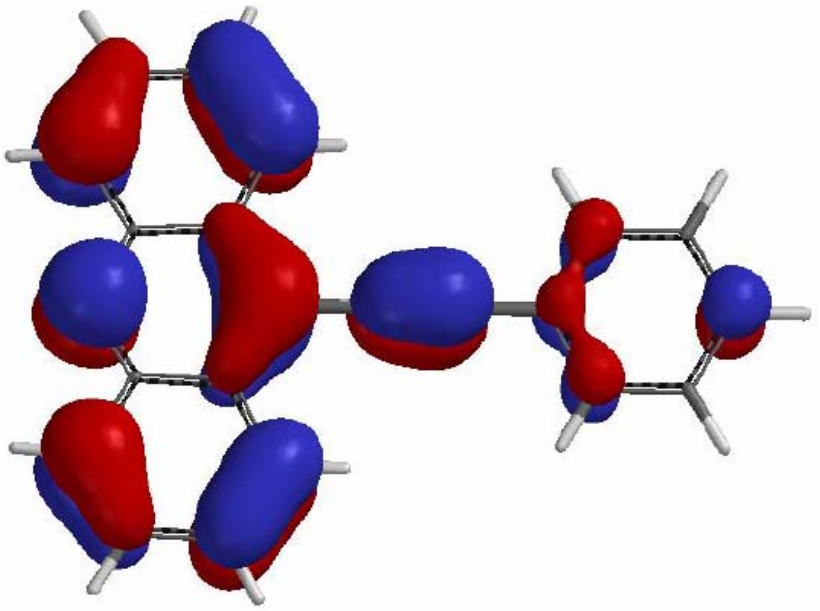
ECL spectrum of **5**. Pulse rates: anode: 1.0s; cathode:0.8s; hold: 0.9s



