Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Dimerization-Cyclization Reactions of Isocyanoaryl-Tethered Alkylidenecyclobutanes via a Triplet Biradical Mediated Process

Le-Yi Tao, Yin Wei, and Min Shi*

State Key Laboratory of Organometallic Chemistry, Center for Excellence in Molecular Synthesis, University of Chinese Academy of Sciences, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Ling-Ling Lu, Shanghai, 200032, China.

weiyin@sioc.ac.cn *Fax* 86-21-64166128.

Supporting Information

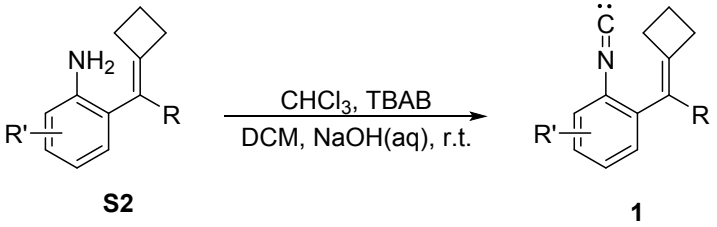
Index

(A) General Information

^{1}H NMR spectra were recorded on Agilent 400 MR DD2 and BRUKER AVANCE III HD 400MHz spectrometer for solution in $CDCl_3$ with tetramethylsilane (TMS) as an internal standard; coupling constants J are given in Hz. ^{13}C NMR spectra were recorded on Agilent 400 MR DD2 and BRUKER AVANCE III HD 400MHz spectrophotometers (100 MHz) with complete proton decoupling spectrophotometers ($CDCl_3$: 77.0 ppm). ^{19}F NMR spectra were recorded on Agilent 400 MR DD2 and BRUKER AVANCE III HD 400MHz for solution in $CDCl_3$. Data are presented as follows: chemical shift (ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants in Hertz (Hz) and integration. Mass and High resolution mass spectra (HRMS) spectra were recorded by ESI or DART method. Infrared spectra were recorded on a Perkin-Elmer PE-983 spectrometer with absorption in cm^{-1}. Melting points were determined on a digital melting point apparatus and temperatures were uncorrected. The employed solvents were dry up by standard methods when necessary. Commercially obtained reagents were used without further purification. For thin-layer chromatography (TLC), silica gel plates (Huanghai GF254) were used. Flash column chromatography was carried out using 300-400 mesh silica gel at increased pressure.

(B) General Procedure for the Preparation of Substrates

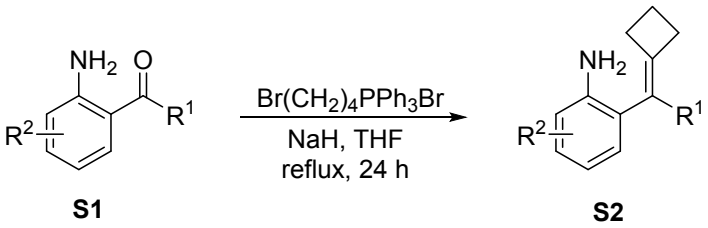
The substrates were prepared according to Scheme S1:



Scheme S1

Compound **1** was prepared according to the synthetic procedure shown above (TBAB = tetrabutylammonium bromide).[1] The synthesis of substrate **S2** is described as follows. Substrates **1a**, **1c**, **1d**, **1k**, **1n-1q**, **1s** and **1t** were synthesized according to the pathway 1, and other substrates were synthesized according to the pathway 2.

Pathway 1 of synthesizing substrate S2



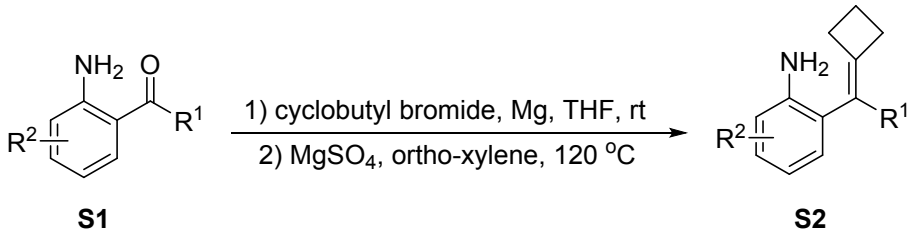
Scheme S2

Substrats **S1a-S1d**, **S1n**, **S1o**, **S1s** and **S1t** were commercially available. Other substrates were prepared according to the previous reported literature.[2]

The product **S2** was synthesized according to the previous literature.[3] A solution of (4-bromobutyl)triphenylphosphonium bromide (1.5 equiv) and NaH (3.0 equiv) in THF (50 mL) was stirred at 75 ^{o}C for 12 h. Afterwards compound **S1** (1.0 equiv) in THF (20 mL) was added and the reaction solution was stirred at 75 ^{o}C for another 12 h. Then the reaction mixture was cooled to room temperature, and the mixture was filtered through a celite pad. Finnaly, the solvent was

removed under reduced pressure and the residue was purified by a silica gel flash chromatography (eluent: petroleum ether / ethyl acetate = 100:1-20:1) to afford the product **S2** in moderate yield.

Pathway 2 of synthesizing substrate S2



S1 **S2**

Scheme S3

Procedure for the preparation of Grignard reagent

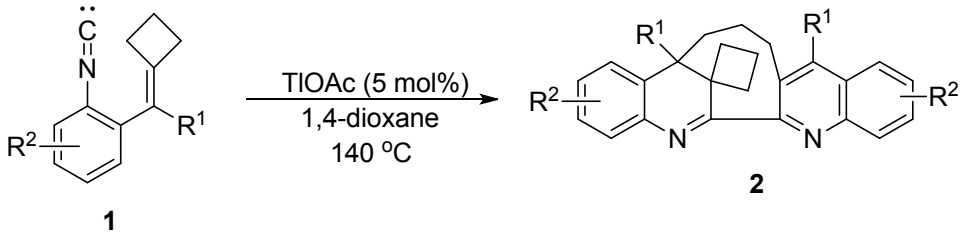
To a dried 100 mL three-neck flask, Mg turnings (1.2 equiv), a grain of iodine and THF (2.0 M relating to the cyclobutyl bromide) were added. Then, adding a small amount of cyclobutyl bromide to the reaction system. The reaction was triggered upon heating to 40 °C. After that, the residual cyclobutyl bromide was added dropwise. The reaction mixture was stirred at 80 °C for 2 hours and preserved at 40 °C for further using.

Procedure for the preparation of substrate S2

The solution of above Grignard reagent (50 mmol, 5.0 equiv) was added dropwise to a solution of **S1** (10 mmol, 1.0 equiv) in THF (20 mL) at 0 °C, and the reaction mixture was stirred at room temperature overnight. The reaction was quenched by adding a saturated aqueous NH_4Cl (10 mL) solution. Then the mixture was extracted with EtOAc (3 x 10 mL) and washed by brine (10 mL). The combined extracts were dried over anhydrous Na_2SO_4. Subsequently, the solvent was removed under reduced pressure to obtain the crude product, which was used for the next reaction without further purification.

The crude product and $MgSO_4$ (50 mmol, 5.0 equiv) were combined in *ortho*-xylene (20 mL) and the reaction mixture was heated at 120 °C for 12 hours. Then the solvent was removed under reduced pressure and the residue was purified by a silica gel flash chromatography (eluent: petroleum ether / ethyl acetate = 50:1) to furnish the desired product in good yield.

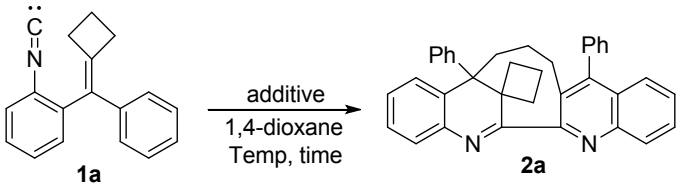
(C) General Procedure for the dimerization-cyclization reaction of substrate 1



Scheme S4

A 10 mL flame-vacuum dried screwed-tube equipped with a magnetic stirring bar was charged with **1** (2 mmol, 1.0 equiv.), TlOAc (0.1 mmol, 0.05 equiv.) and the degassed 1,4-dioxane (4.0 mL) under argon atmosphere. The reaction mixture was stirred at 140 °C for 24 hours in a pre-heated oil bath. After reaction finished, the reaction mixture was cooled to ambient temperature. Then, organic solvent was removed under reduced pressure and the resulting residue was purified through a silica-gel column chromatography (eluent: petroleum ether / ethyl acetate = 10:1-4:1) to provide the desired products **2** in moderate yields.

Table S1. Optimization of the additives

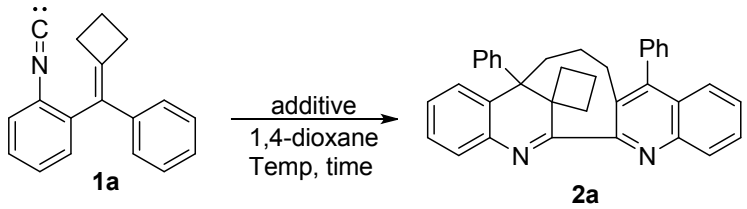


entry[a]	additive (mol%)	solvent	temp (°C)	time (h)	yield/%[b]
1	Ag_2CO_3	1,4-dioxane	140	24	33
2	$AgNTf_2$	1,4-dioxane	140	24	21
3	AgOAc	1,4-dioxane	140	24	32
4	CF_3COOAg	1,4-dioxane	140	24	31
5	$AgSbF_6$	1,4-dioxane	140	24	-
6	$AgNO_3$	1,4-dioxane	140	24	26
7	$AgBF_4$	1,4-dioxane	140	24	-
8	AgOTf	1,4-dioxane	140	24	19
9	$Bi(OTf)_3$	1,4-dioxane	140	24	20
10	$Yb(OTf)_3$	1,4-dioxane	140	24	13
11	$Cu(OTf)_2$	1,4-dioxane	140	24	-
12	$La(OTf)_3$	1,4-dioxane	140	24	-
13	$Ha(OTf)_4$	1,4-dioxane	140	24	-
14	$Ce(OTf)_3$	1,4-dioxane	140	24	-
15	$In(OTf)_3$	1,4-dioxane	140	24	-
16	$Fe(OTf)_2$	1,4-dioxane	140	24	20
17	$Ga(OTf)_3$	1,4-dioxane	140	24	-
18	$Zn(OTf)_2$	1,4-dioxane	140	24	-
19	$BF_3 \cdot Et_2O$	1,4-dioxane	140	24	-
20	CuBr	1,4-dioxane	140	24	26
21	$Zn(NTf_2)_2$	1,4-dioxane	140	24	-
22	iPrAuCl	1,4-dioxane	140	24	36
23	TlOAc	1,4-dioxane	140	24	42
24	$B(C_6F_5)_3$	1,4-dioxane	140	24	27

25	AIBN	1,4-dioxane	140	24	10
26	$TiCl_4$	1,4-dioxane	140	24	32
27	$AuCl_3$	1,4-dioxane	140	24	-
28	$PtCl_2$	1,4-dioxane	140	24	-
29	-	1,4-dioxane	140	24	37

[a]Unless otherwise specified, all reactions were carried out using **1a** (0.1 mmol), additive (5 mol%) in solvent (1.0 mL), 140 °C, 24 h. [b]Yields were determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as an internal standard.

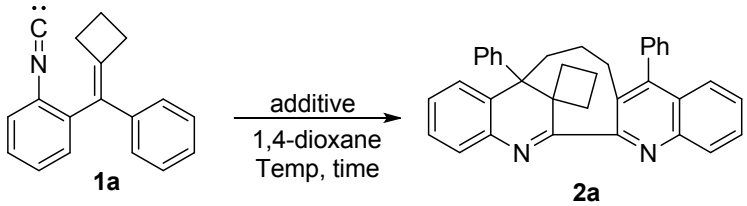
Table S2. Optimization of the solvent



entry[a]	additive (mol%)	solvent	temp (°C)	time (h)	yield/%[b]
1	TlOAc	1,4-dioxane	140	24	42
2	TlOAc	Toluene	140	24	42
3	TlOAc	DMF	140	24	37
4	TlOAc	DMSO	140	24	39
5	TlOAc	PhCl	140	24	42
6	TlOAc	Anisole	140	24	42
7	TlOAc	Cyclohexanone	140	24	32
8	TlOAc	1-Methyl-2-pyrrolidinone	140	24	39
9	TlOAc	Butyronitrile	140	24	36
10	TlOAc	2-Methoxyethanol	140	24	27
11	TlOAc	1,1,2,2-Tetrachloroethane	140	24	24
12	TlOAc	Ethylene glycol diethyl ether	140	24	35
13	TlOAc	1-Butanol	140	24	37

[a]Unless otherwise specified, all reactions were carried out using **1a** (0.1 mmol), additive (5 mol%) in solvent (1.0 mL), 140 °C, 24 h. [b]Yields were determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as an internal standard.

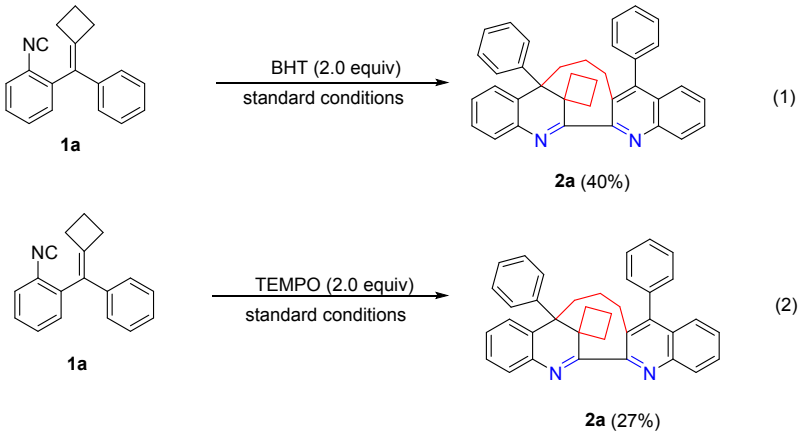
Table S3. Optimization of the reaction conditions



entry[a]	additive (mol%)	solvent	temp (°C)	time (h)	yield/%[b]
1	TlOAc	1,4-dioxane	140	24	42
2	TlOAc (20 mol%)	1,4-dioxane	140	24	41
3	TlOAc	1,4-dioxane	150	24	37
4	TlOAc	1,4-dioxane	130	24	20
5	TlOAc	1,4-dioxane	120	24	21
6	TlOAc	1,4-dioxane	140	36	40
7	TlOAc	1,4-dioxane	140	12	18
8	TlOAc	1,4-dioxane (2 mL)	140	24	18
9	TlOAc	1,4-dioxane (4 mL)	140	24	20
10[c]	**TlOAc**	**1,4-dioxane**	**140**	**24**	**45 (40)**
11[d]	TlOAc	1,4-dioxane	140	24	39

[a]Unless otherwise specified, all reactions were carried out using **1a** (0.1 mmol), additive (5 mol%) in solvent (1.0 mL), 140 °C, 24 h. [b]Yields were determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as an internal standard. [c]Purging oxygen gas in the solvent. [d]Adding molecular sieves 4Å (50 mg).

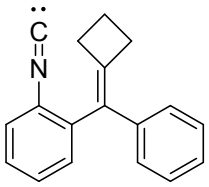
(D) The Control Experiments



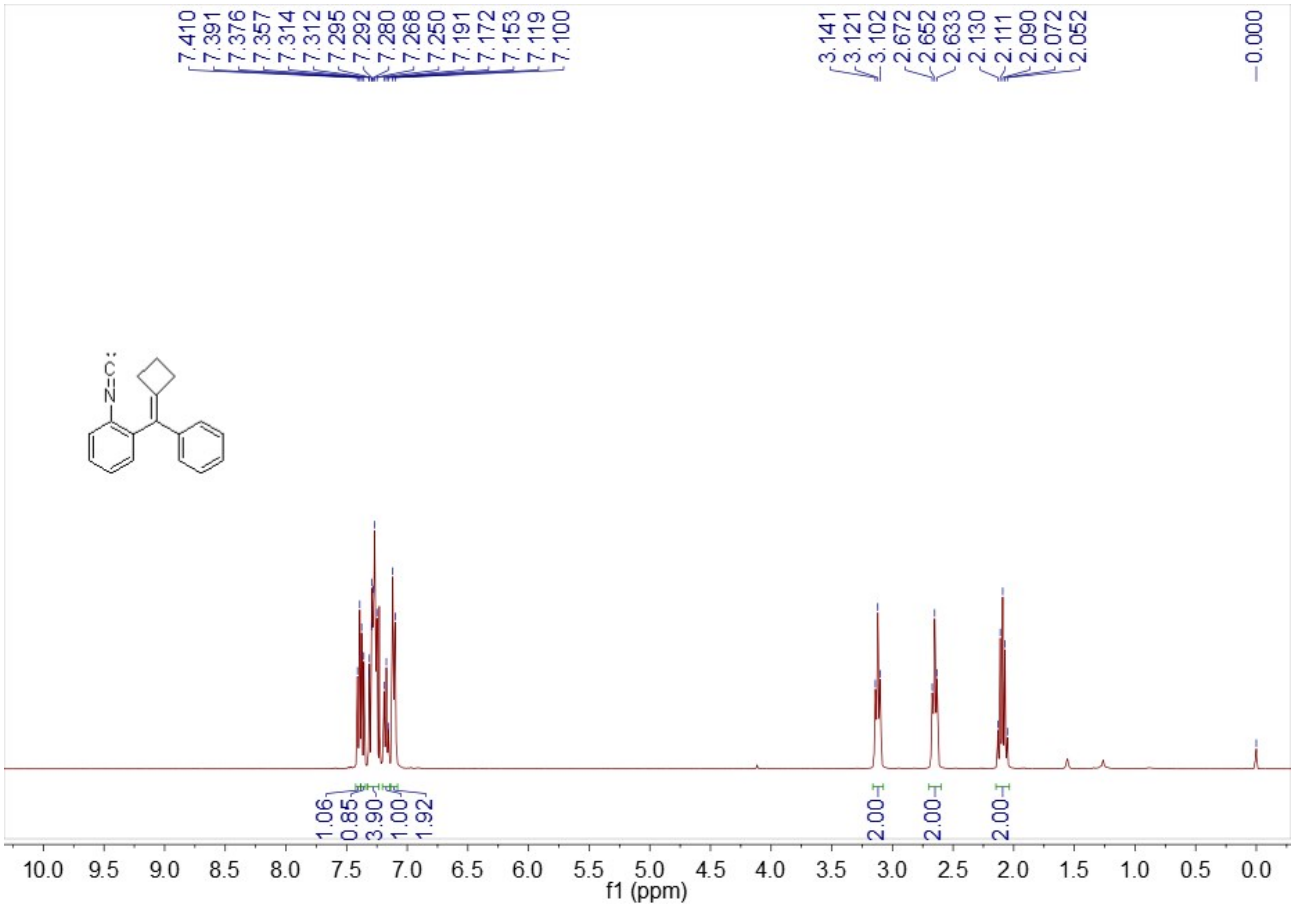
Scheme S5

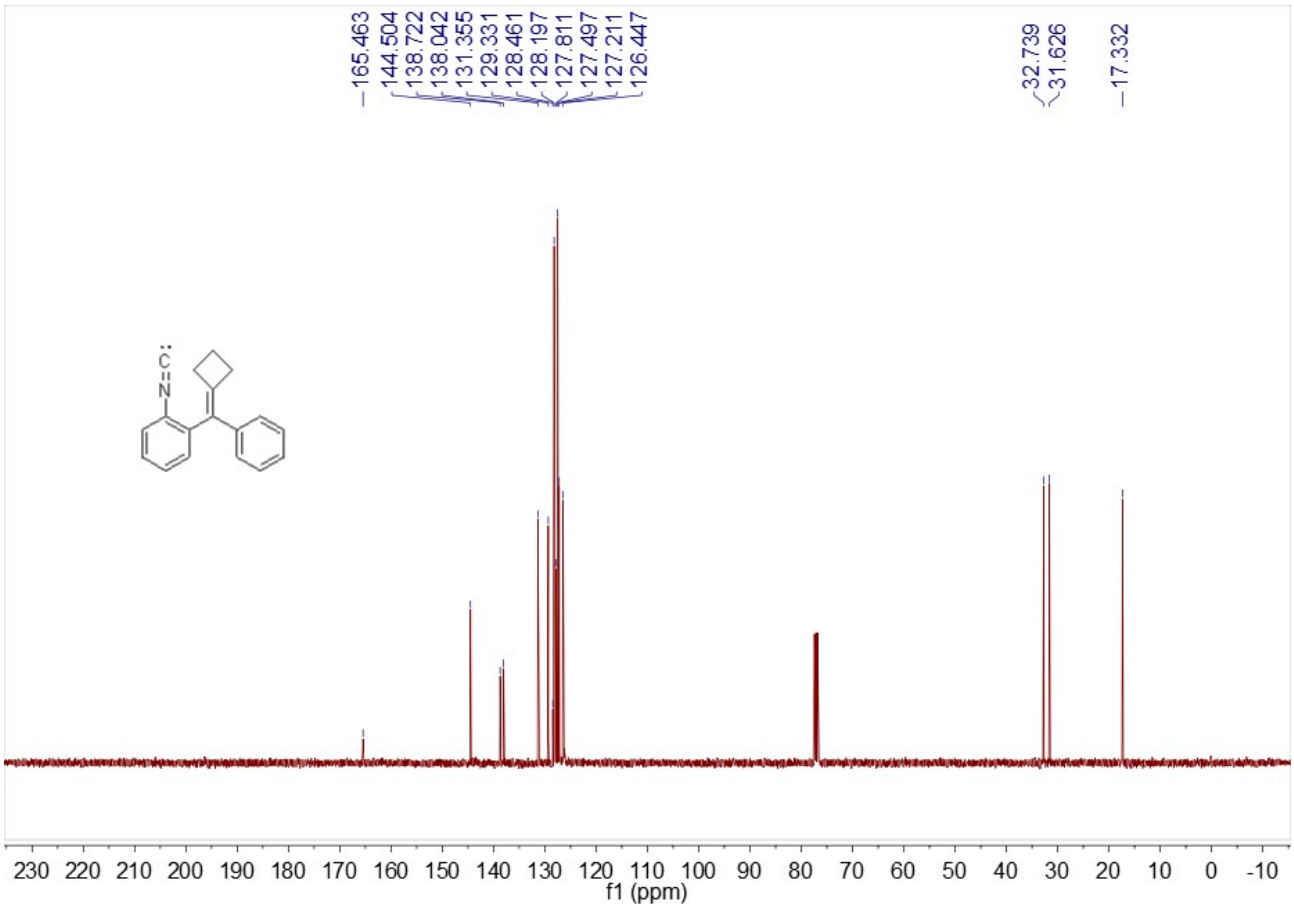
A 10 mL flame-vacuum dried screwed-tube equipped with a magnetic stirring bar was charged with **1a** (2 mmol, 1.0 equiv.), TlOAc (0.1 mmol, 0.05 equiv.), BHT or TEMPO (4 mmol, 2.0 equiv) and the degassed 1,4-dioxane (4.0 mL) under argon atmosphere. The reaction mixture was stirred at 140 ^{o}C for 24 hours in a pre-heated oil bath. After reaction finished, the reaction mixture was cooled to ambient temperature. Then, organic solvent was removed under reduced pressure and the resulting residue was purified through a silica-gel column chromatography (eluent: petroleum ether / ethyl acetate = 10:1-4:1) to provide the desired products **2a**.