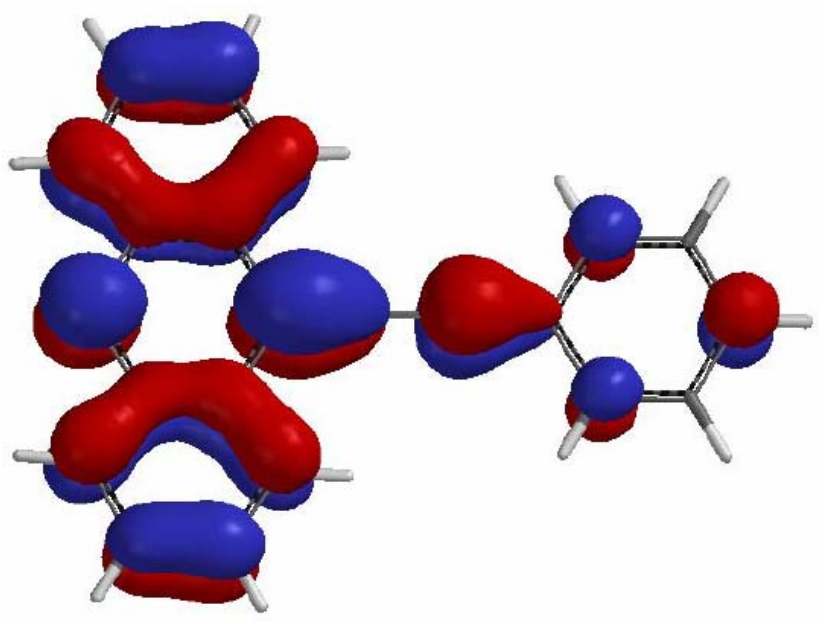


ECL spectrum of **6**. Pulse rates: anode = 0.9s; cathode = 1.0s; hold: 3s

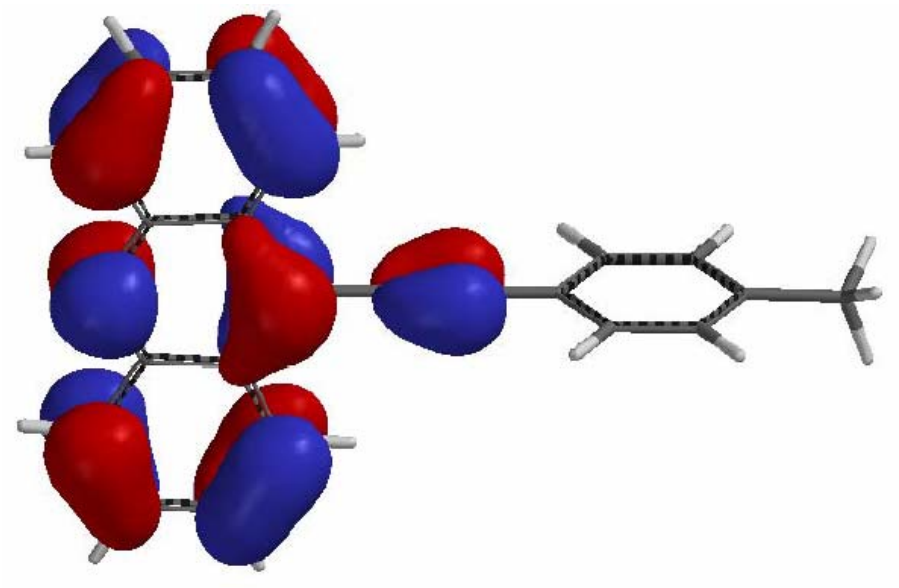
HOMO surface of **1**