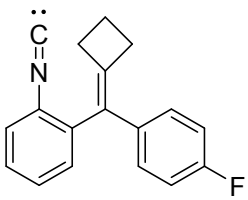
(E) Spectroscopic Data of Substrates and Products



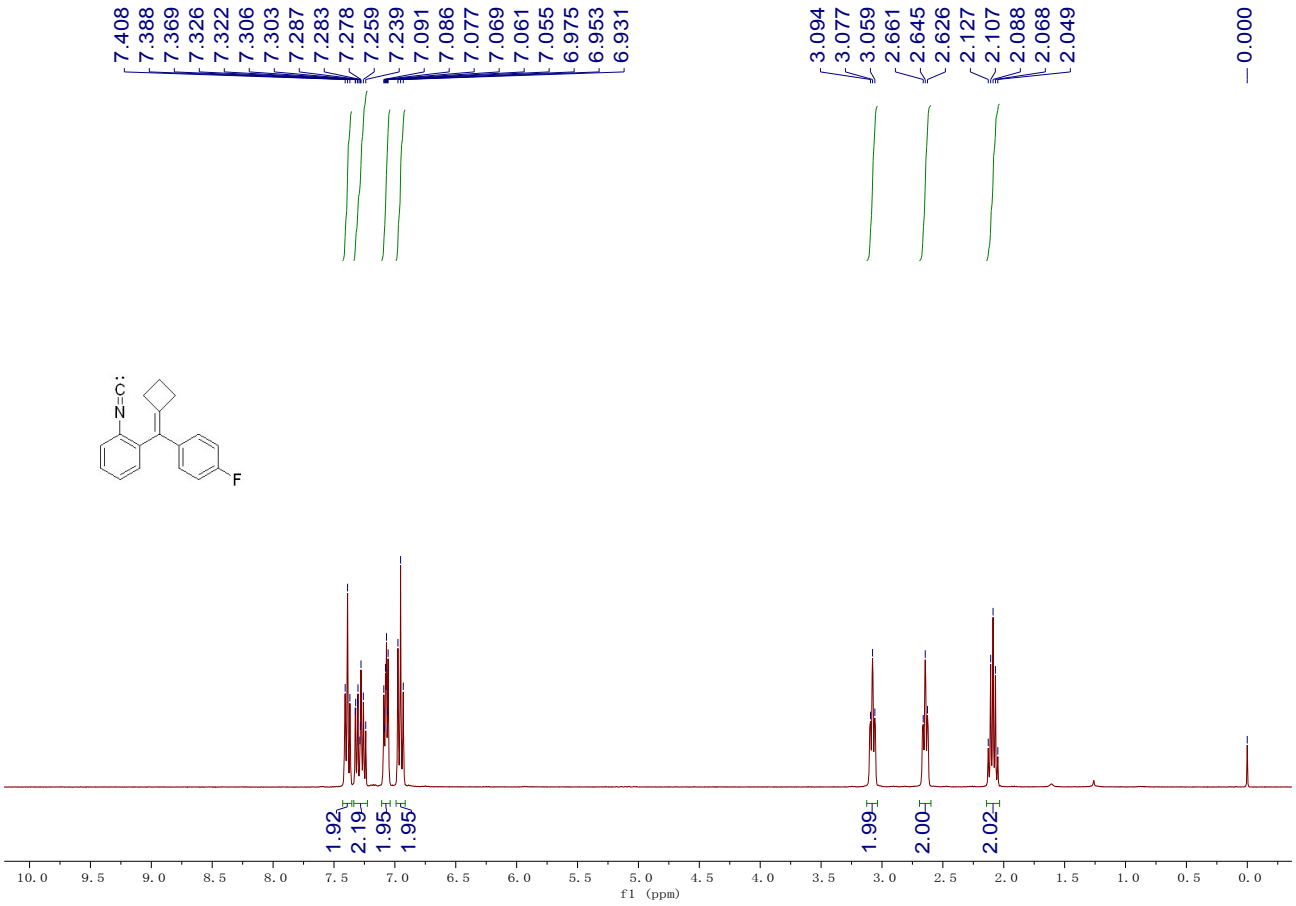
Compound **1a**: Yield: 0.871 g; A brown solid; m.p. 70-72 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.05-2.13 (m, 2H), 2.65 (t, *J* = 7.6 Hz, 2H), 3.12 (t, *J* = 7.6 Hz, 2H), 7.11 (d, *J* = 7.6 Hz, 2H), 7.17 (t, *J* = 7.6 Hz, 1H), 7.25-7.31 (m, 4H), 7.37 (d, *J* = 7.6 Hz, 1H), 7.40 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.3, 31.6, 32.7, 126.4, 127.2, 127.5, 127.8, 128.2, 128.5, 129.3, 131.4, 138.0, 138.7, 144.5, 165.5; IR (CH_3COCH_3): ν 3056, 2952, 2906, 2120, 1598, 1494, 1483, 1443, 1411, 1317, 1190, 1095, 1077, 1033, 951, 903 cm^{-1}; MS (ESI) m/z 246.1 $(M+H)^{+}$; HRMS (ESI) Calcd. for $C_{18}H_{16}N$: 246.1277, Found: 246.1279.

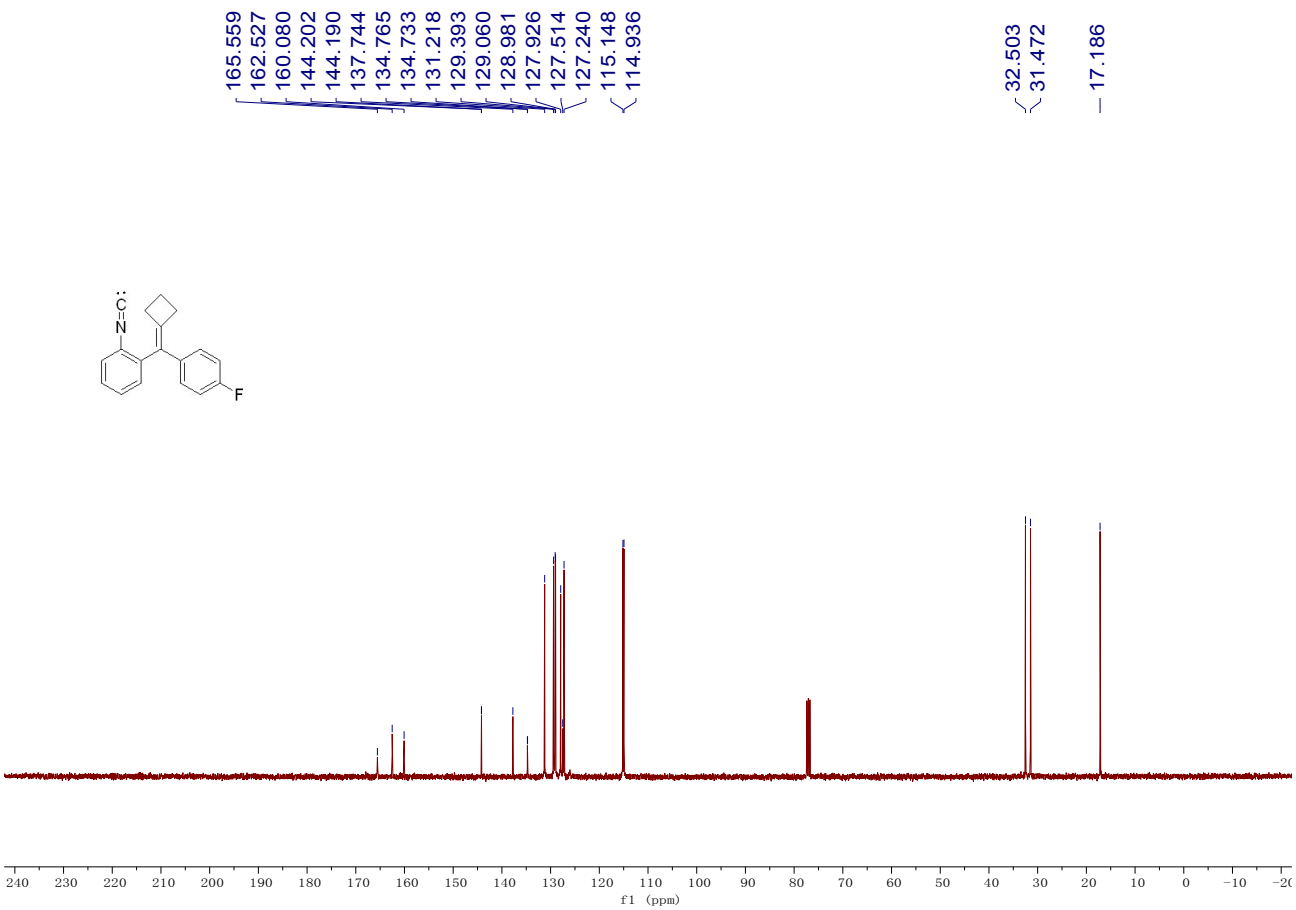


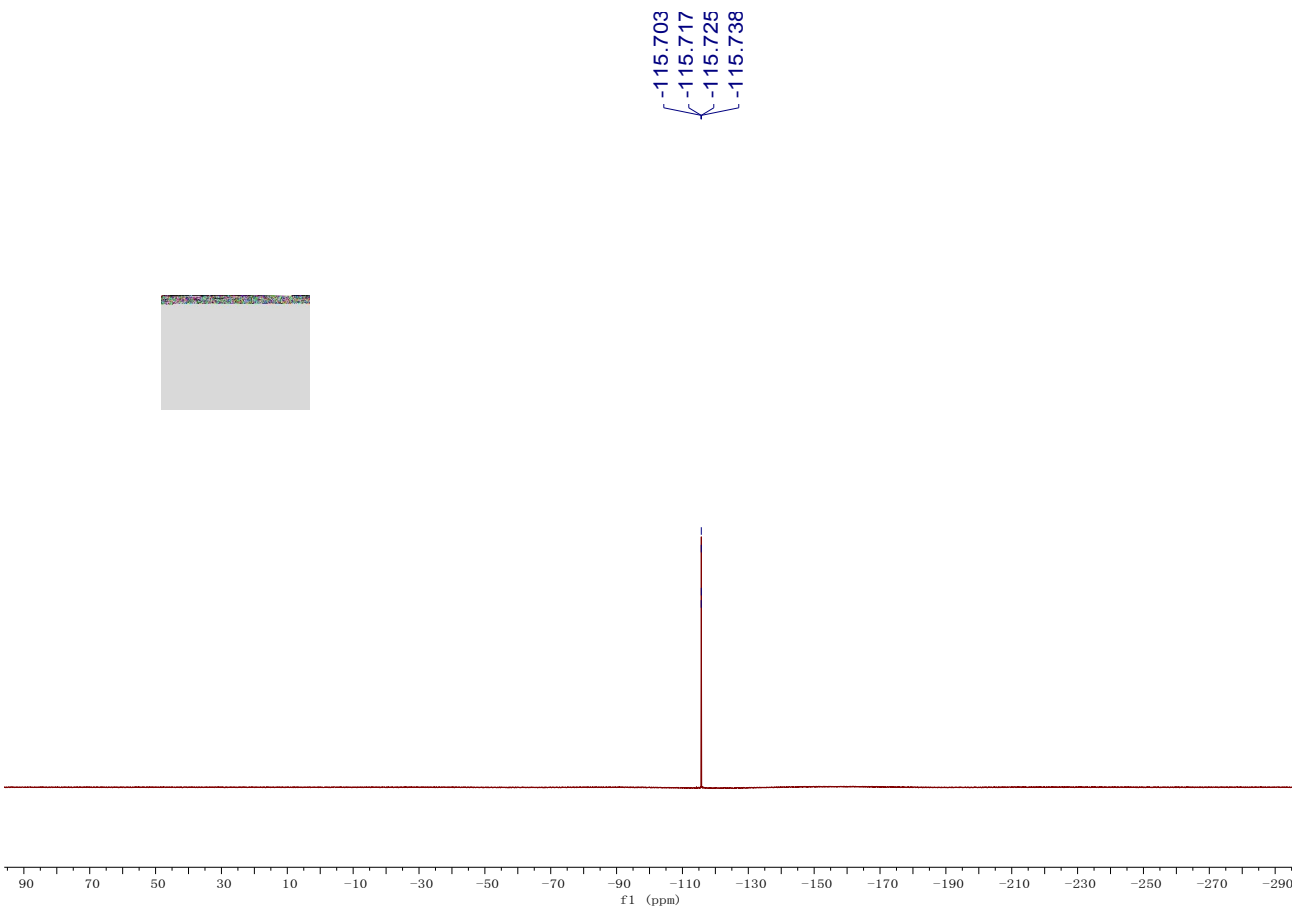


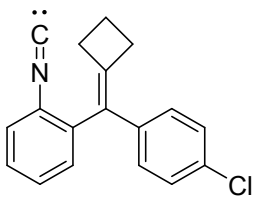


Compound **1b**: Yield: 2.563 g; A brown solid; m.p. 65-67 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.05-2.13 (m, 2H), 2.65 (t, J = 7.0 Hz, 2H), 3.08 (t, J = 7.0 Hz, 2H), 6.95 (t, J = 8.8 Hz, 2H), 7.06-7.09 (m, 2H), 7.24-7.33 (m, 2H), 7.39 (t, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.2, 31.5, 32.5, 115.0 (d, $J_{C\text{-}F}$ = 21.2 Hz), 127.2, 127.5, 127.9, 129.0 (d, $J_{C\text{-}F}$ = 7.9 Hz), 129.4, 131.2, 134.8 (d, $J_{C\text{-}F}$ = 3.2 Hz), 137.7, 144.2 (d, $J_{C\text{-}F}$ = 1.2 Hz) , 161.3 (d, $J_{C\text{-}F}$ = 244.7 Hz), 165.6; ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$): δ -115.7 (m); IR (CH_3COCH_3): ν 2990, 2953, 2909, 2120, 1659, 1602, 1506, 1483, 1442, 1407, 1314, 1223, 1158, 1097, 1037, 1013, 905, 834, 805, 758, 719 cm^{-1}; MS (ESI) m/z 264.1 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{18}H_{15}NF$: 264.11830, Found: 264.11879.

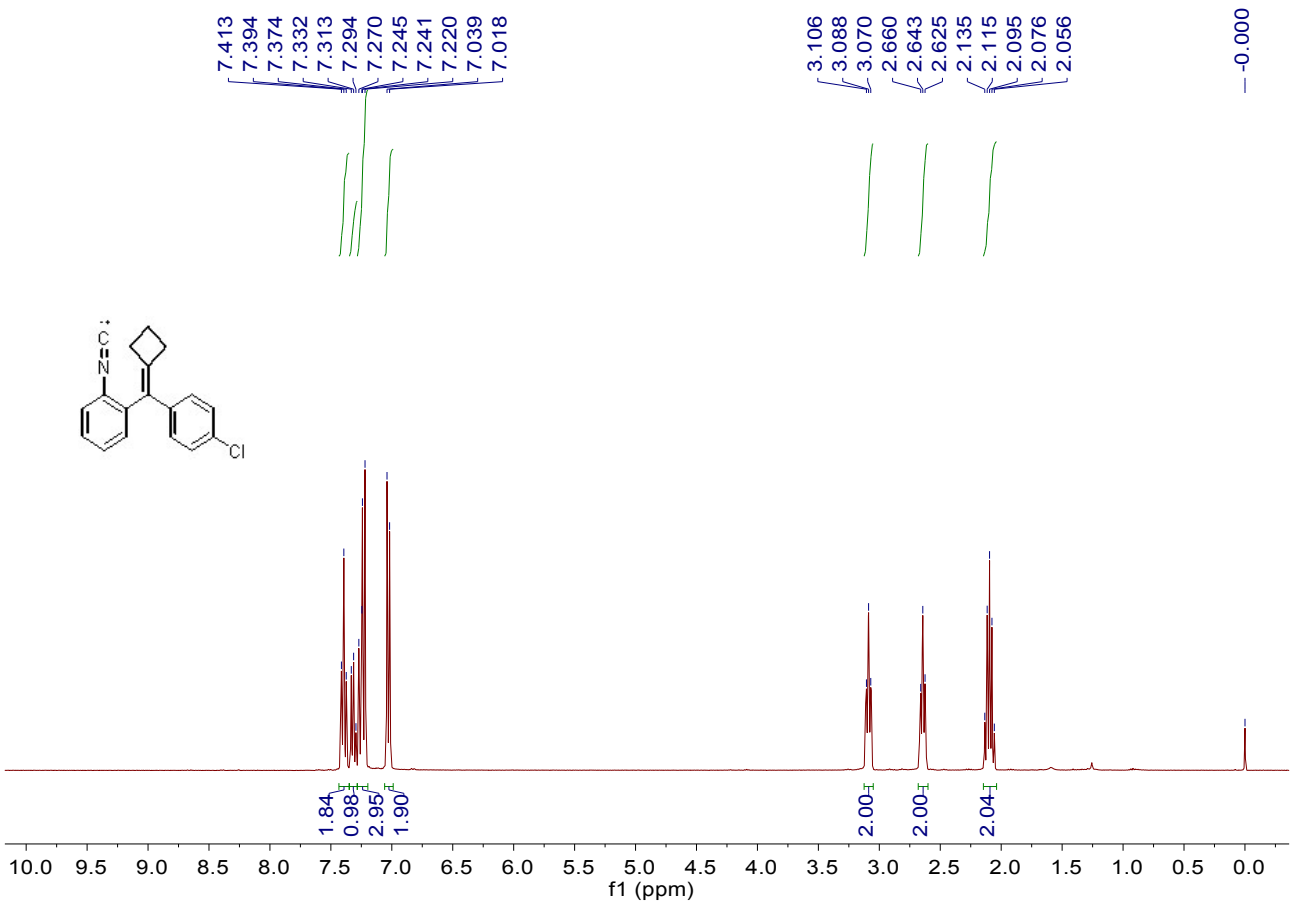

7.408
7.388
7.369
7.326
7.322
7.306
7.303
7.287
7.283
7.278
7.259
7.239
7.091
7.086
7.077
7.069
7.061
7.055
6.975
6.953
6.931
3.094
3.077
3.059
2.661
2.645
2.626
2.127
2.107
2.088
2.068
2.049
0.000
N
F
1.92
2.19
1.95
1.95
1.99
2.00
2.02
f1 (ppm)

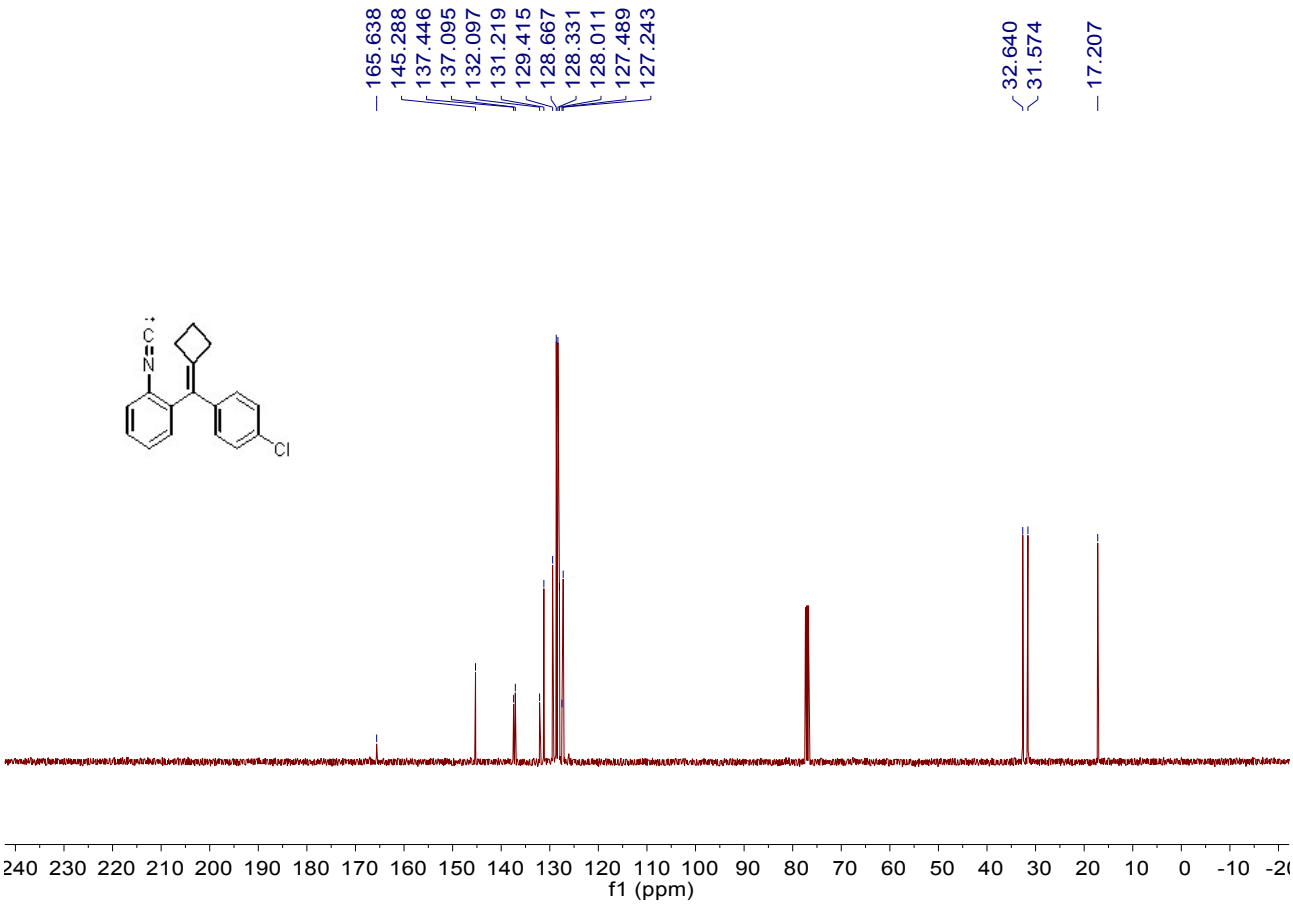

165.559
162.527
160.080
144.202
144.190
137.744
134.765
134.733
131.218
129.393
129.060
128.981
127.926
127.514
127.240
115.148
114.936
32.503
31.472
17.186
N
F
f1 (ppm)

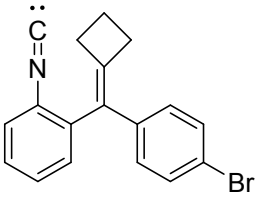




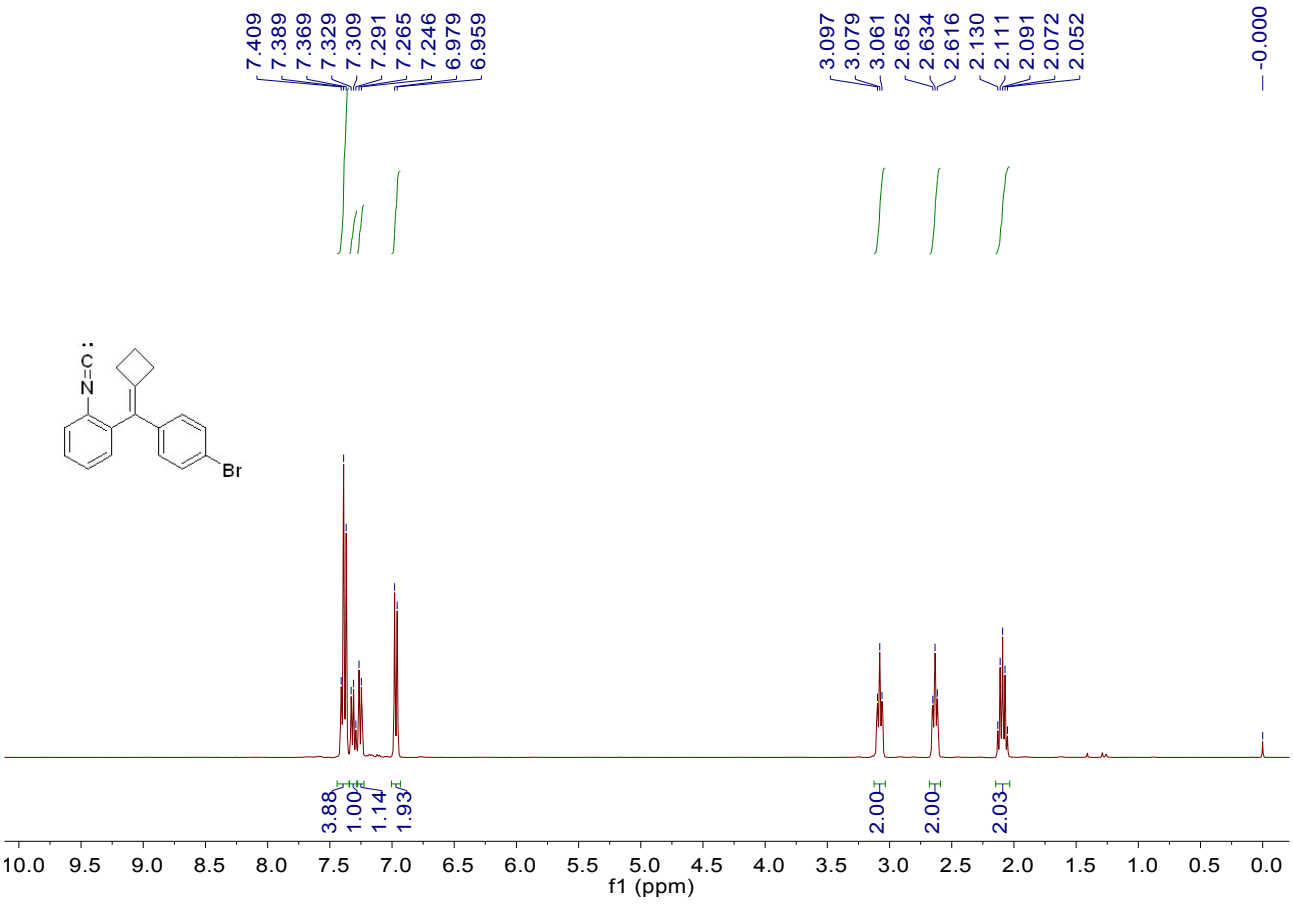
Compound **1c**: Yield: 1.762 g; A brown solid; m.p. 72-74 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.06-2.14 (m, 2H), 2.64 (t, J = 7.0 Hz, 2H), 3.09 (t, J = 7.2 Hz, 2H), 7.03 (d, J = 8.4 Hz, 2H), 7.22-7.27 (m, 3H), 7.31 (t, J = 7.6 Hz, 1H), 7.39 (t, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.2, 31.6, 32.6, 127.2, 127.5, 128.0, 128.3, 128.7, 129.4, 131.2, 132.1, 137.1, 137.4, 145.3, 165.6; IR (CH_3COCH_3): ν 2982, 2953, 2909, 2120, 1655, 1490, 1444, 1399, 1092, 1012, 951, 904, 828, 759, 717 cm^{-1}; MS (ESI) m/z 280.1 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{18}H_{15}NCl$: 280.0888, Found: 280.0890.

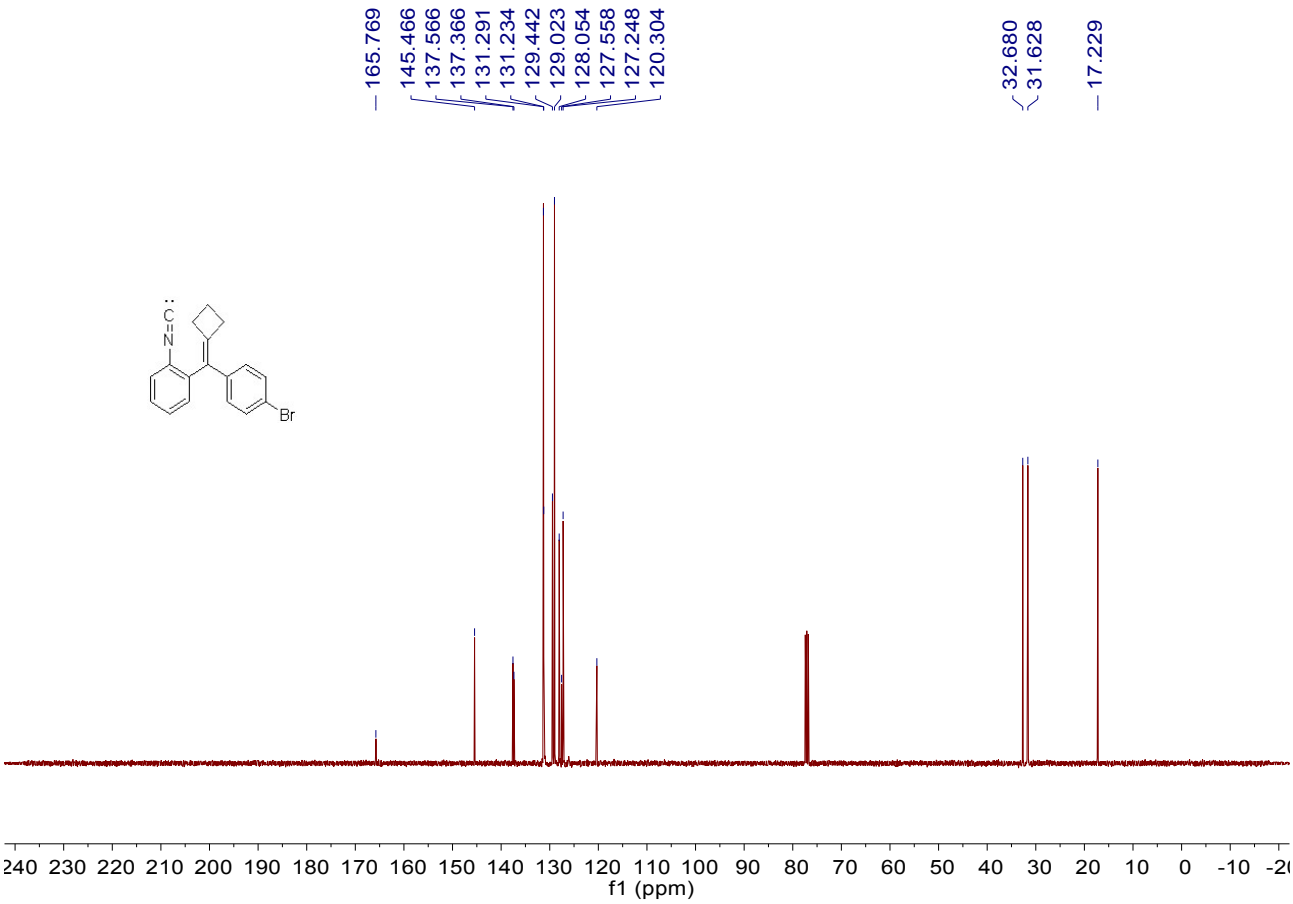

7.413
7.394
7.374
7.332
7.313
7.294
7.270
7.245
7.241
7.220
7.039
7.018
3.106
3.088
3.070
2.660
2.643
2.625
2.135
2.115
2.095
2.076
2.056
-0.000
N
Cl
1.84
0.98
2.95
1.90
2.00
2.00
2.04
f1 (ppm)

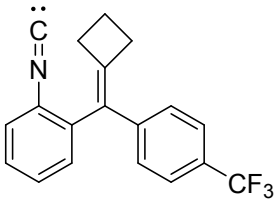

165.638
145.288
137.446
137.095
132.097
131.219
129.415
128.667
128.331
128.011
127.489
127.243
32.640
31.574
17.207
N
Cl
f1 (ppm)



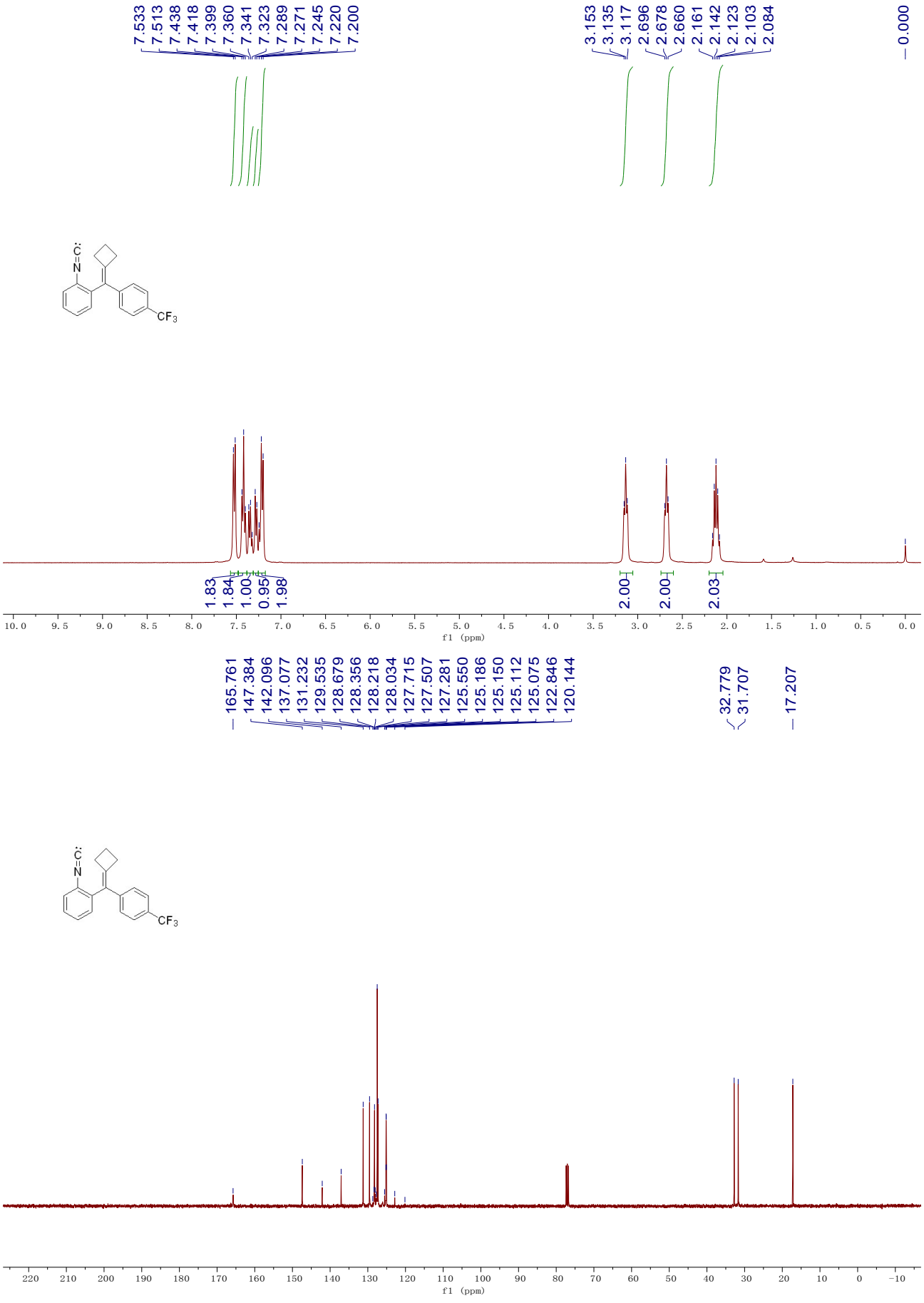
Compound **1d**: Yield: 1.274g , 47%; A brown solid; m.p. 94-96 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.05-2.13 (m, 2H), 2.63 (t, *J* = 7.2 Hz, 2H), 3.08 (t, *J* = 7.2 Hz, 2H), 6.97 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 7.6 Hz, 1H), 7.31 (t, *J* = 7.8 Hz, 1H), 7.37-7.41 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.2, 31.6, 32.7, 120.3, 127.2, 127.6, 128.1, 129.0, 129.4, 131.2, 131.3, 137.4, 137.6, 145.5, 165.8; IR (CH_3COCH_3): ν 2980, 2953, 2906, 2120, 1655, 1583, 1485, 1443, 1409, 1395, 1173, 1096, 1073, 1037, 1008, 903, 825, 759, 714 cm^{-1}; MS (ESI) m/z 324.0 $(M+H)^{+}$; HRMS (ESI) Calcd. for $C_{18}H_{15}NBr$: 324.0382, Found: 324.0381.

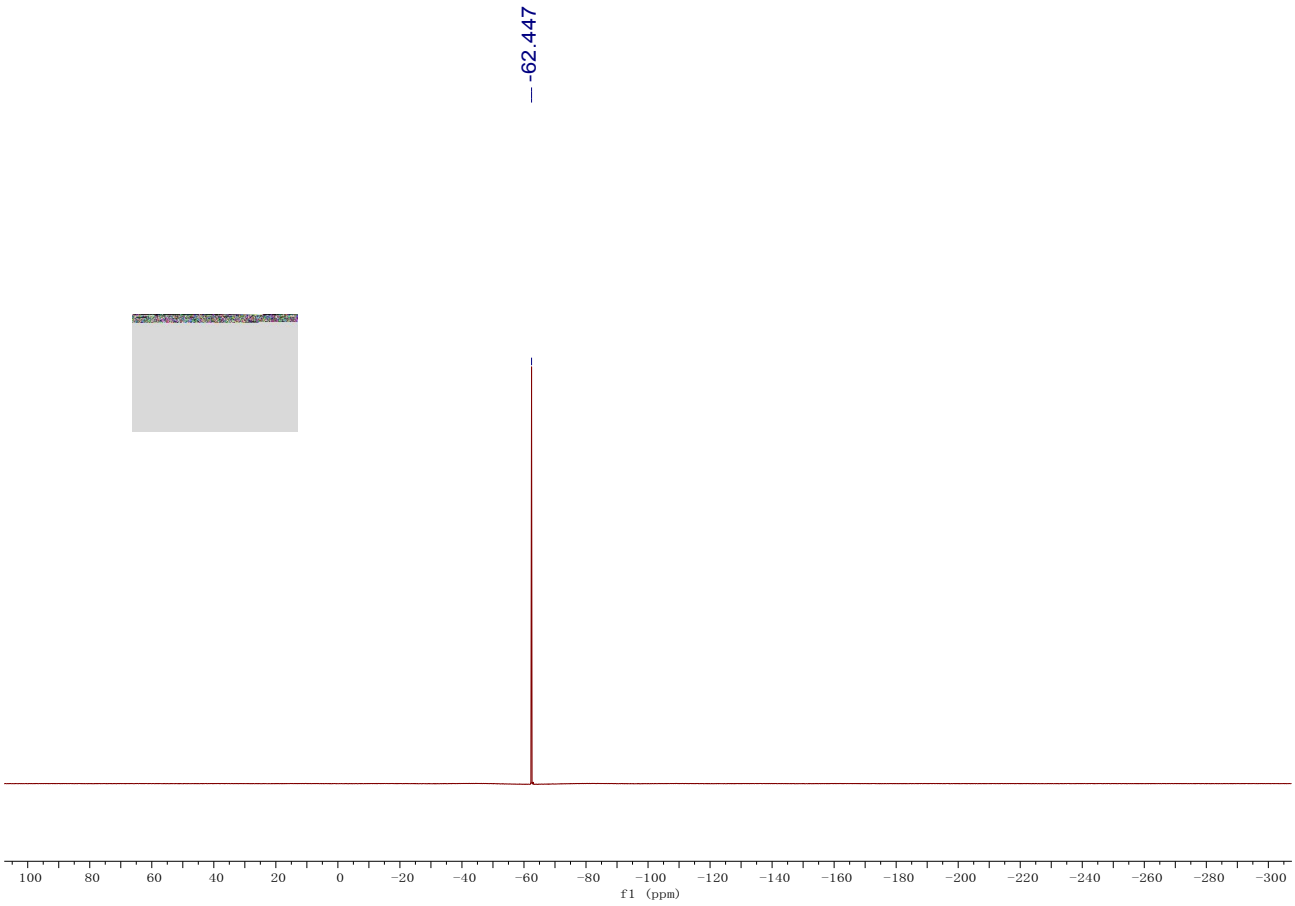


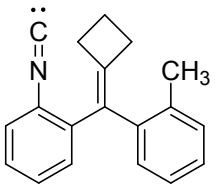




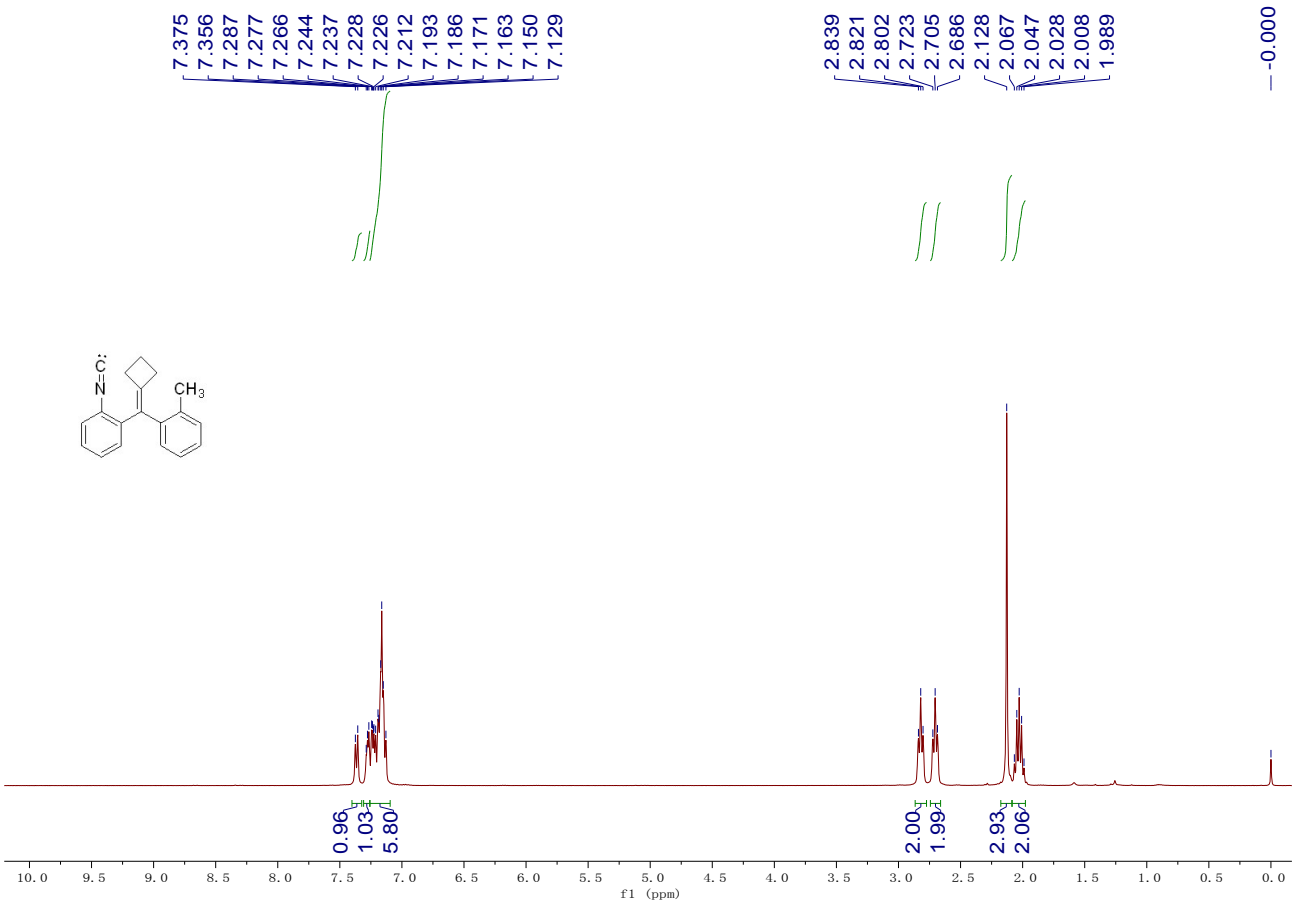
Compound **1e**: Yield: 1.661 g; A brown solid; m.p. 71-73 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.08-2.16 (m, 2H), 2.68 (t, J = 7.2 Hz, 2H), 3.14 (t, J = 7.2 Hz, 2H), 7.20-7.25 (m, 2H), 7.28 (d, J = 7.2 Hz, 1H), 7.34 (t, J = 7.4 Hz, 1H), 7.42 (t, J = 7.8 Hz, 2H), 7.52 (d, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.2, 31.7, 32.8, 124.2 (q, $J_{C\text{-}F}$ = 270.4 Hz), 125.1 (q, $J_{C\text{-}F}$ = 3.6 Hz), 127.3, 127.5, 128.20 (q, $J_{C\text{-}F}$ = 32.2 Hz), 128.22, 129.5, 131.2, 137.1, 142.1, 147.4, 165.8; ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$): δ -62.4 (s); IR (CH_3COCH_3): ν 2988, 2957, 2914, 2121, 1713, 1615, 1483, 1444, 1409, 1361, 1323, 1221, 1164, 1118, 1067, 1015, 906, 843, 760, 673 cm^{-1}; MS (ESI) m/z 314.1 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{19}H_{15}NF_3$: 314.11511, Found: 314.11559.