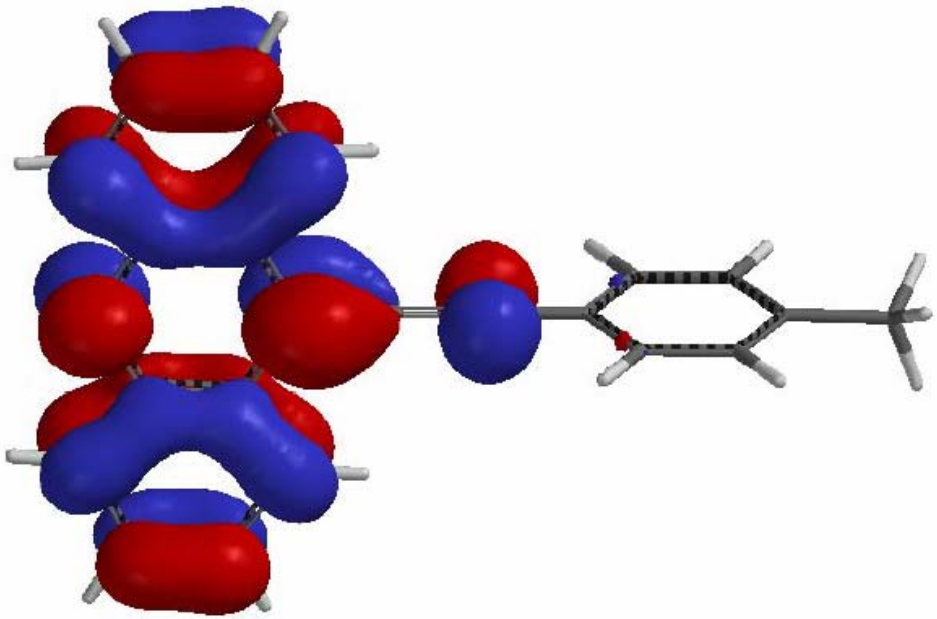
LUMO surface of **1**



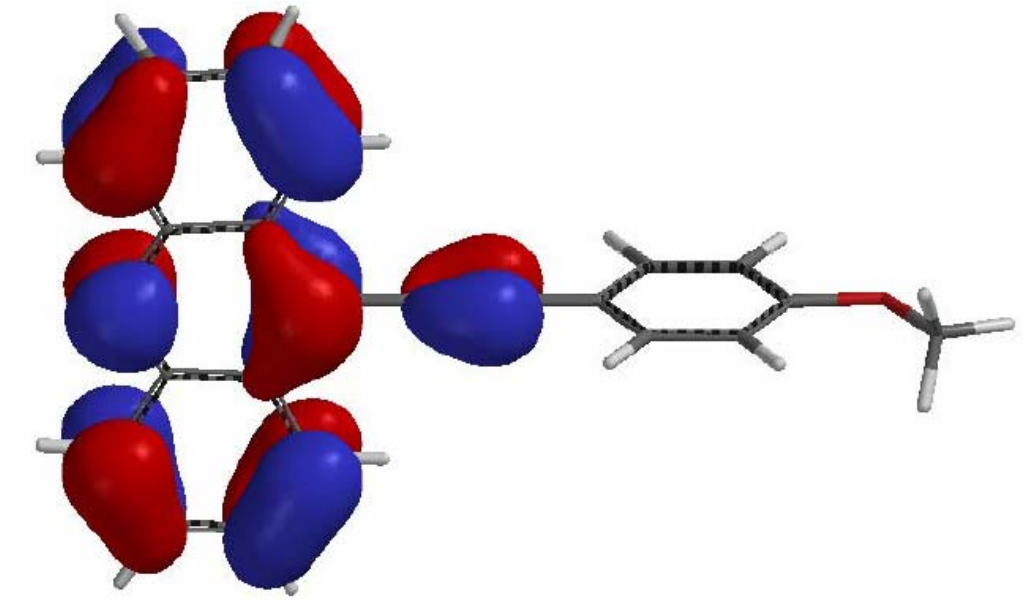
HOMO surface of **2**



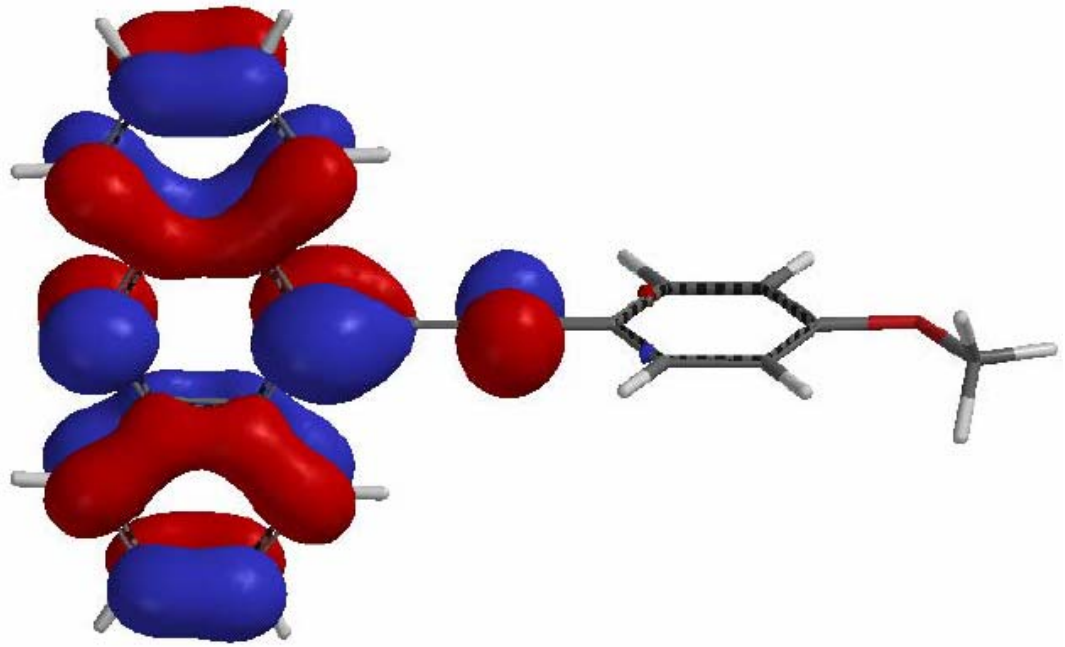
LUMO surface of **2**



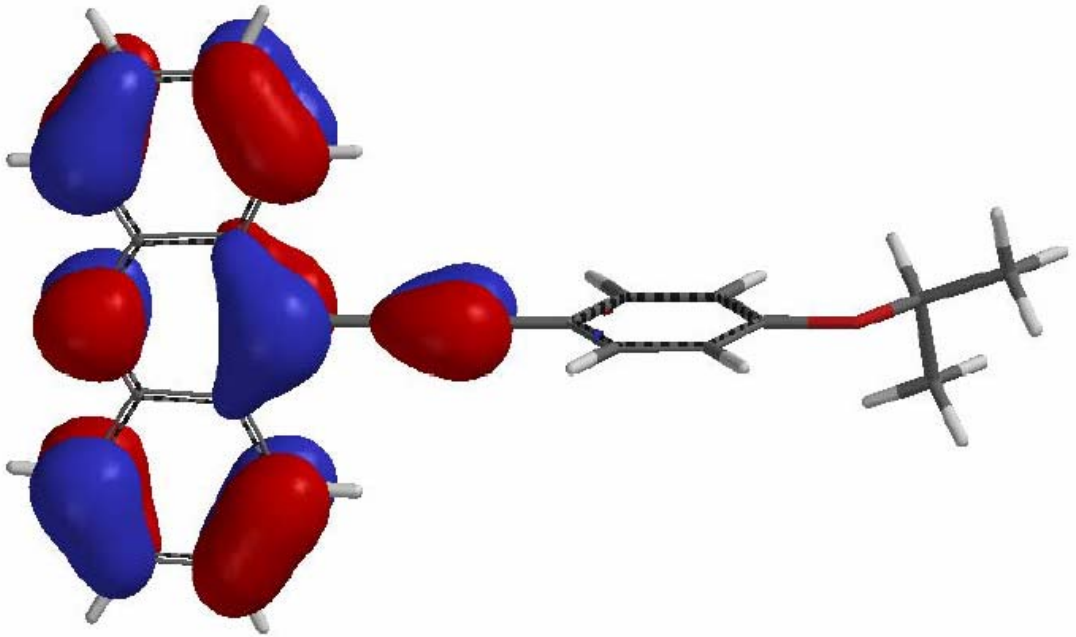
HOMO surface of **3**



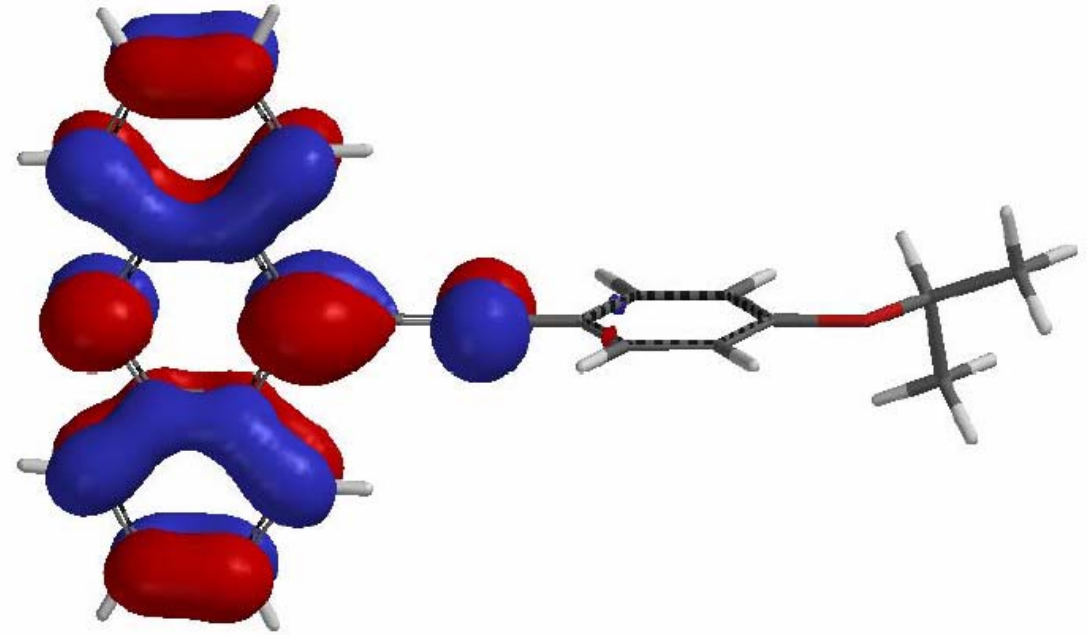
LUMO surface of **3**