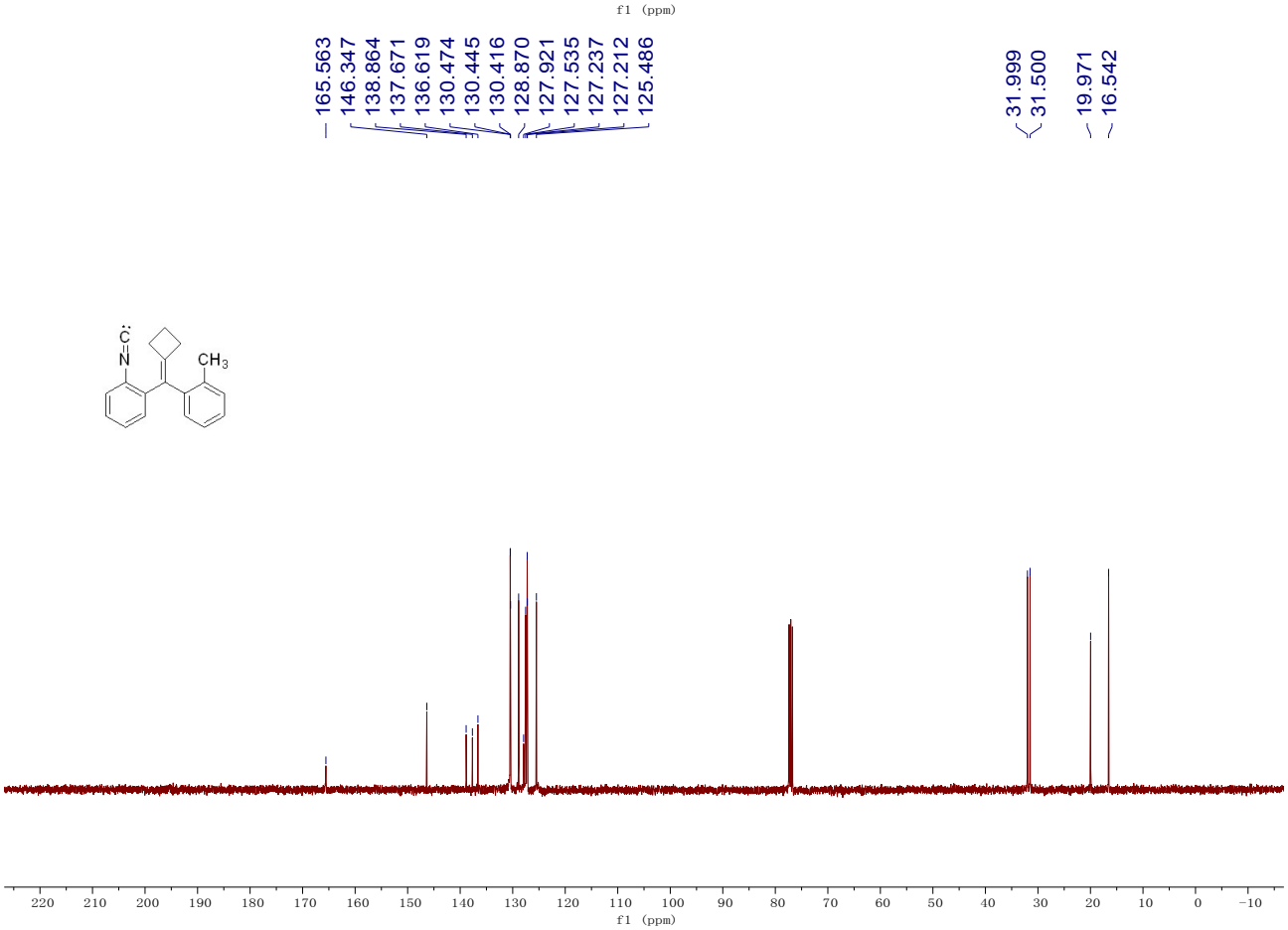

7.533
7.513
7.438
7.418
7.399
7.360
7.341
7.323
7.289
7.271
7.245
7.220
7.200
3.153
3.135
3.117
2.696
2.678
2.660
2.161
2.142
2.123
2.103
2.084
0.000
CF3
1.83
1.84
1.00
0.95
1.98
2.00
2.00
2.03
f1 (ppm)
165.761
147.384
142.096
137.077
131.232
129.535
128.679
128.356
128.218
128.034
127.715
127.507
127.281
125.550
125.186
125.150
125.112
125.075
122.846
120.144
32.779
31.707
17.207
CF3
f1 (ppm)

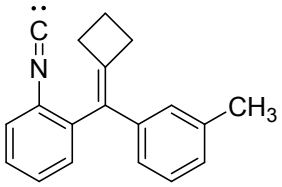




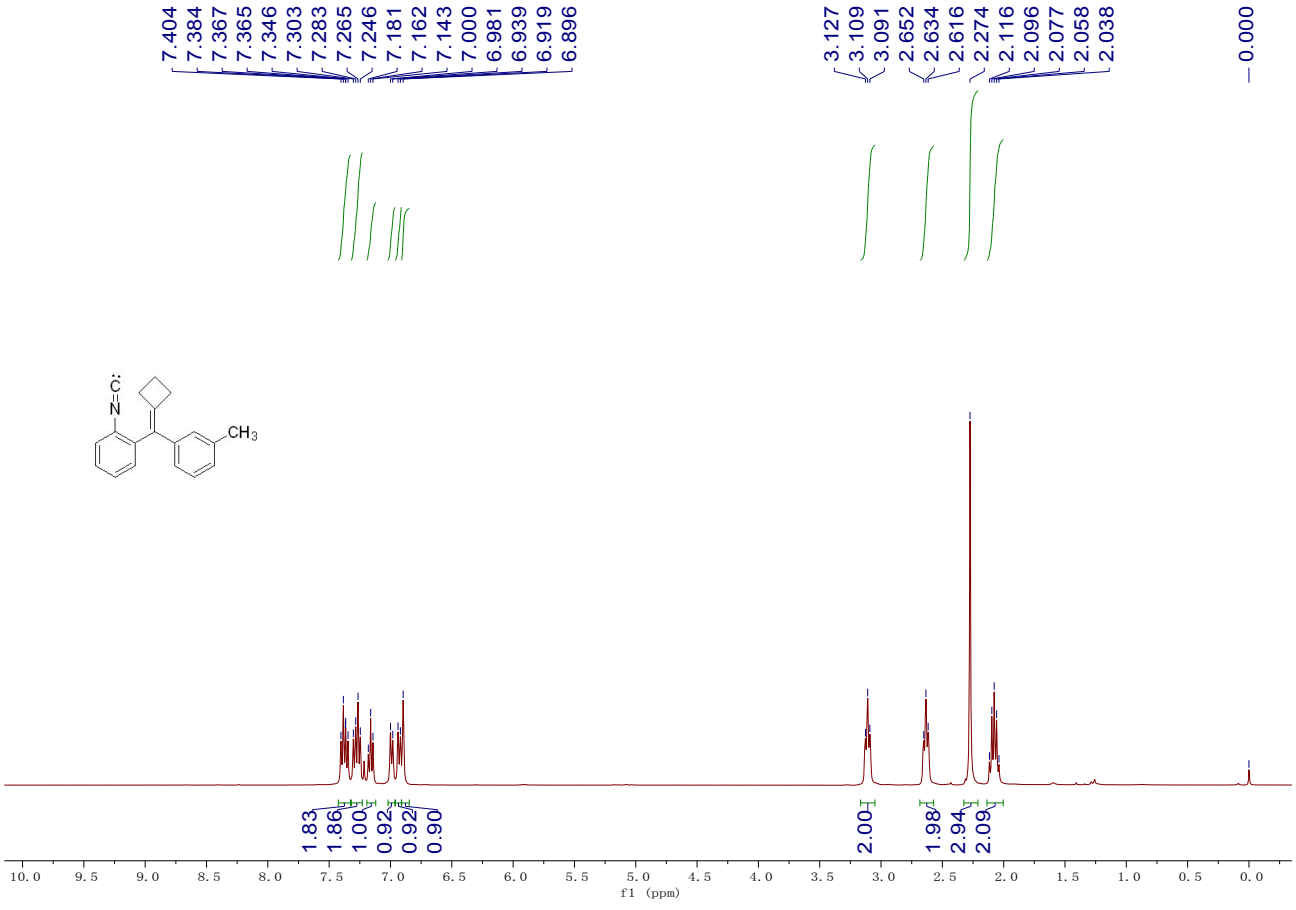
Compound **1f**: Yield: 1.289 g; A brown solid; m.p. 73-75 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.99-2.07 (m, 2H), 2.13 (s, 3H), 2.70 (t, *J* = 7.4 Hz, 2H), 2.82 (t, *J* = 7.4 Hz, 2H), 7.13-7.24 (m, 6H), 7.27-7.29 (s, 1H), 7.37 (d *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.5, 20.0, 31.5, 32.0, 125.5, 127.21, 127.24, 127.5, 127.9, 128.9, 130.42, 130.45, 130.5, 136.6, 137.7, 138.9, 146.3, 165.6; IR (CH_3COCH_3): ν 2985, 2952, 2914, 2119, 1713, 1671, 1483, 1440, 1360, 1219, 1094, 1039, 974, 949, 905, 753, 734 cm^{-1}; MS (ESI) m/z 260.1 $(M+H)^{+}$; HRMS (ESI) Calcd. for $C_{19}H_{18}N$: 260.14338, Found: 260.14337.

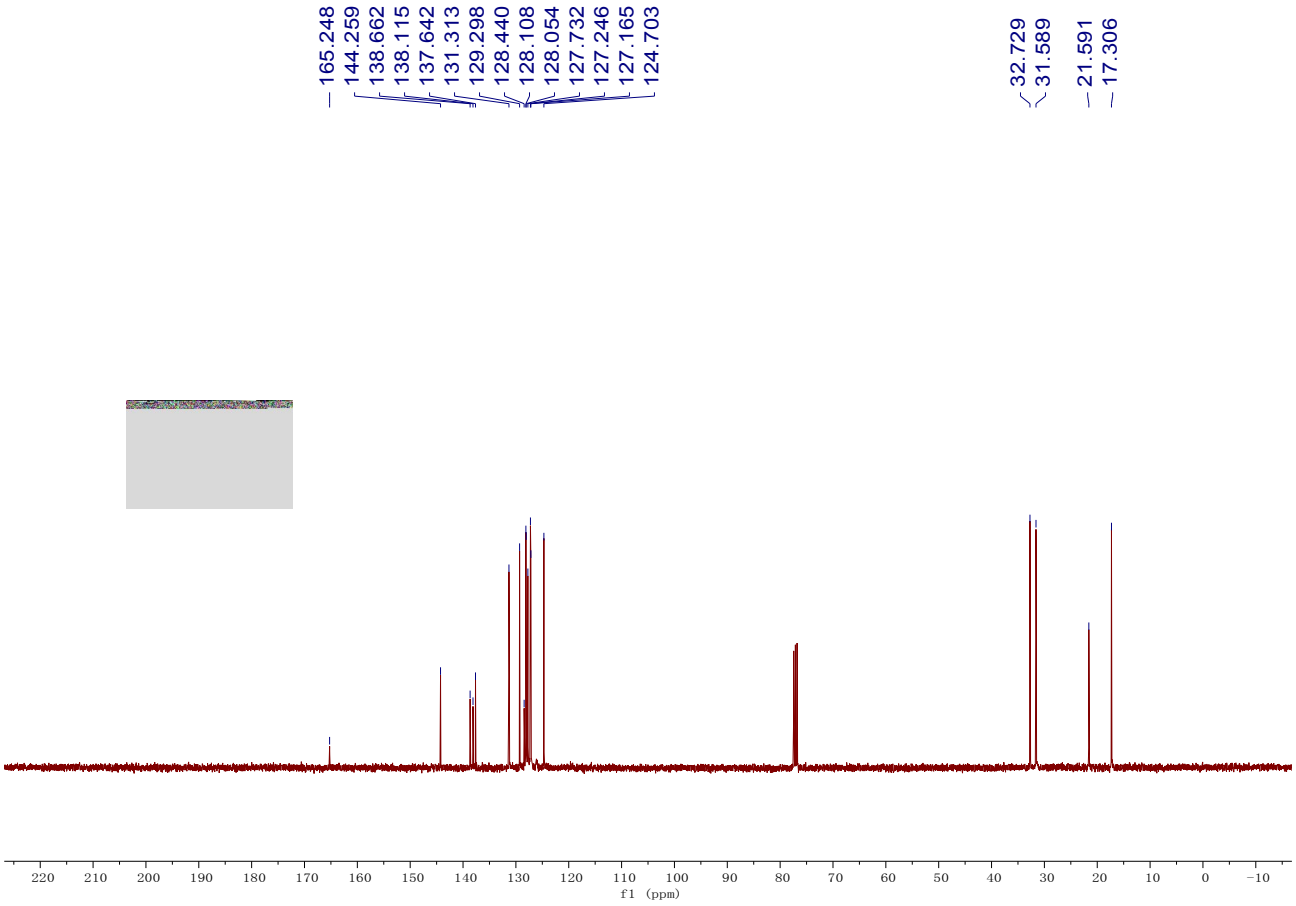

7.375
7.356
7.287
7.277
7.266
7.244
7.237
7.228
7.226
7.212
7.193
7.186
7.171
7.163
7.150
7.129
2.839
2.821
2.802
2.723
2.705
2.686
2.128
2.067
2.047
2.028
2.008
1.989
-0.000
CH3
0.96
1.03
5.80
2.00
1.99
2.93
2.06
f1 (ppm)

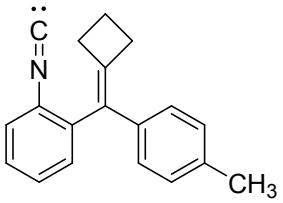

165.563
146.347
138.864
137.671
136.619
130.474
130.445
130.416
128.870
127.921
127.535
127.237
127.212
125.486
31.999
31.500
19.971
16.542
CH3
f1 (ppm)



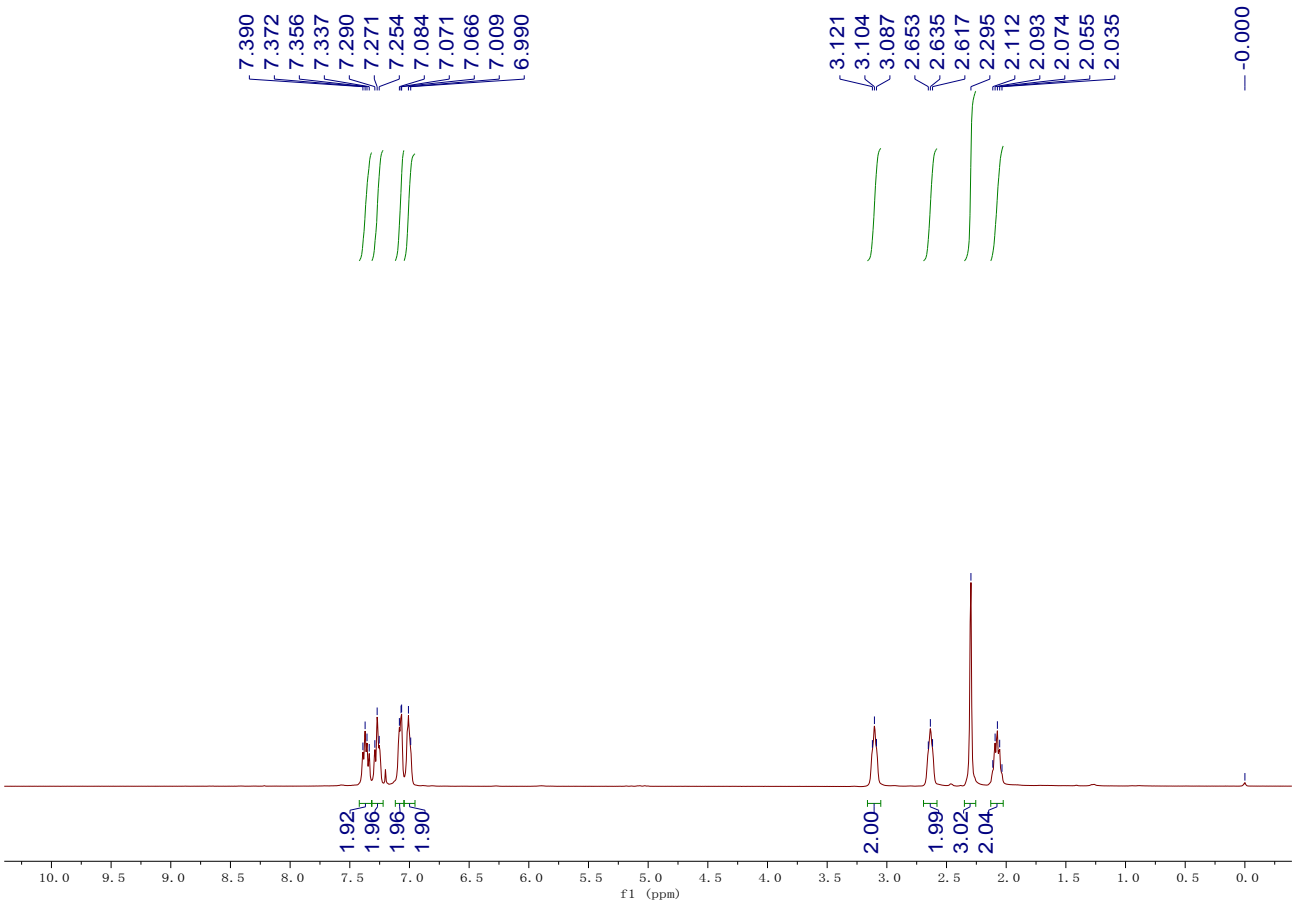
Compound **1g**: Yield: 2.193 g; Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.04-2.12 (m, 2H), 2.27 (s, 3H), 2.63 (t, *J* = 7.2 Hz, 2H), 3.11 (t, *J* = 7.2 Hz, 2H), 6.90 (s, 1H), 6.93 (d, *J* = 8.0 Hz, 1H) 6.99 (d, *J* = 7.6 Hz, 1H), 7.16 (t, *J* = 7.6 Hz, 1H), 7.25-7.30 (m, 2H), 7.35-7.40 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.3, 21.6, 31.6, 32.7, 124.7, 127.17, 127.25, 127.7, 128.05, 128.11, 128.4, 129.3, 131.3, 137.6, 138.1, 138.7, 144.3, 165.2; IR (CH_3COCH_3): ν 2982, 2951, 2912, 2120, 1702, 1601, 1483, 1442, 1410, 1309, 1185, 1095, 1037, 950, 878, 786, 758, 699, 660 cm^{-1}; MS (ESI) m/z 260.1 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{19}H_{18}N$: 260.14338, Found: 260.14382.

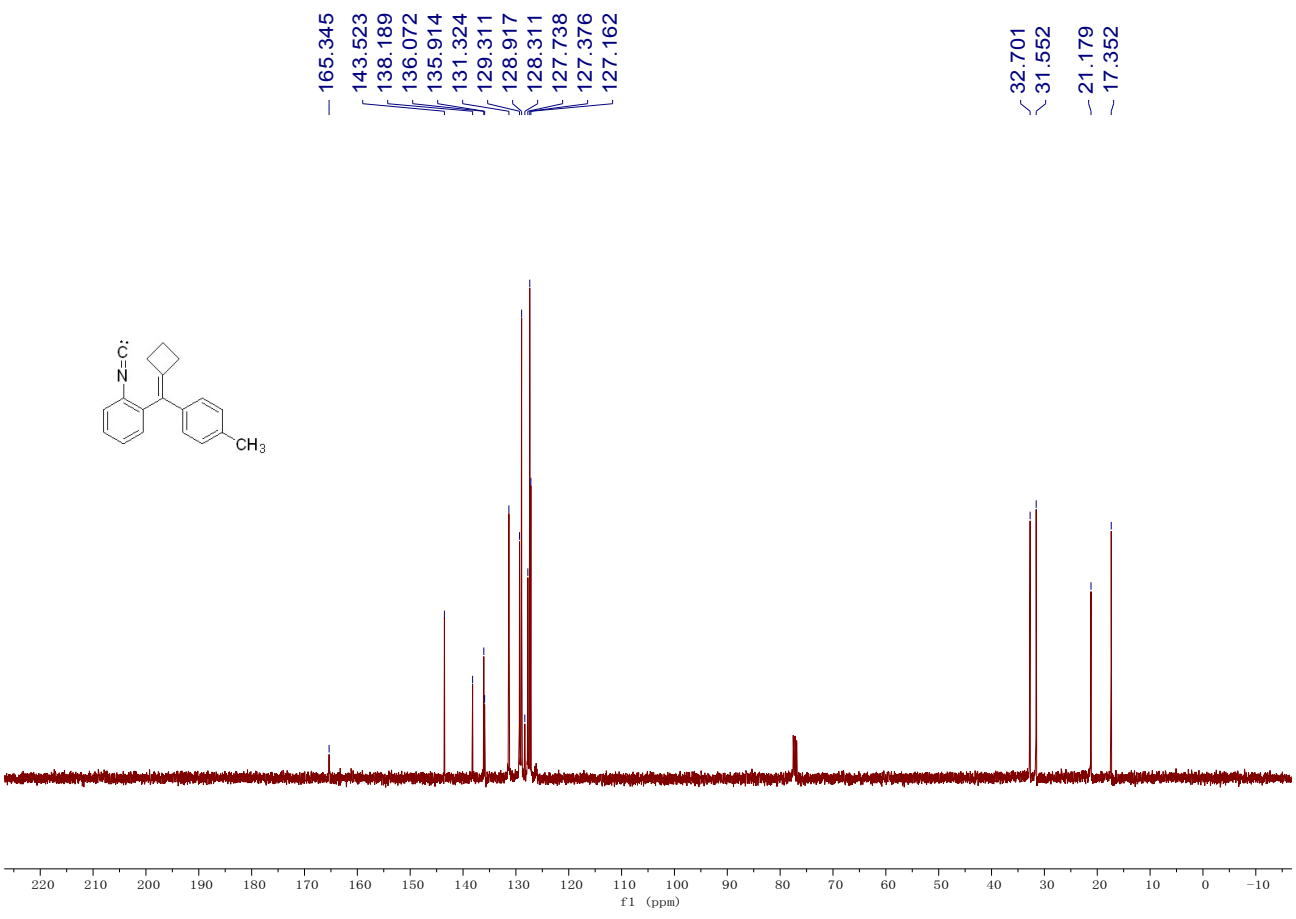


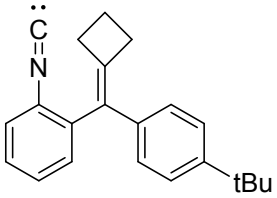




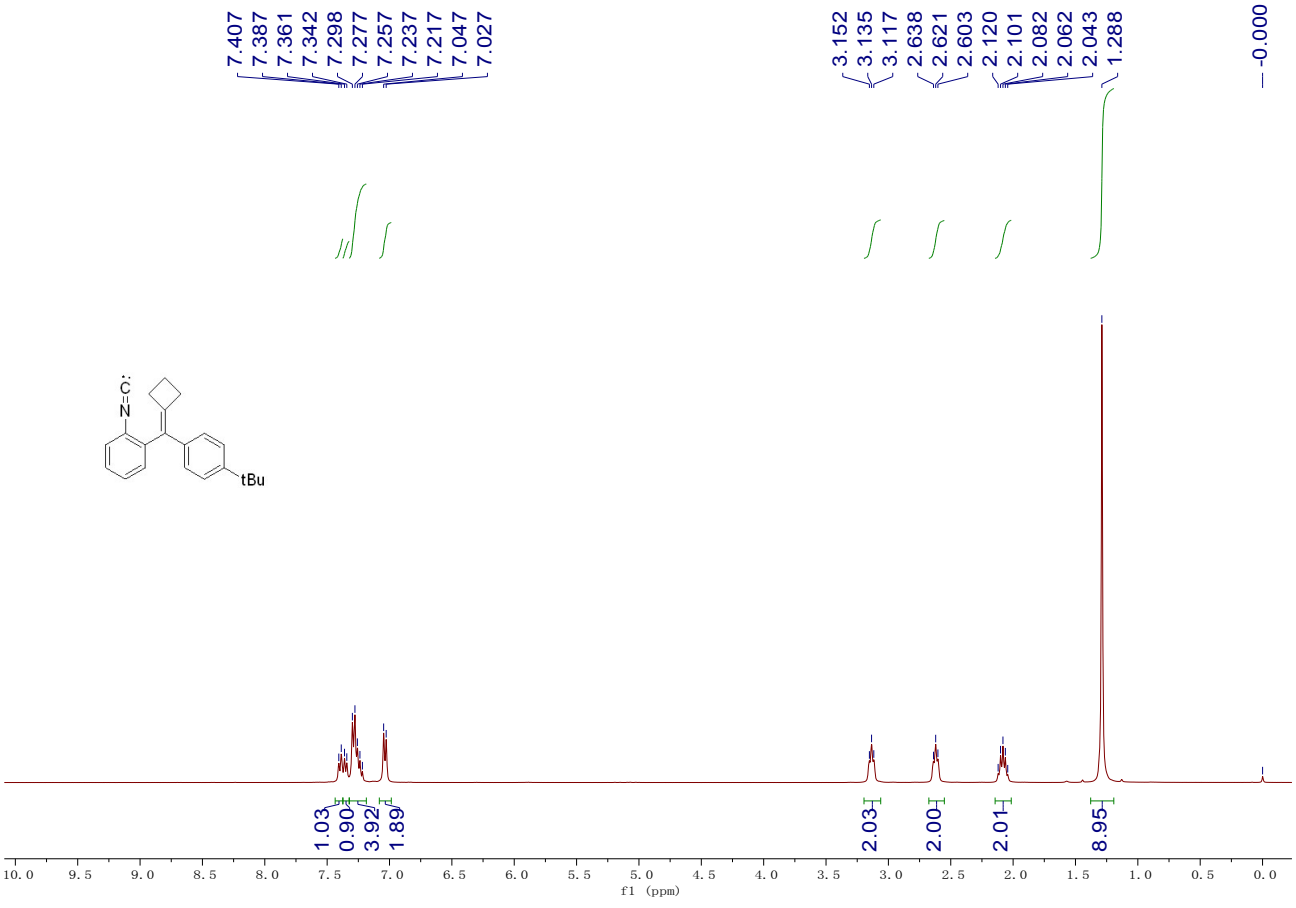
Compound **1h**: Yield: 1.670 g; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.04-2.11 (m, 2H), 2.30 (s, 3H), 2.64 (t, *J* = 7.2 Hz, 2H), 3.10 (t, *J* = 7.2 Hz, 2H), 7.00 (d, *J* = 8.6 Hz, 2H), 7.07-7.08 (m, 2H), 7.27 (t, *J* = 7.2 Hz, 2H), 7.34-7.39 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.4, 21.2, 31.6, 32.7, 127.2, 127.4, 127.7, 128.3, 128.9, 129.3, 131.3, 135.9, 136.1, 138.2, 143.5, 165.3; IR (CH_3COCH_3): ν 2984, 2952, 2912, 2120, 1713, 1511, 1482, 1442, 1411, 1360, 1219, 1096, 1037, 905, 818, 759, 717 cm^{-1}; MS (ESI) m/z 260.1 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{19}H_{18}N$: 260.14338, Found: 260.14363.