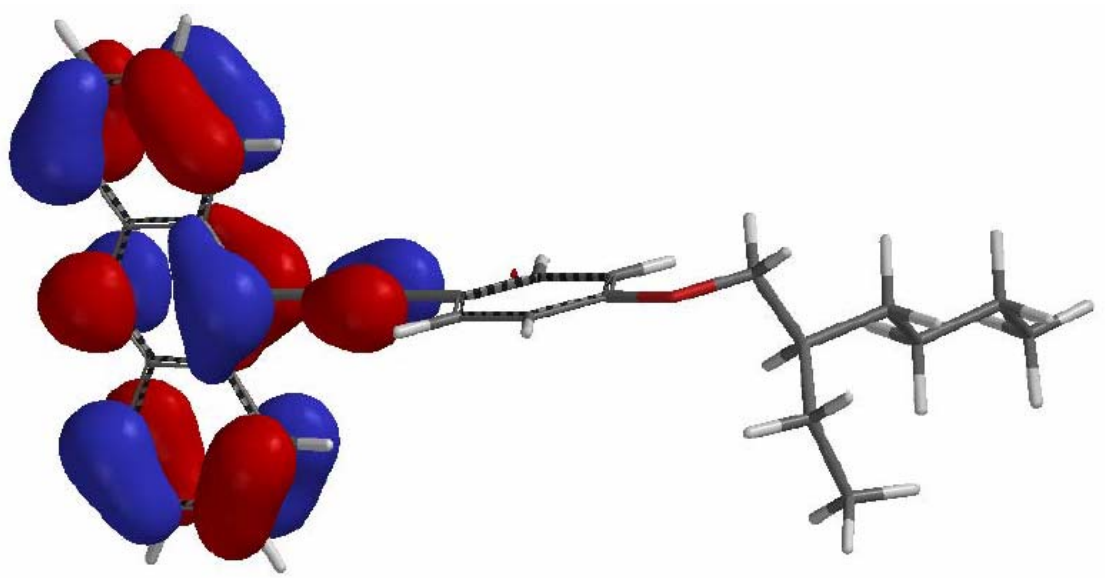
HOMO surface of **4**



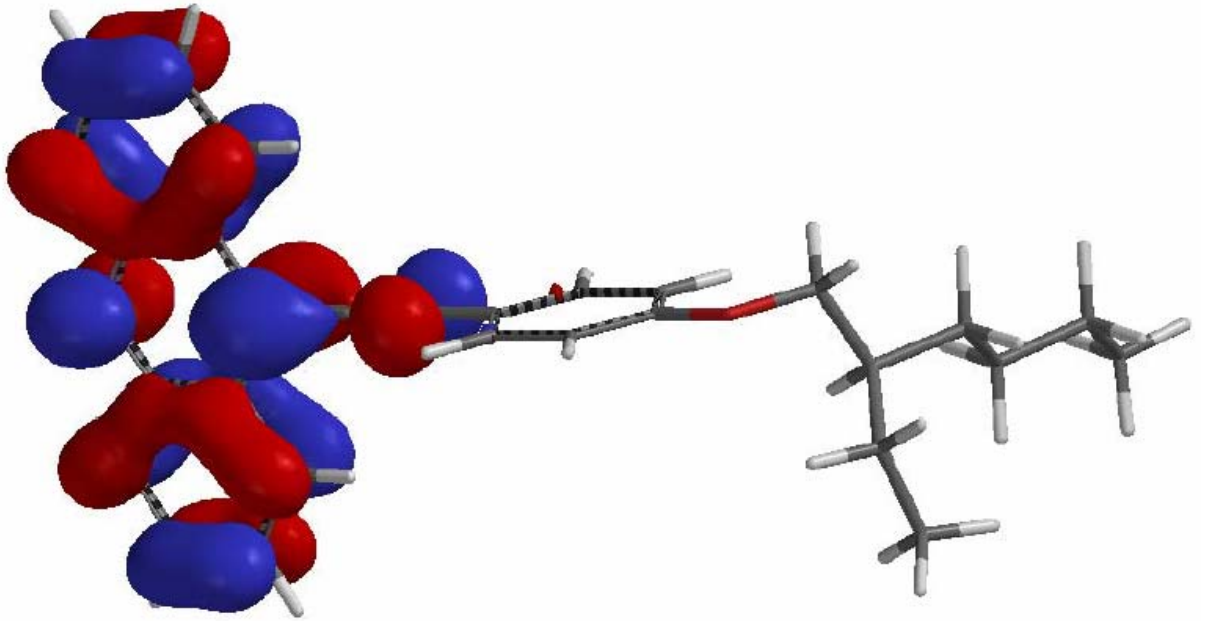
LUMO surface of **4**



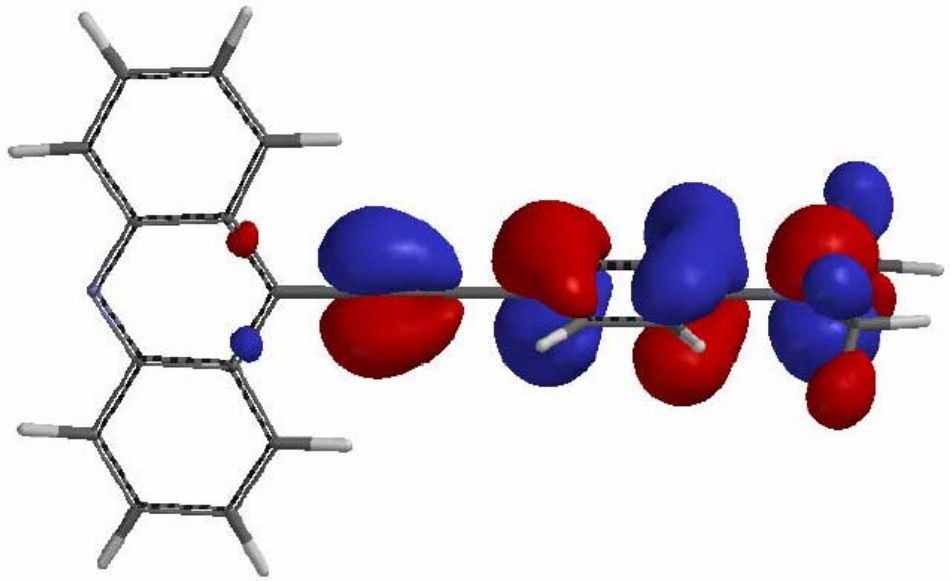
HOMO surface of **5**



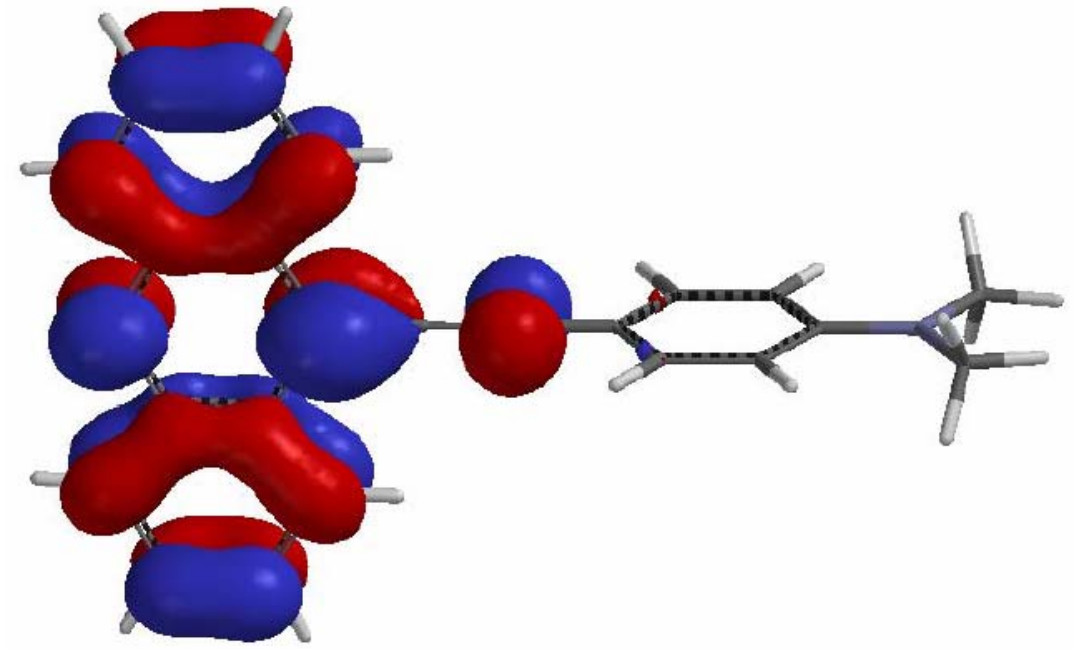
LUMO surface of **5**



HOMO surface of **6**



LUMO surface of **6**



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