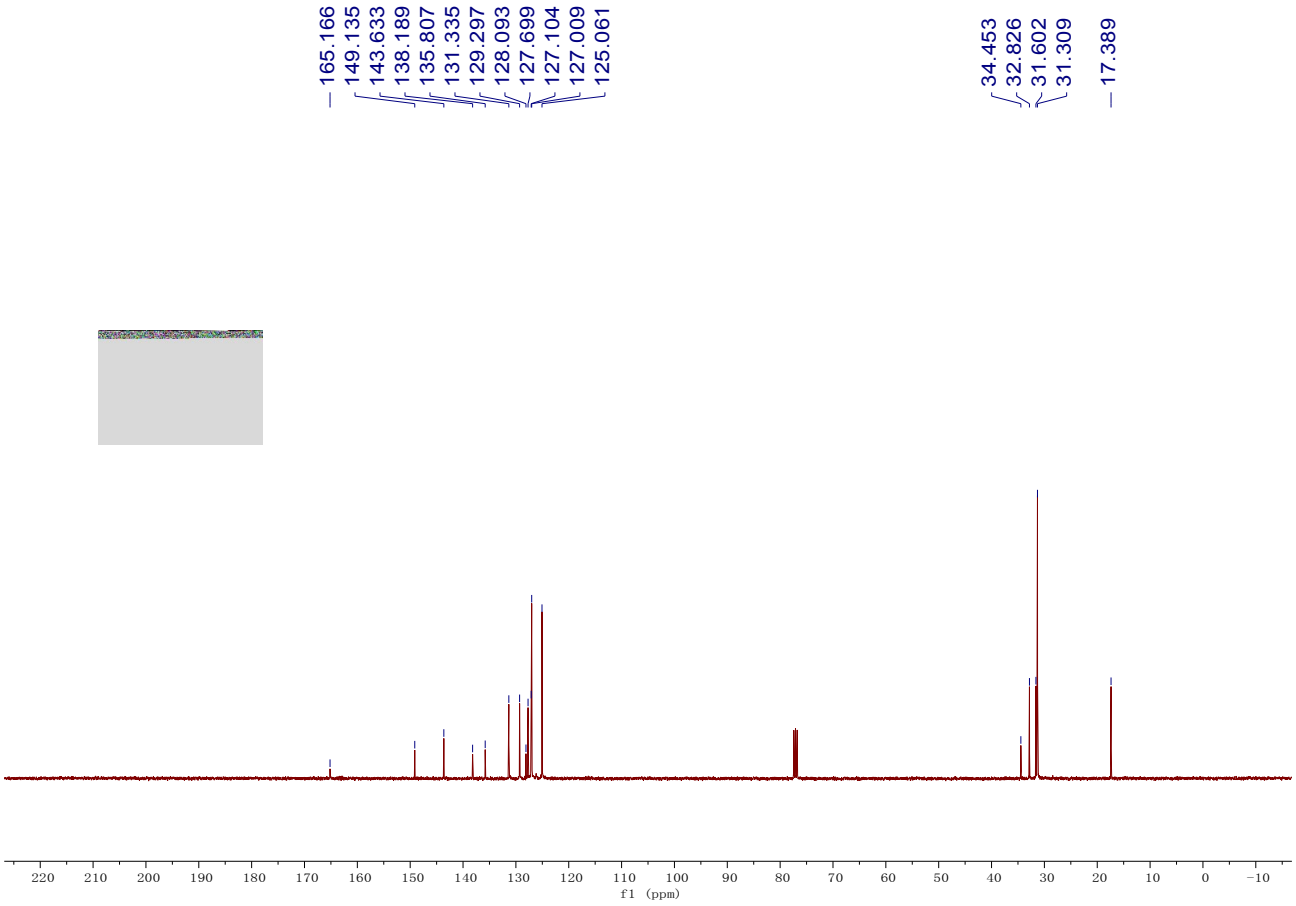

7.390
7.372
7.356
7.337
7.290
7.271
7.254
7.084
7.071
7.066
7.009
6.990
3.121
3.104
3.087
2.653
2.635
2.617
2.295
2.112
2.093
2.074
2.055
2.035
-0.000
1.92
1.96
1.96
1.90
2.00
1.99
3.02
2.04
f1 (ppm)

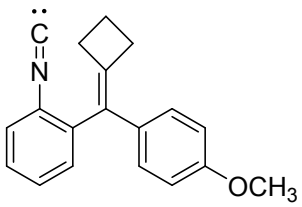

165.345
143.523
138.189
136.072
135.914
131.324
129.311
128.917
128.311
127.738
127.376
127.162
32.701
31.552
21.179
17.352
N
CH3
f1 (ppm)



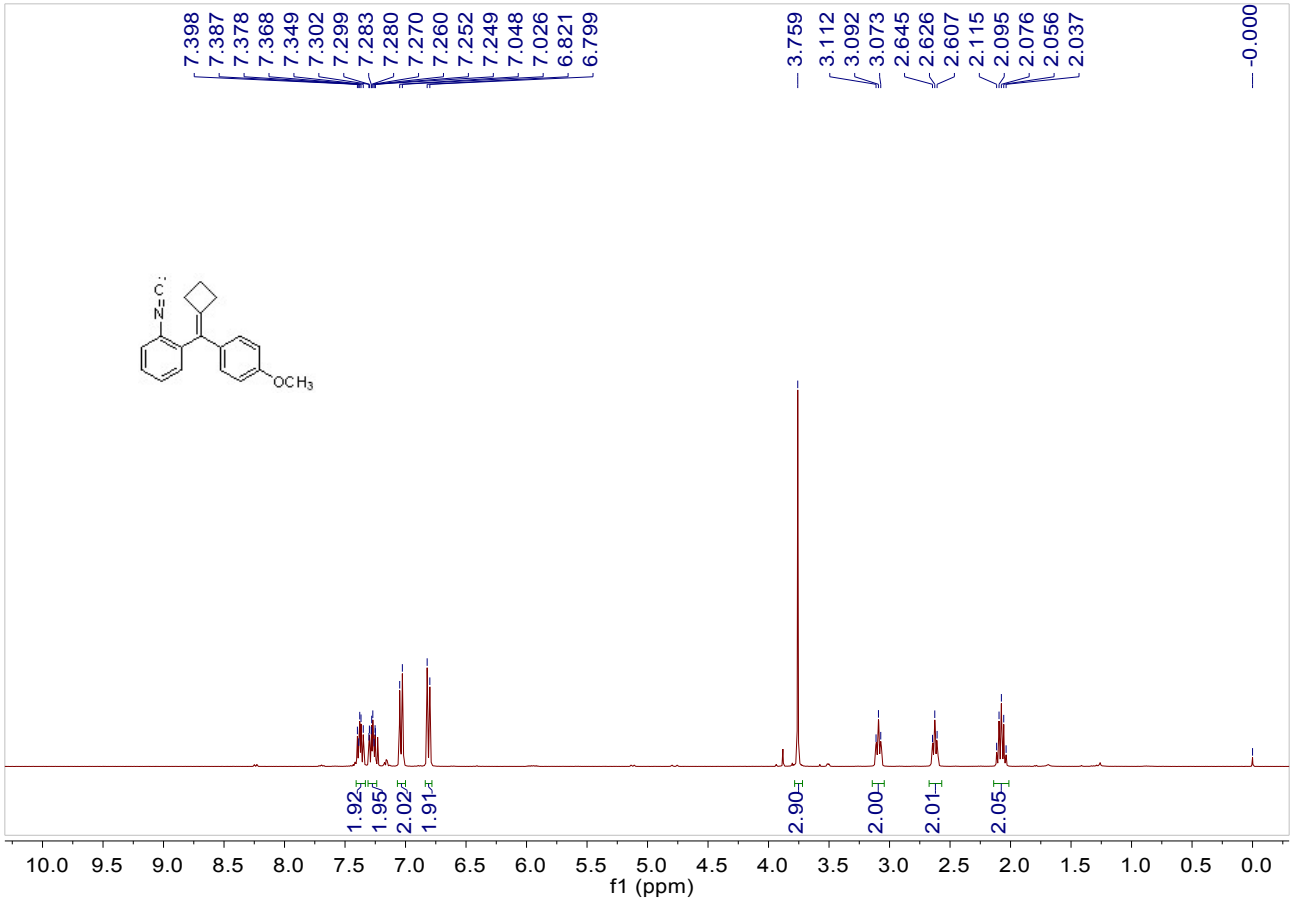
Compound **1i**: Yield: 2.867 g; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.29 (s, 9H), 2.04-2.12 (m, 2H), 2.62 (t, *J* = 7.0 Hz, 2H), 3.13 (t, *J* = 7.0 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 7.22-7.30 (m, 4H), 7.35 (d, *J* = 7.6 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.4, 31.3, 31.6, 32.8, 34.5, 125.1, 127.0, 127.1, 127.7, 128.1, 129.3, 131.3, 135.8, 138.2, 143.6, 149.1, 165.2; IR (CH_3COCH_3): ν 2960, 2901, 2868, 2121, 1713, 1514, 1482, 1462, 1442, 1408, 1361, 1270, 1219, 1095, 1017, 906, 836, 761 cm^{-1}; MS (ESI) m/z 302.2 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{22}H_{24}N$: 302.19033, Found: 302.19009.

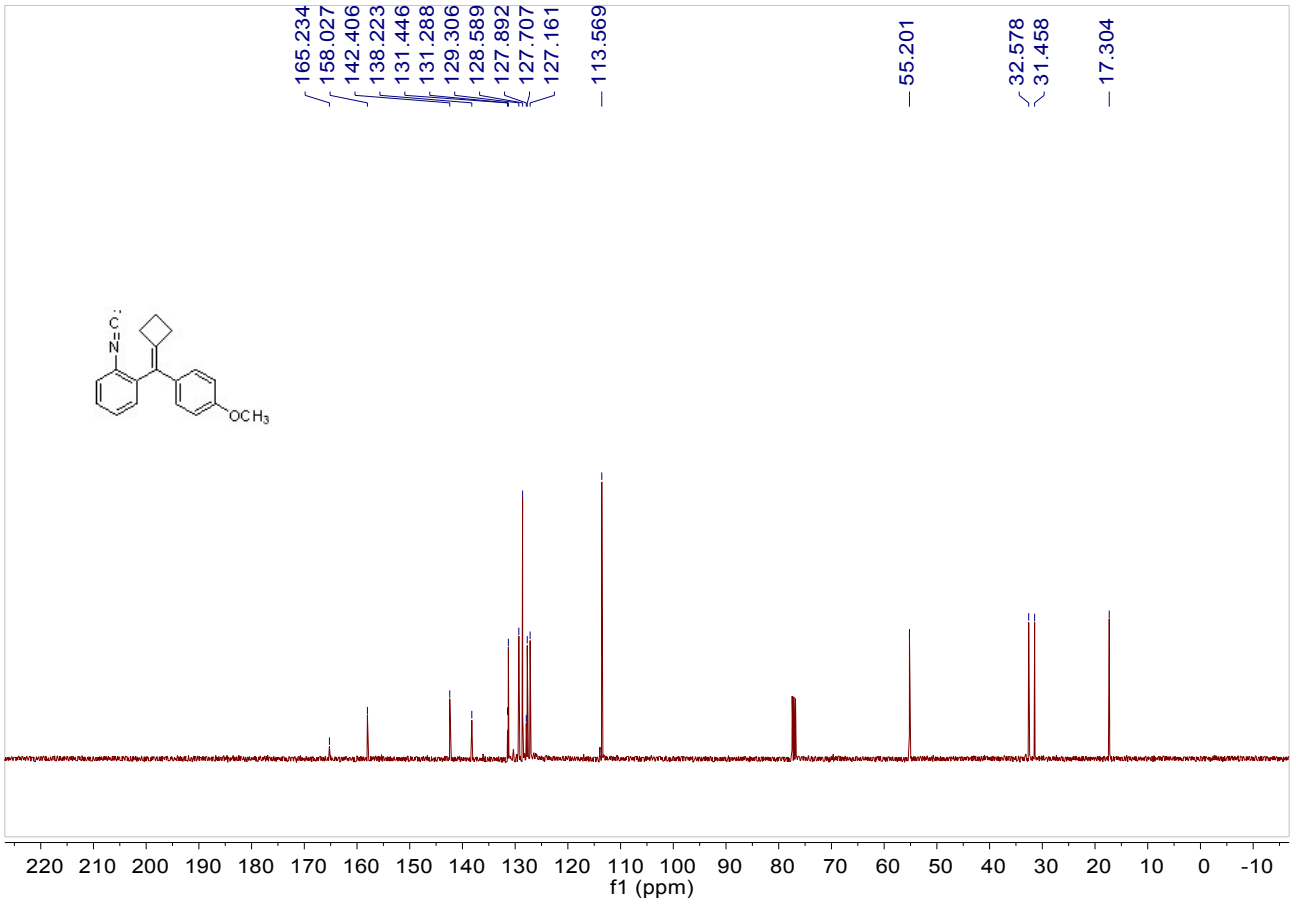


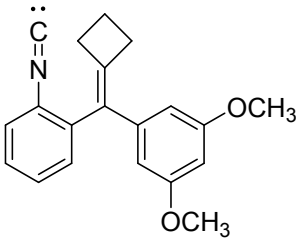




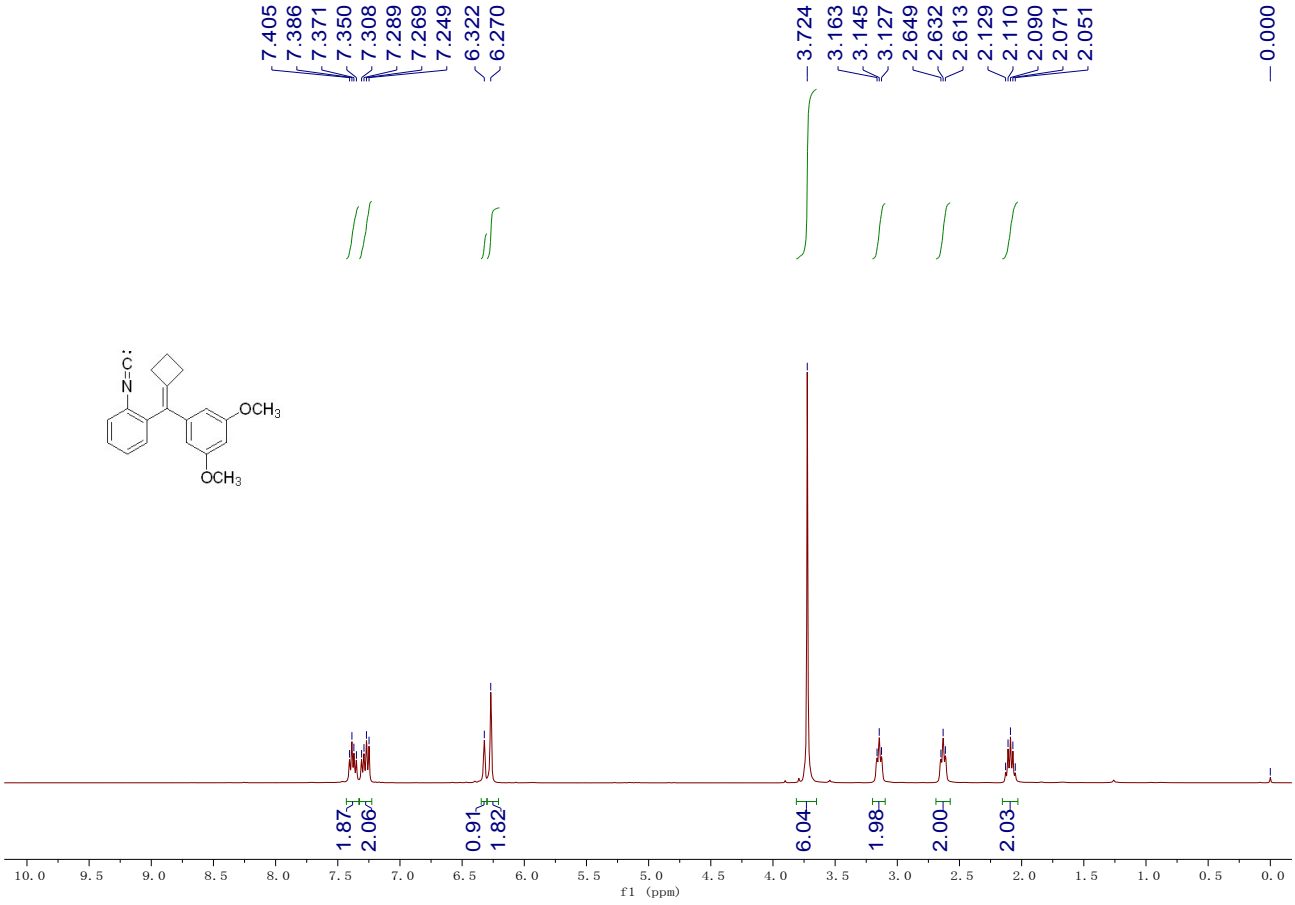
Compound **1j**: Yield: 1.975 g; A brown solid; m.p. 77-79 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.04-2.12 (m, 2H), 2.63 (t, *J* = 7.6 Hz, 2H), 3.09 (t, *J* = 7.8 Hz, 2H), 3.76 (s, 3H), 6.81 (d, *J* = 8.8 Hz, 2H), 7.04 (d, *J* = 8.8 Hz, 2H), 7.25-7.30 (m, 2H), 7.35-7.40 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.3, 31.5, 32.6, 55.2, 113.6, 127.2, 127.7, 127.9, 128.6, 129.3, 131.3, 131.4, 138.2, 142.4, 158.0, 165.2; IR (CH_3COCH_3): ν 2953, 2903, 2835, 2120, 1712, 1606, 1509, 1482, 1463, 1442, 1360, 1320, 1247, 1220, 1180, 1111, 1033, 905, 830, 789, 759 cm^{-1}; MS (ESI) m/z 276.1 $(M+H)^{+}$; HRMS (ESI) Calcd. for $C_{19}H_{18}NO$: 276.1383, Found: 276.1385.

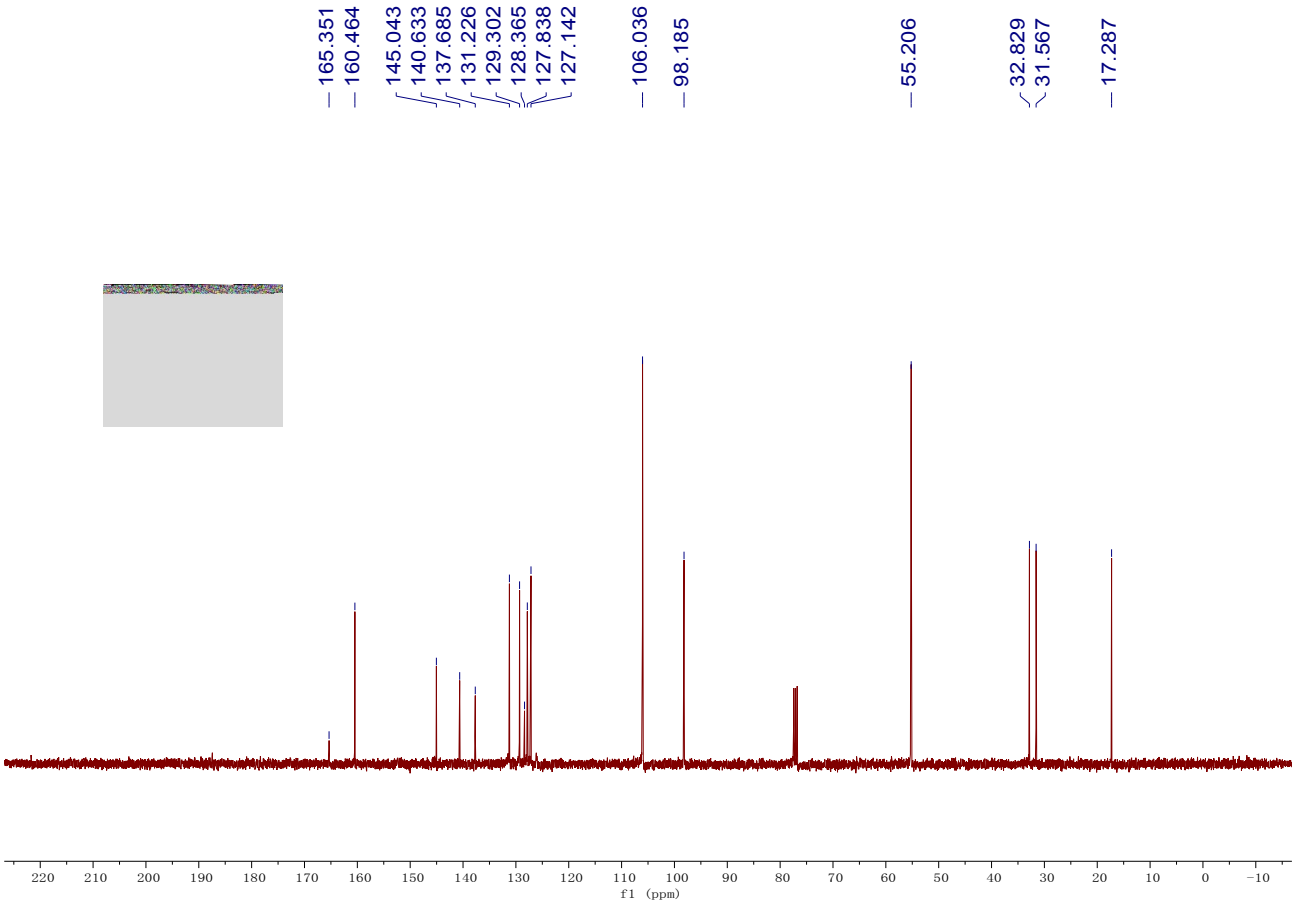

7.398
7.387
7.378
7.368
7.349
7.302
7.299
7.283
7.280
7.270
7.260
7.252
7.249
7.048
7.026
6.821
6.799
3.759
3.112
3.092
3.073
2.645
2.626
2.607
2.115
2.095
2.076
2.056
2.037
-0.000
1.92
1.95
2.02
1.91
2.90
2.00
2.01
2.05
OCH3
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

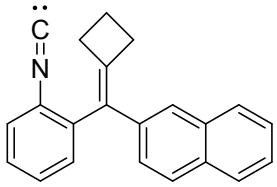

165.234
158.027
142.406
138.223
131.446
131.288
129.306
128.589
127.892
127.707
127.161
113.569
55.201
32.578
31.458
17.304
OCH3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



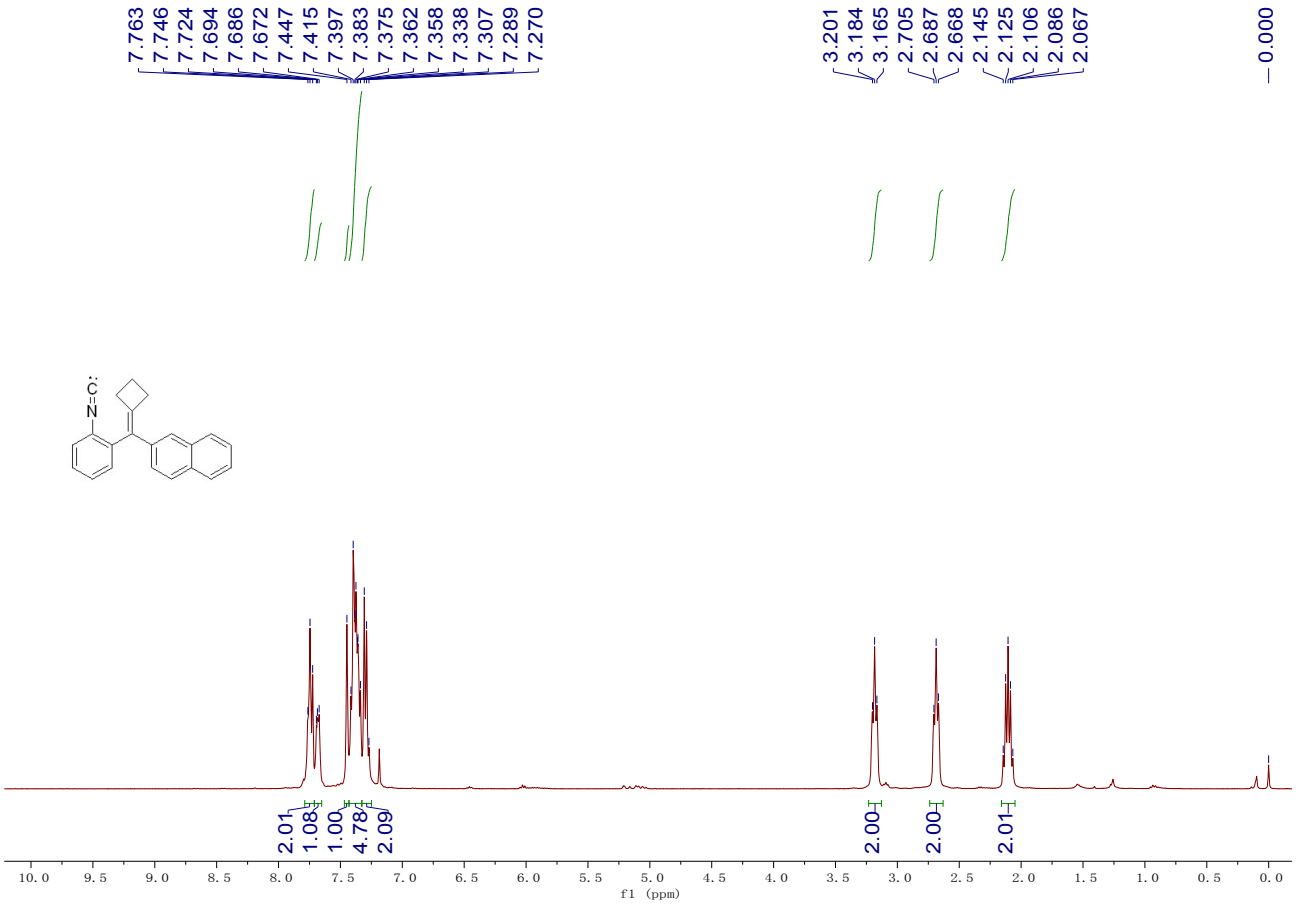
Compound **1k**: Yield: 1.670 g; A brown solid; m.p. 59-61 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.05-2.13 (m, 2H), 2.63 (t, J = 7.2 Hz, 2H), 3.15 (t, J = 7.2 Hz, 2H), 3.72 (s, 6H), 6.27 (s, 2H), 6.32 (s, 1H), 7.25-7.31 (m, 2H), 7.35-7.41 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.3, 31.6, 32.8, 55.2, 98.2, 106.0, 127.1, 127.8, 128.4, 129.3, 131.2, 137.7, 140.6, 145.0, 160.5, 165.4; IR (CH_3COCH_3): ν 3000, 2956, 2838, 2122, 1711, 1589, 1454, 1422, 1358, 1334, 1220, 1203, 1151, 1093, 1060, 986, 929, 833, 759, 693 cm^{-1}; MS (ESI) m/z 306.1 $(M+H)^{+}$; HRMS (ESI) Calcd. for $C_{20}H_{20}NO_2$: 306.14886, Found: 306.14815.

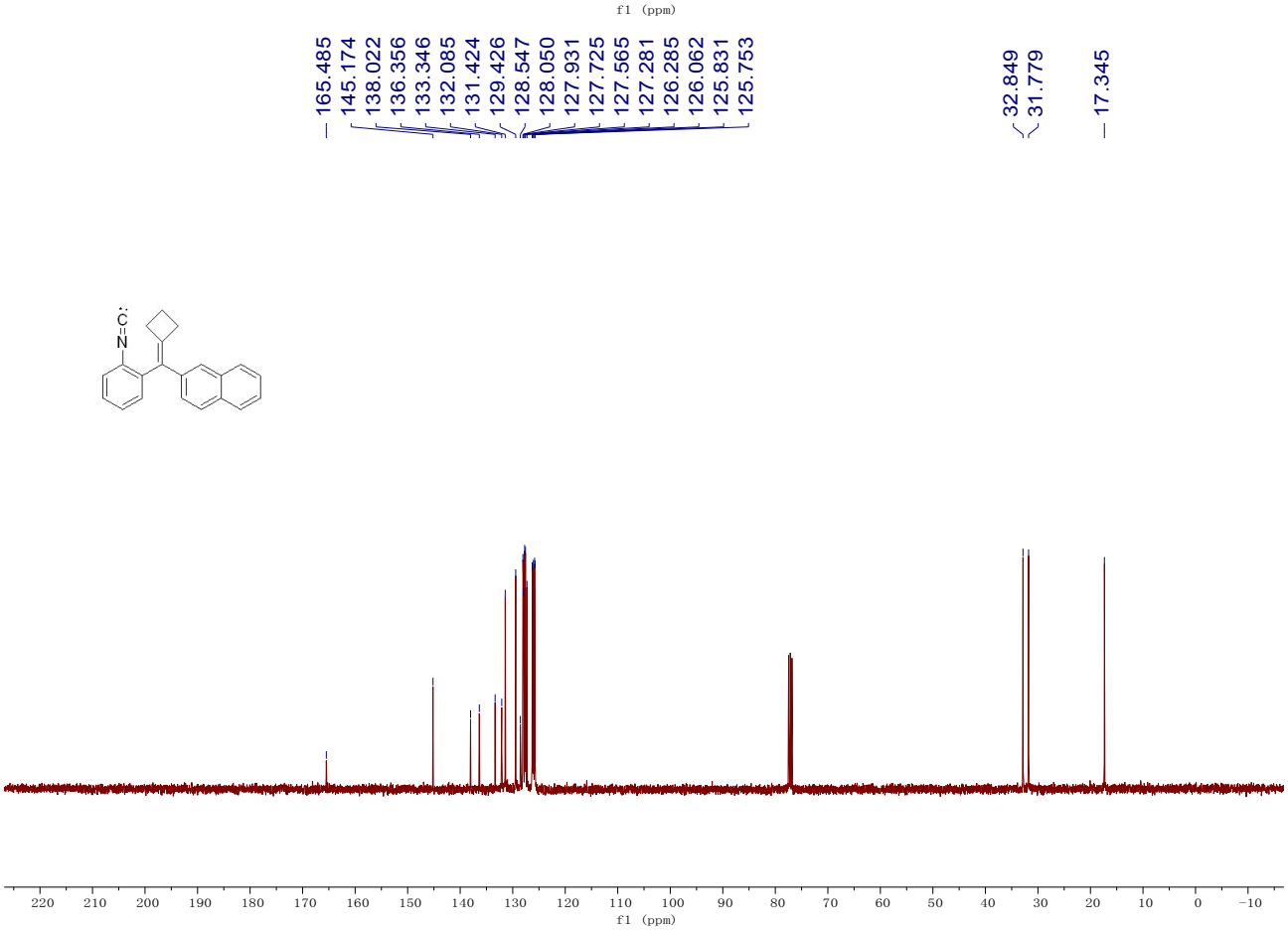


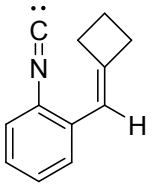




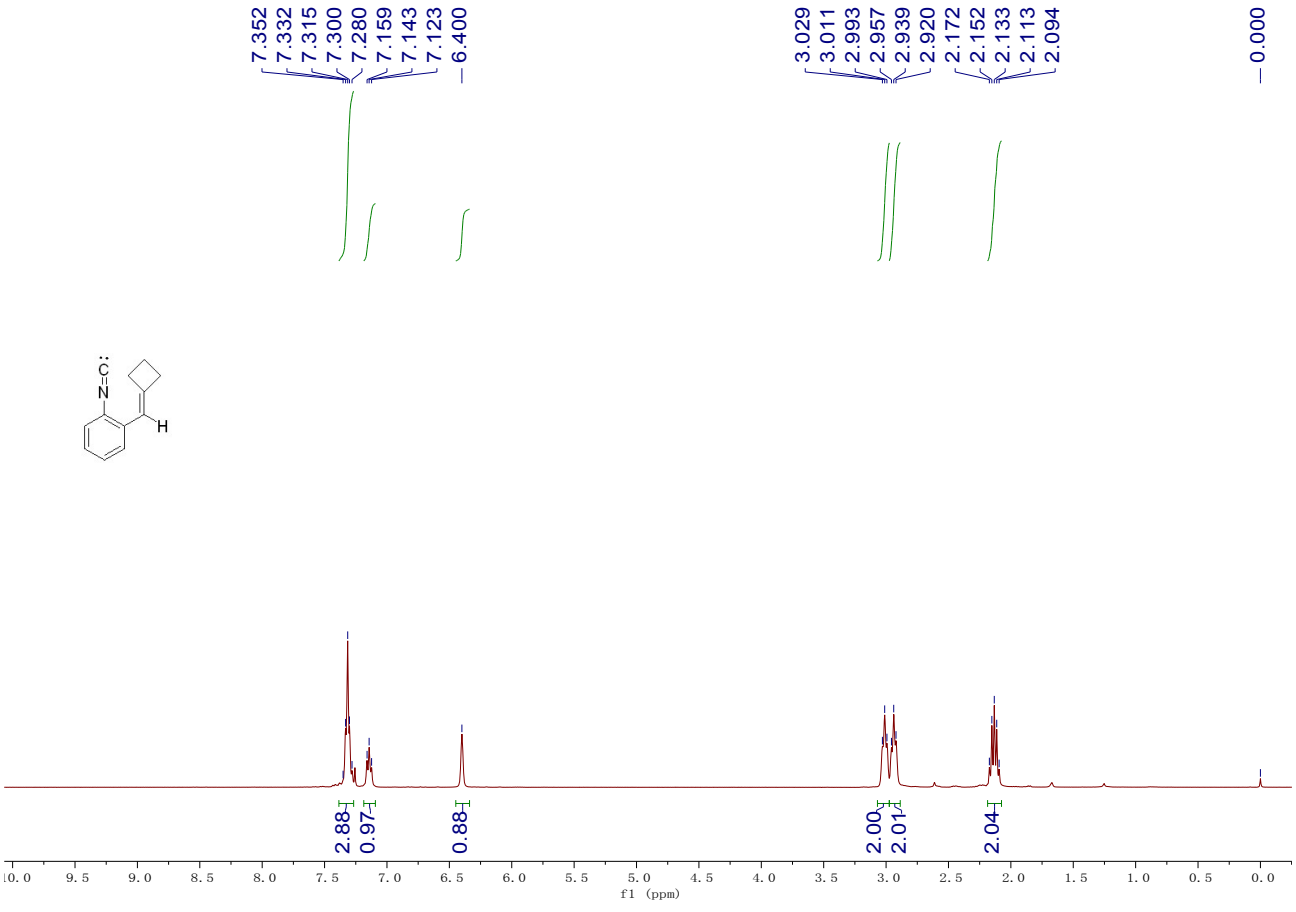
Compound **1l**: Yield: 3.147 g; A brown solid; m.p. 113-115 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.07-2.15 (m, 2H), 2.69 (t, *J* = 7.4 Hz, 2H), 3.18 (t, *J* = 7.2 Hz, 2H), 7.27-7.31 (m, 2H), 7.34-7.42 (m, 5H), 7.45 (s, 1H), 7.67-7.69 (m, 1H), 7.72-7.76 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.3, 31.8, 32.8, 125.8, 125.8, 126.1, 126.3, 127.3, 127.6, 127.7, 127.9, 128.1, 128.5, 129.4, 131.4, 132.1, 133.3, 136.4, 138.0, 145.2, 165.5; IR (CH_3COCH_3): ν 3055, 2985, 2955, 2909, 2120, 1712, 1597, 1505, 1483, 1442, 1360, 1220, 1160, 1095, 1036, 951, 894, 858, 818, 674 cm^{-1}; MS (ESI) m/z 296.1 $(M+H)^{+}$; HRMS (ESI) Calcd. for $C_{22}H_{18}N$: 296.14338, Found: 296.14332.

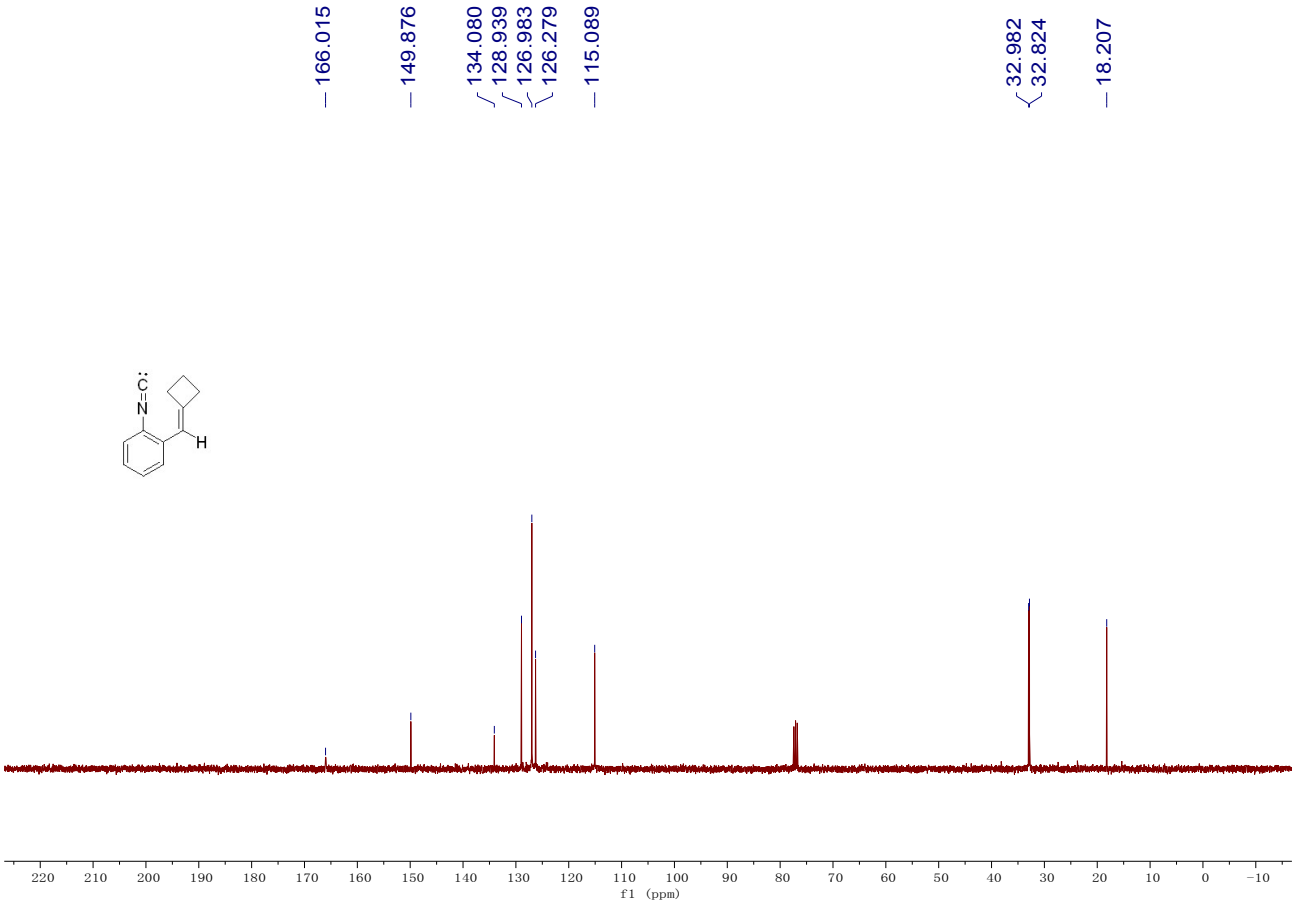

7.763
7.746
7.724
7.694
7.686
7.672
7.447
7.415
7.397
7.383
7.375
7.362
7.358
7.338
7.307
7.289
7.270
3.201
3.184
3.165
2.705
2.687
2.668
2.145
2.125
2.106
2.086
2.067
0.000
2.01
1.08
1.00
4.78
2.09
2.00
2.00
2.01
f1 (ppm)

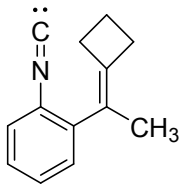

165.485
145.174
138.022
136.356
133.346
132.085
131.424
129.426
128.547
128.050
127.931
127.725
127.565
127.281
126.285
126.062
125.831
125.753
32.849
31.779
17.345
f1 (ppm)



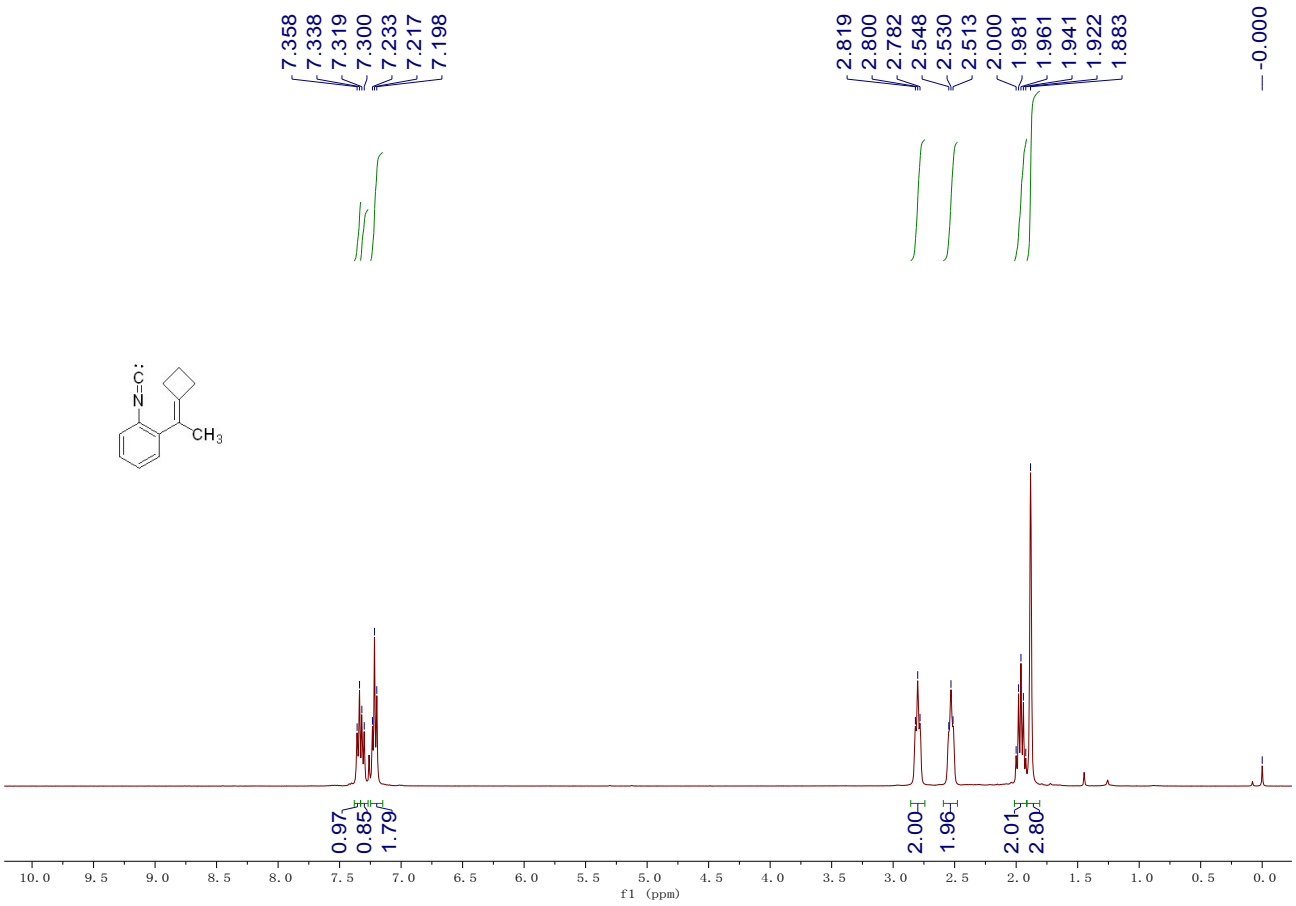
Compound **1m**: Yield: 2.146 g; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.09-2.17 (m, 2H), 2.94 (t, *J* = 7.4 Hz, 2H), 3.01 (t, *J* = 7.2 Hz, 2H), 6.40 (s, 1H), 7.14 (t, *J* = 7.2 Hz, 1H), 7.28-7.35 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 18.2, 32.8, 33.0, 115.1, 126.3, 127.0, 128.9, 134.1, 149.9, 166.0; IR (CH_3COCH_3): ν 2982, 2954, 2909, 2117, 1713, 1668, 1595, 1481, 1447, 1360, 1289, 1220, 1176, 1109, 1040, 946, 873, 853, 755 cm^{-1}; MS (DART) m/z 170.1 $(M+H)^+$; HRMS (DART) Calcd. for $C_{12}H_{12}N$: 170.0964, Found: 170.0964.

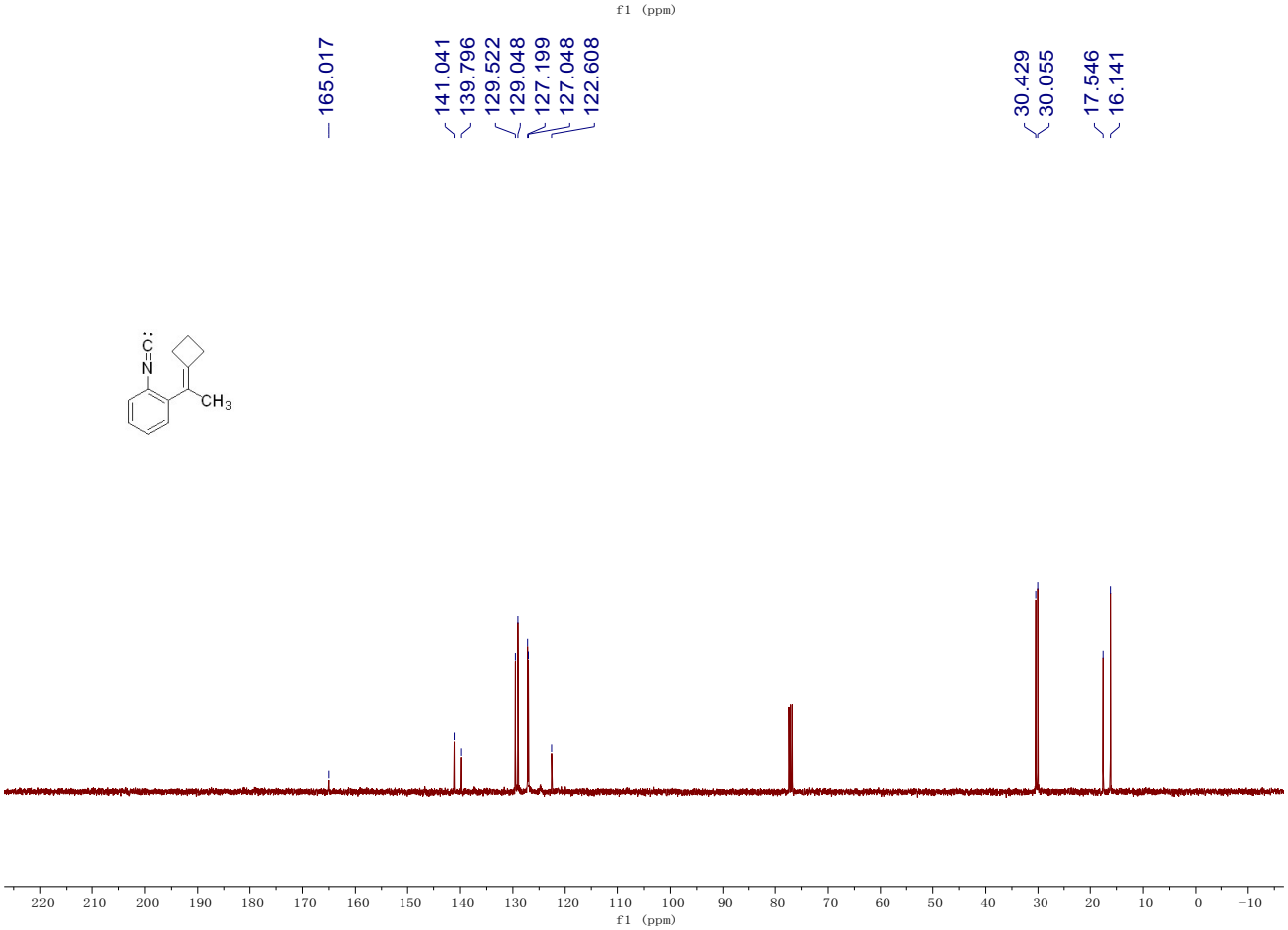


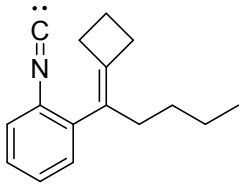




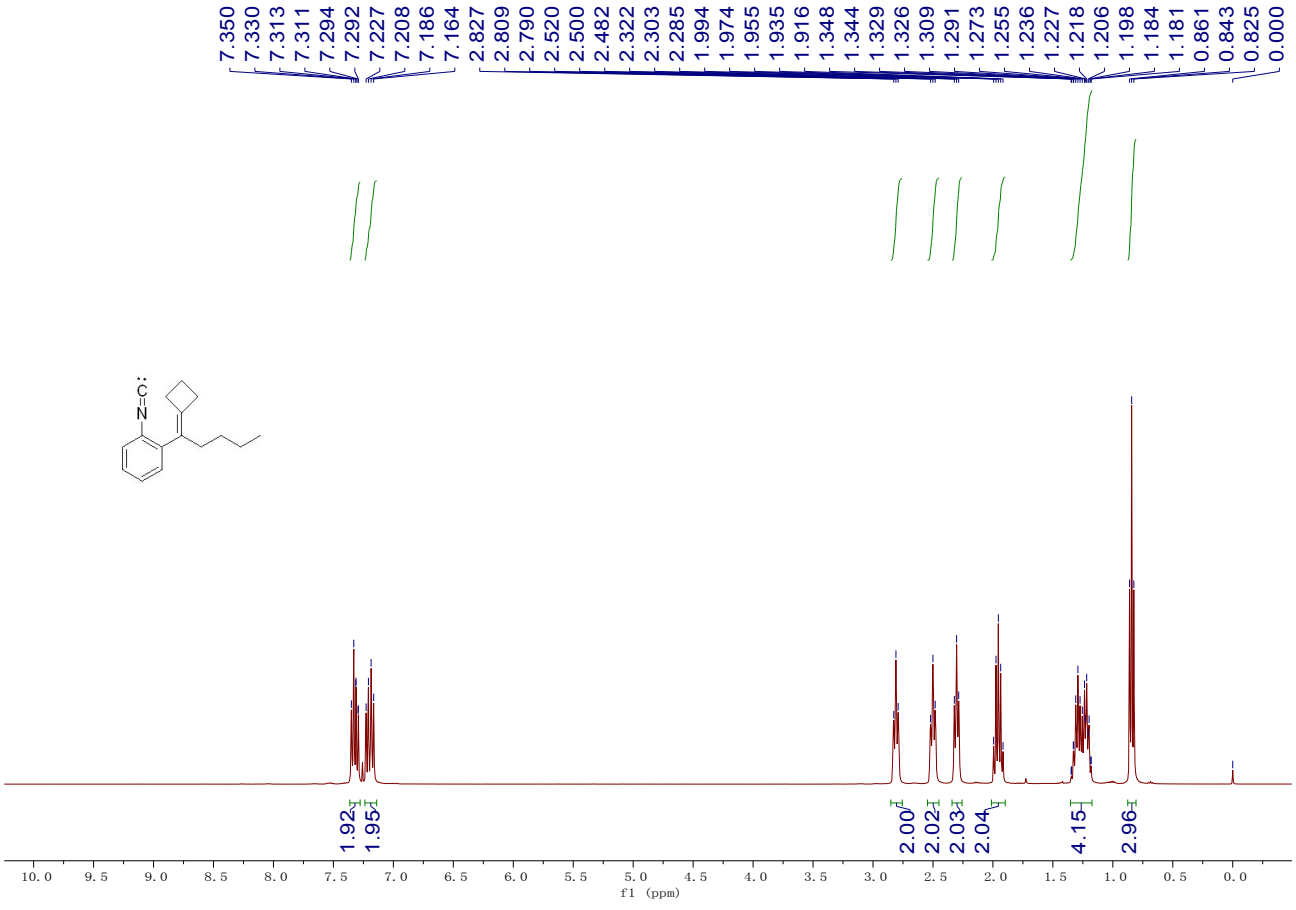
Compound **1n**: Yield: 2.826 g; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.88 (s, 3H), 1.88-2.00 (m, 2H), 2.53 (t, *J* = 7.0 Hz, 2H), 2.80 (t, *J* = 7.4 Hz, 2H), 7.22 (d, *J* = 7.0 Hz, 2H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.1, 17.5, 30.1, 30.4, 122.6, 127.0, 127.2, 129.0, 129.5, 139.8, 141.0, 165.0; IR (CH_3COCH_3): ν 2979, 2951, 2914, 2120, 1713, 1483, 1440, 1414, 1360, 1219, 1185, 1070, 1029, 948, 759 cm^{-1}; MS (DART) m/z 184.1 $(M+H)^+$; HRMS (DART) Calcd. for $C_{13}H_{14}N$: 184.1121, Found: 184.1120.

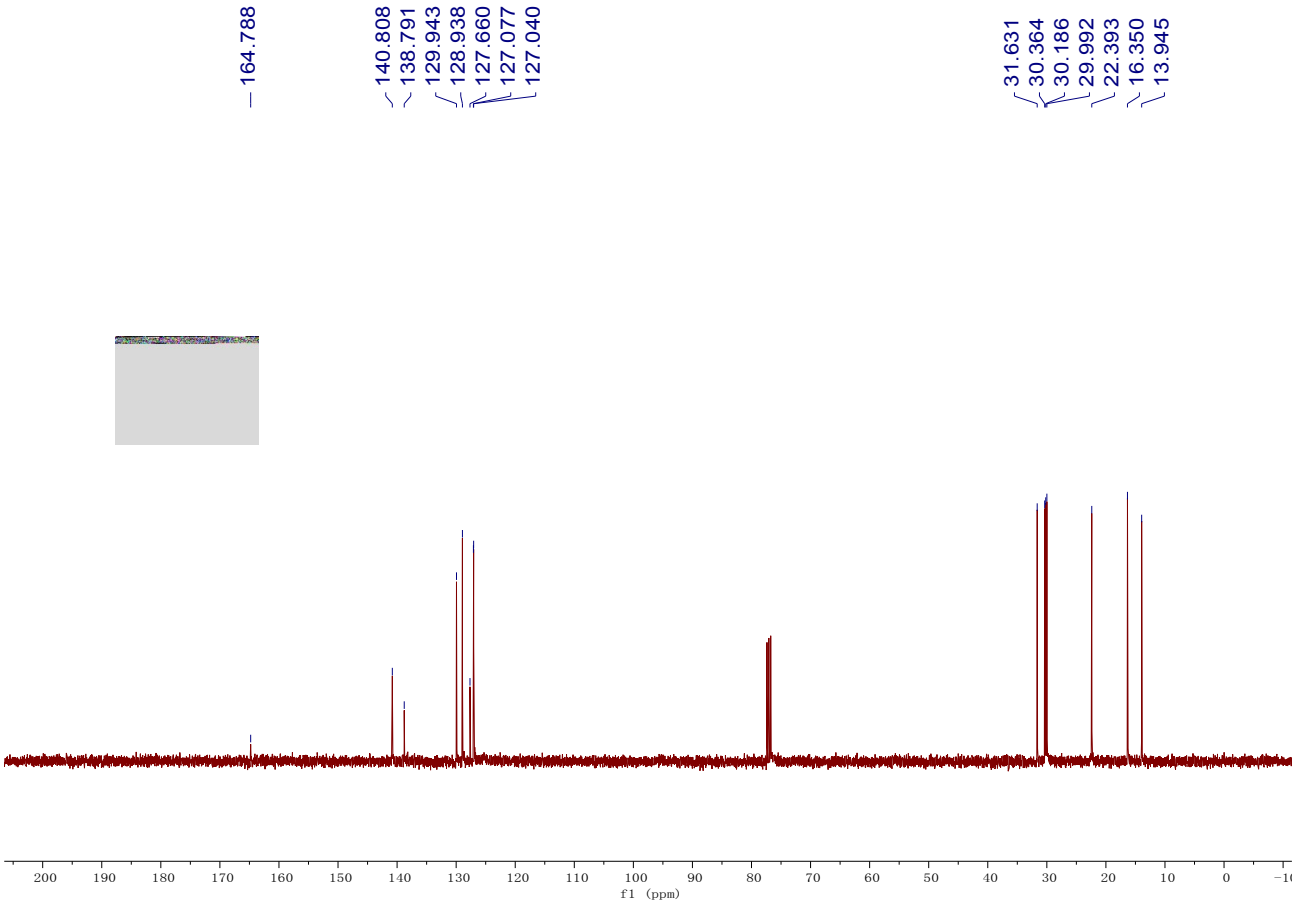

7.358
7.338
7.319
7.300
7.233
7.217
7.198
2.819
2.800
2.782
2.548
2.530
2.513
2.000
1.981
1.961
1.941
1.922
1.883
-0.000
0.97
0.85
1.79
2.00
1.96
2.01
2.80
f1 (ppm)

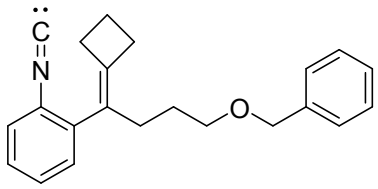

165.017
141.041
139.796
129.522
129.048
127.199
127.048
122.608
30.429
30.055
17.546
16.141
f1 (ppm)



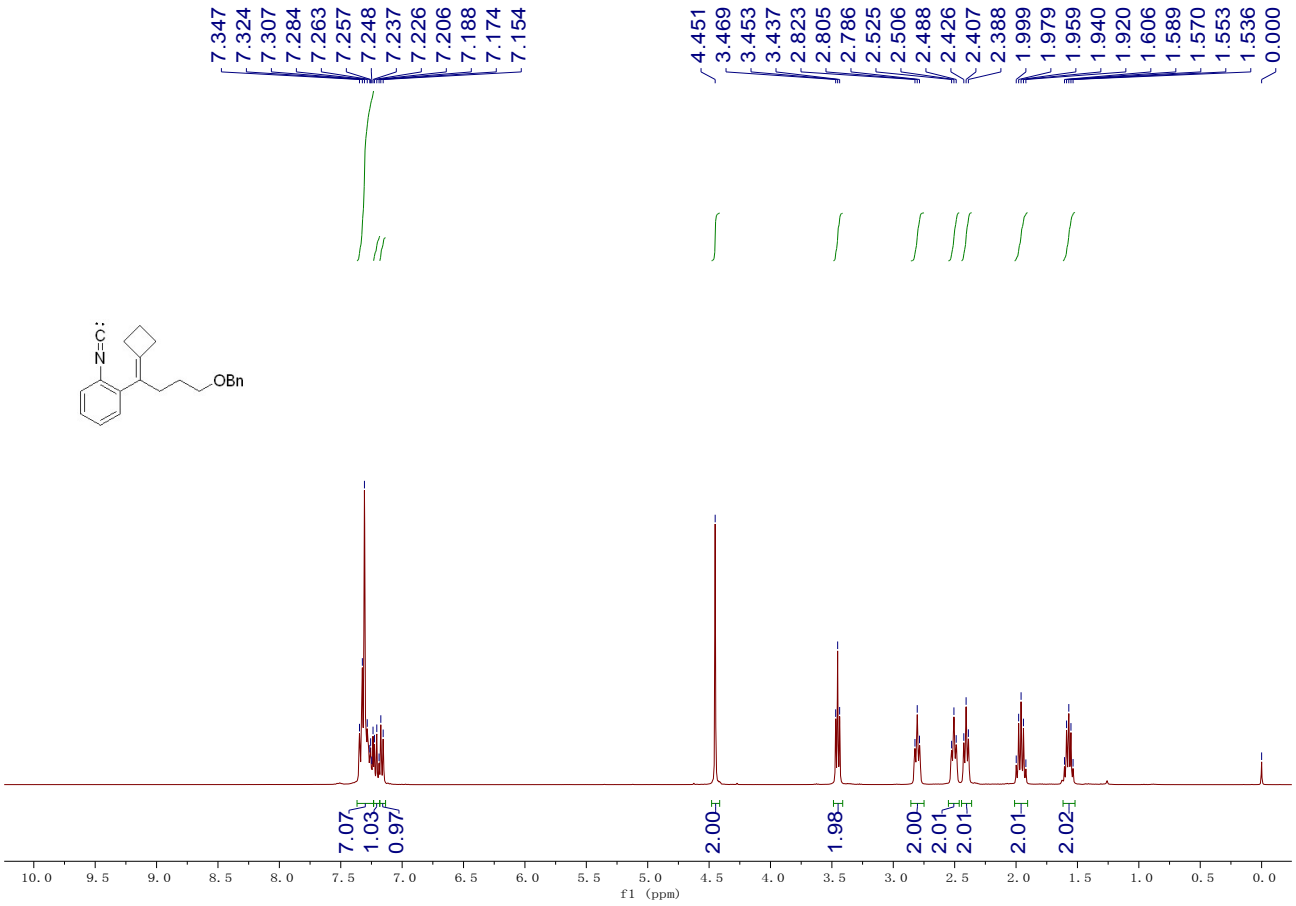
Compound **1o**: Yield: 2.424 g; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.84 (t, *J* = 7.2 Hz, 3H), 1.18-1.35 (m, 4H), 1.92-1.99 (m, 2H), 2.30 (t, *J* = 7.4 Hz, 2H), 2.50 (t, *J* = 7.6 Hz, 2H), 2.81 (t, *J* = 7.4 Hz, 2H), 7.16-7.23 (m, 2H), 7.29-7.35 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 13.9, 16.3, 22.4, 30.0, 30.2, 30.4, 31.6, 127.0, 127.1, 127.7, 128.9, 129.9, 138.8, 140.8, 164.8; IR (CH_3COCH_3): ν 2955, 2929, 2872, 2857, 2120, 1483, 1465, 1440, 1414, 1378, 1302, 1185, 1093, 1037, 948, 912, 867, 758 cm^{-1}; MS (DART) m/z 226.2 $(M+H)^+$; HRMS (DART) Calcd. for $C_{16}H_{20}N$: 226.1590, Found: 226.1589.

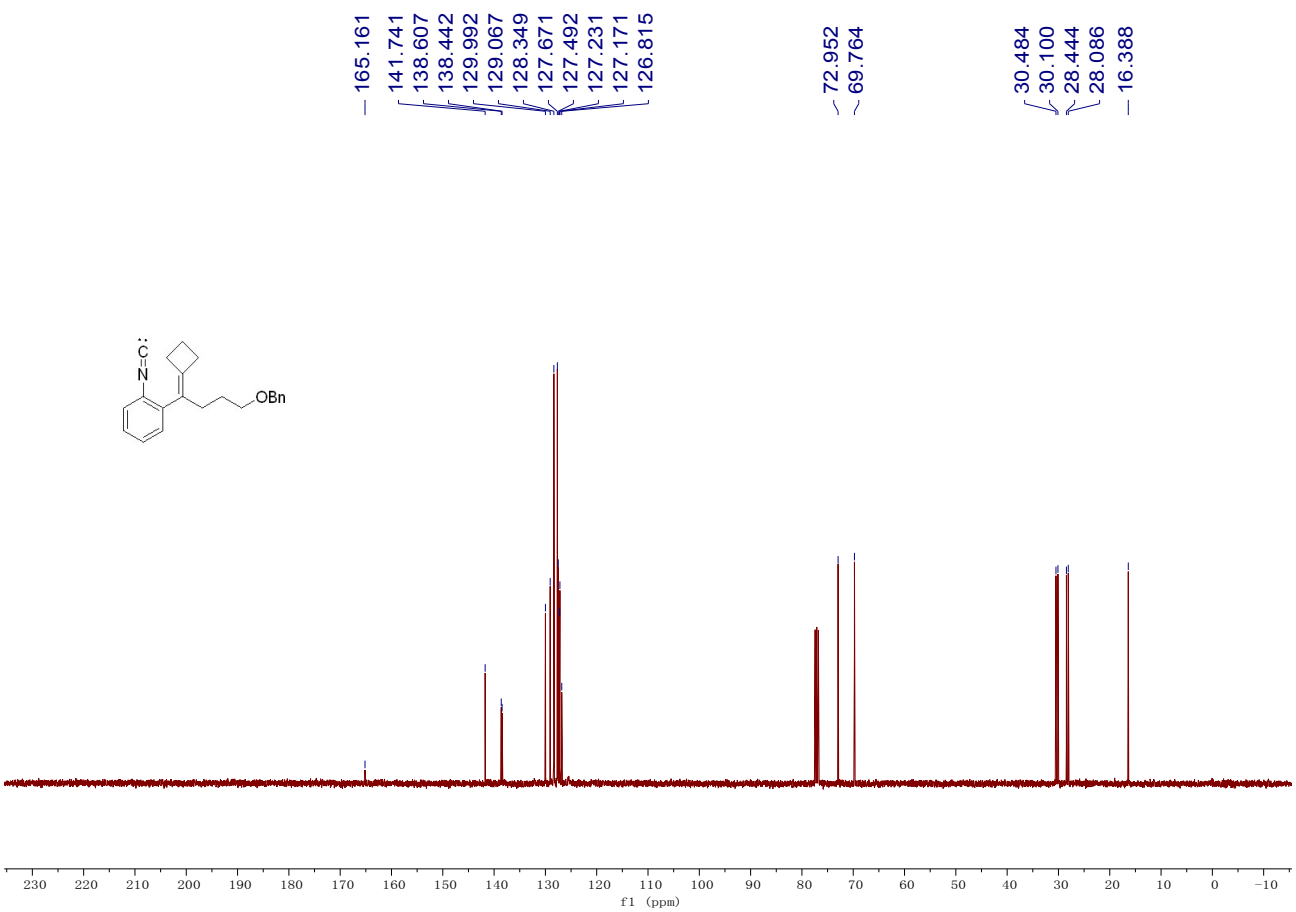


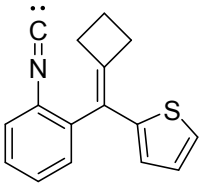




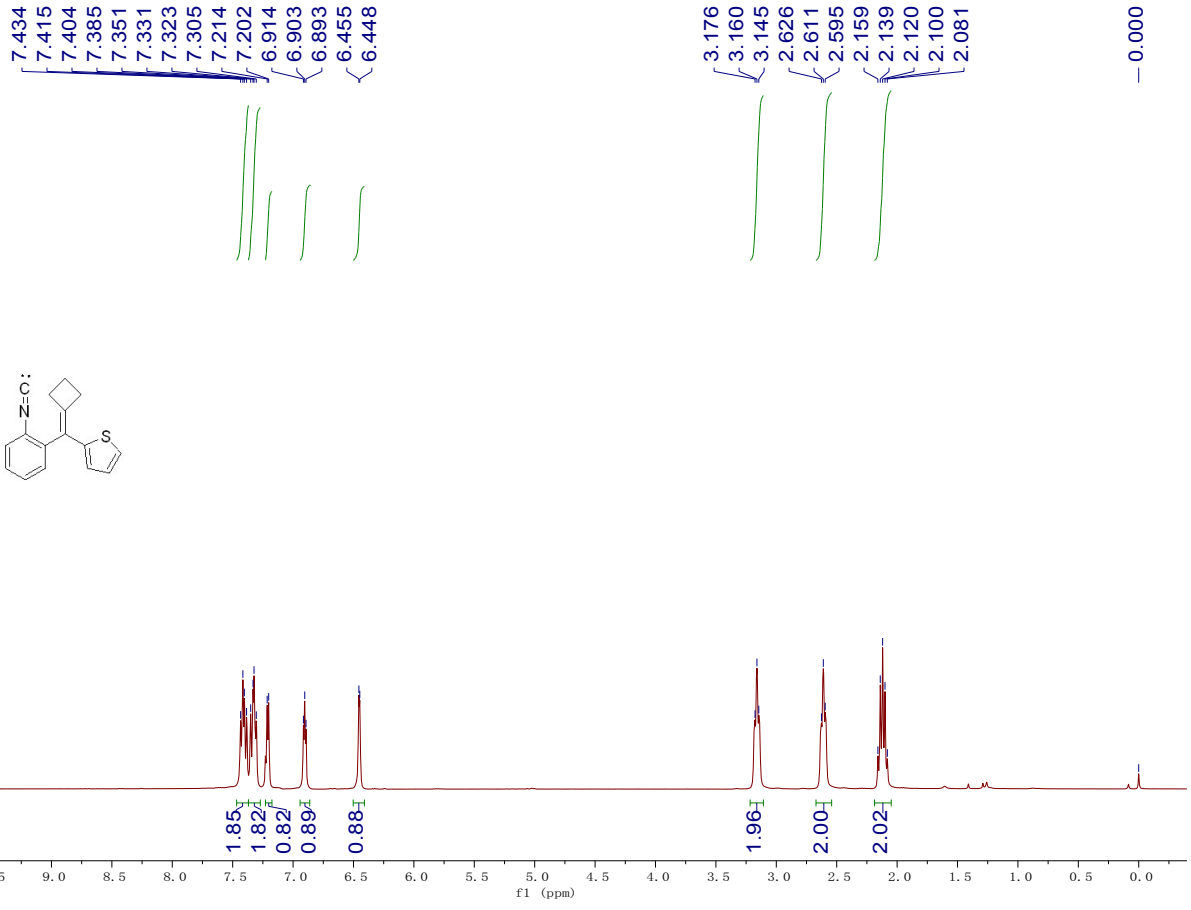
Compound **1p**: Yield: 1.902 g; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.54-1.61 (m, 2H), 1.92-2.00 (m, 2H), 2.41 (t, J = 7.6 Hz, 2H), 2.51 (t, J = 7.4 Hz, 2H), 2.81 (t, J = 7.4 Hz, 2H), 3.45 (t, J = 6.4 Hz, 2H), 4.45 (s, 2H), 7.16 (d, J = 8.0 Hz, 1H), 7.21 (t, J = 7.6 Hz, 1H), 7.23-7.35 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): 16.4, 28.1, 28.4, 30.1, 30.5, 69.8, 73.0, 126.8, 127.17, 127.23, 127.5, 127.7, 128.3, 129.1, 130.0, 138.4, 138.6, 141.7, 165.2; IR (CH_3COCH_3): ν 3066, 3029, 2942, 2853, 2120, 1713, 1495, 1483, 1453, 1414, 1362, 1219, 1100, 1028, 909, 7600, 735, 697 cm^{-1}; MS (DART) m/z 318.2 $(M+H)^+$; HRMS (DART) Calcd. for $C_{22}H_{24}NO$: 318.1852, Found: 318.1851.

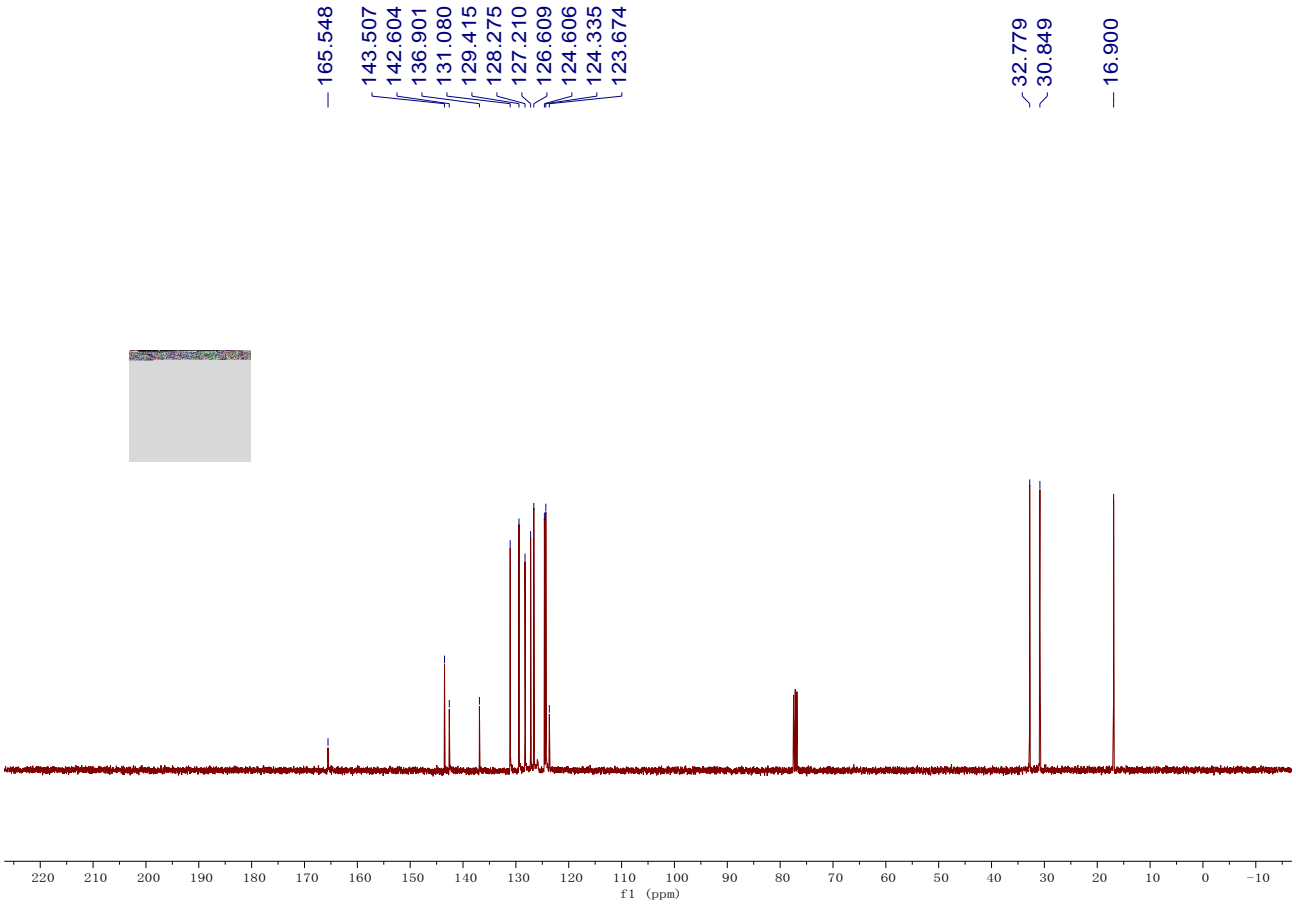

7.347
7.324
7.307
7.284
7.263
7.257
7.248
7.237
7.226
7.206
7.188
7.174
7.154
4.451
3.469
3.453
3.437
2.823
2.805
2.786
2.525
2.506
2.488
2.426
2.407
2.388
1.999
1.979
1.959
1.940
1.920
1.606
1.589
1.570
1.553
1.536
0.000
OBn
7.07
1.03
0.97
2.00
1.98
2.00
2.01
2.01
2.01
2.02
f1 (ppm)

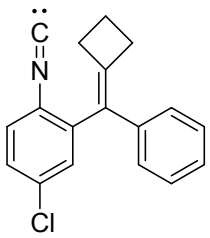

165.161
141.741
138.607
138.442
129.992
129.067
128.349
127.671
127.492
127.231
127.171
126.815
72.952
69.764
30.484
30.100
28.444
28.086
16.388
OBn
f1 (ppm)



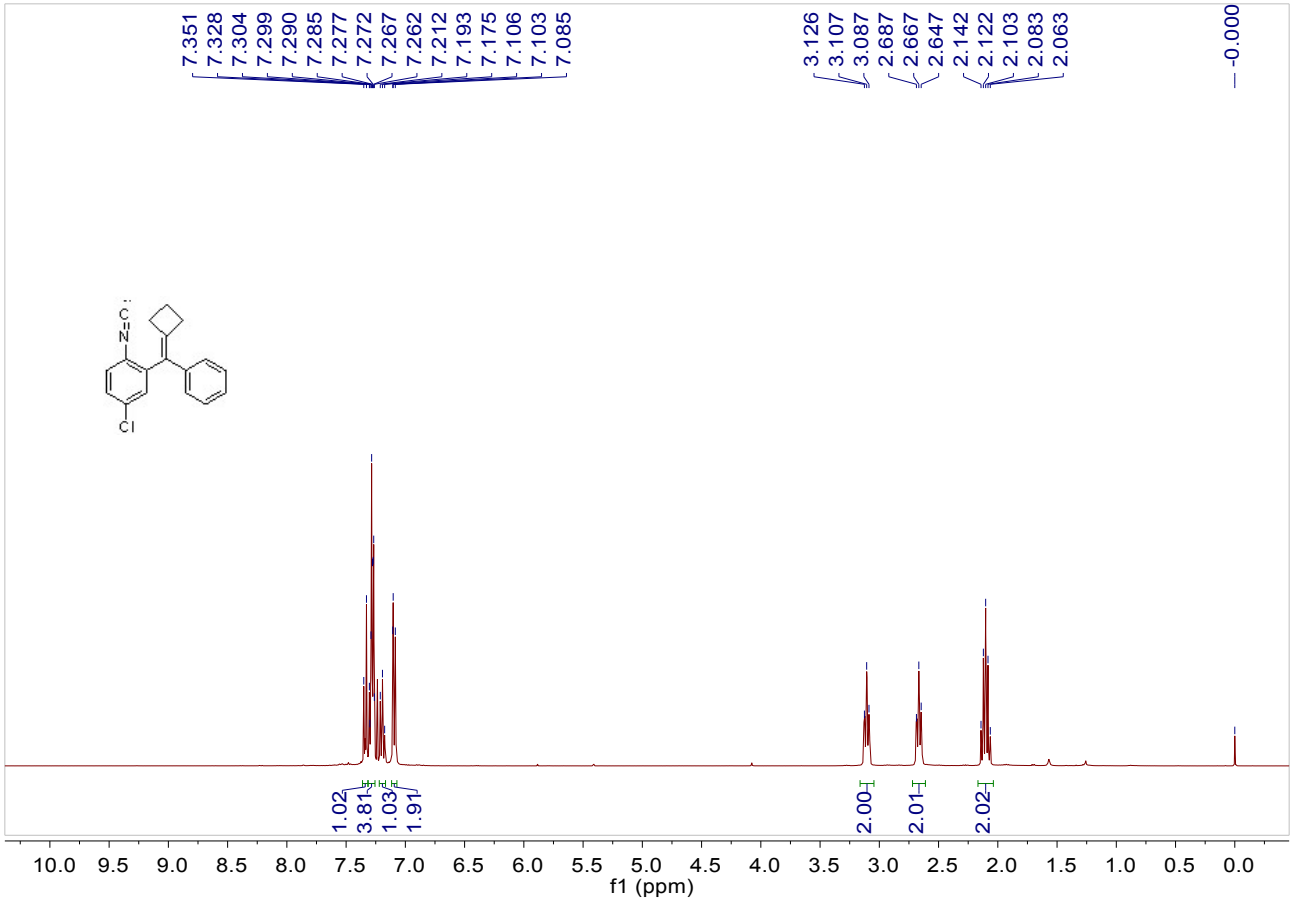
Compound **1q**: Yield: 1.712 g; A brown solid; m.p. 83-85 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.08-2.16 (m, 2H), 2.61 (t, J = 6.2 Hz, 2H), 3.16 (t, J = 6.2 Hz, 2H), 6.45 (d, J = 2.8 Hz, 1H), 6.90 (t, J = 4.2 Hz, 1H), 7.20-7.23 (m, 1H), 7.31-7.35 (m, 2H), 7.39-7.43 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.9, 30.8, 32.8, 123.7, 124.3, 124.6, 126.6, 127.2, 128.3, 129.4, 131.1, 136.9, 142.6, 143.5, 165.5; IR (CH_3COCH_3): ν 3070, 2982, 2954, 2909, 2121, 1712, 1483, 1443, 1360, 1220, 1096, 1047, 952, 825, 760, 695 cm^{-1}; MS (ESI) m/z 252.1 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{16}H_{14}NS$: 252.08415, Found: 252.08412.

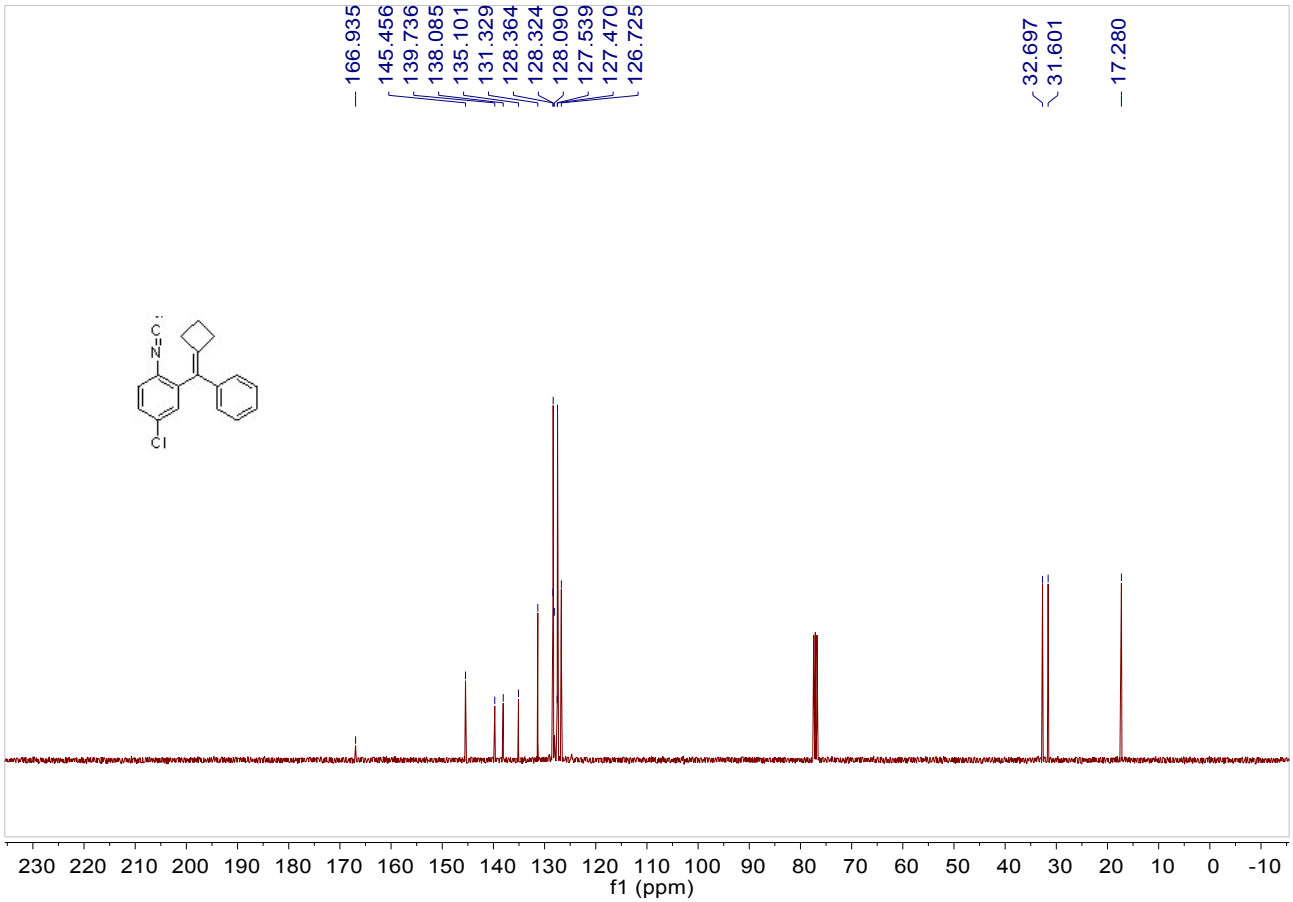


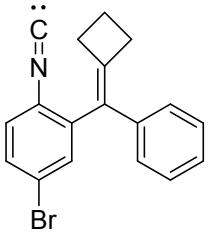




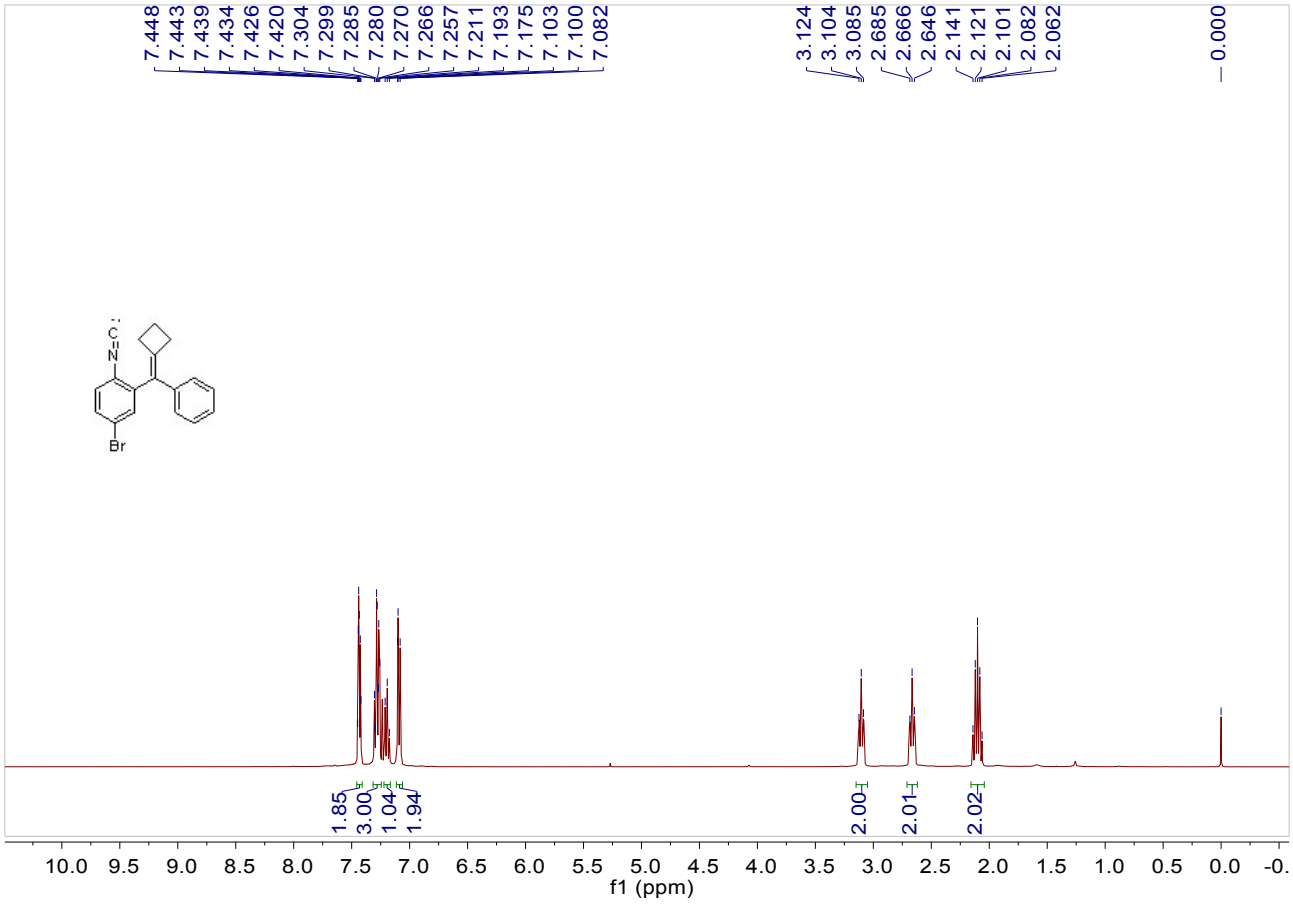
Compound **1r**: Yield: 0.863 g; A brown solid; m.p. 89-91 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.06-2.14 (m, 2H), 2.66 (t, *J* = 8.0 Hz, 2H), 3.11 (t, *J* = 7.8 Hz, 2H), 7.09-7.11 (m, 2H), 7.19 (t, *J* = 7.4 Hz, 1H), 7.26-7.30 (m, 4H), 7.34 (d, *J* = 9.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.3, 31.6, 32.7, 126.7, 127.47, 127.54, 128.1, 128.3, 128.4, 131.3, 135.1, 138.1, 139.7, 145.5, 166.9; IR (CH_3COCH_3): ν 3057, 2979, 2953, 2906, 2119, 1712, 1590, 1560, 1494, 1477, 1444, 1397, 1300, 1268, 1171, 1110, 1083, 1031, 933, 880, 820, 764, 730, 695 cm^{-1}; MS (ESI) m/z 280.0888 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{18}H_{15}NCl$: 280.0888, Found: 280.0888.

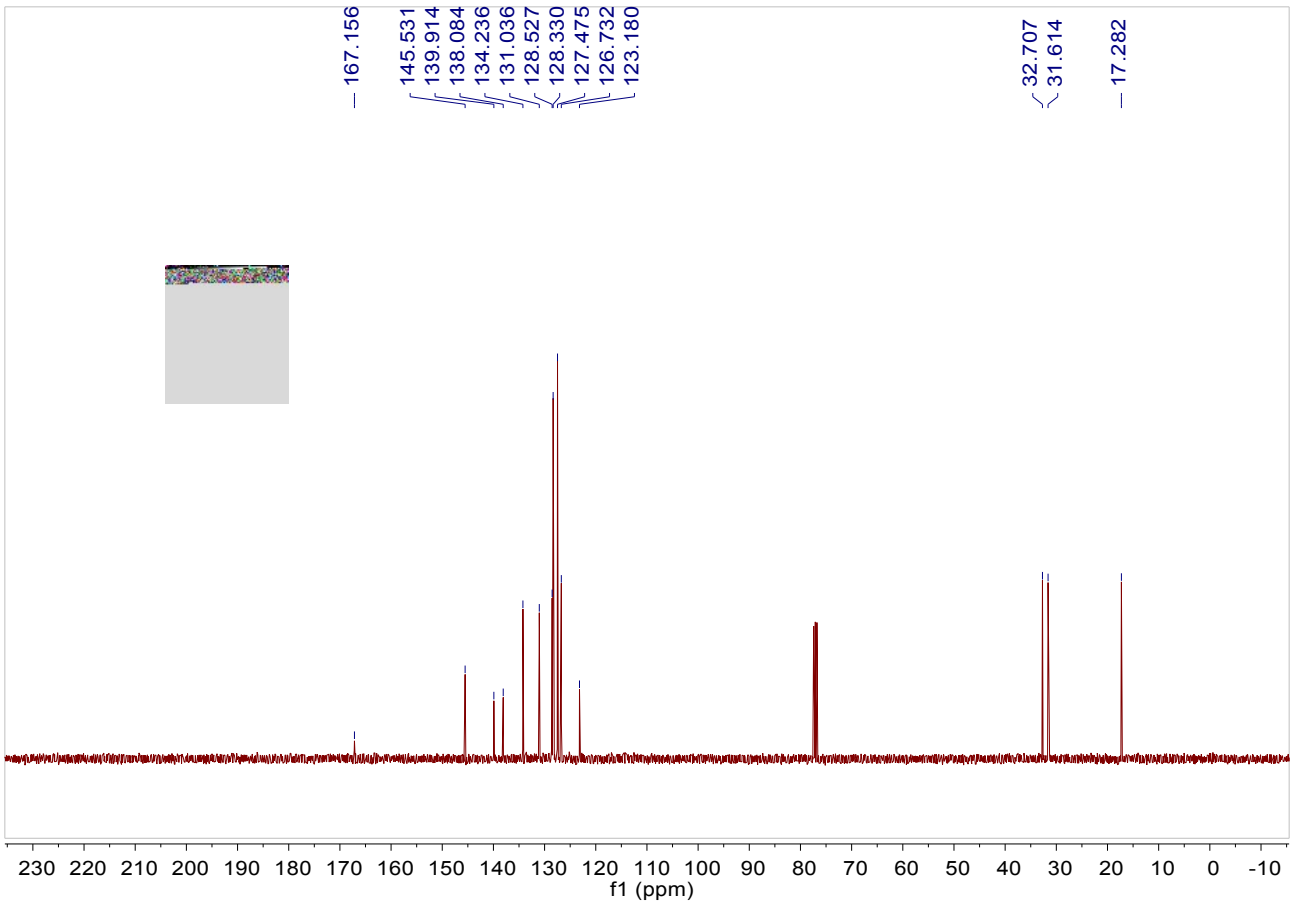

7.351
7.328
7.304
7.299
7.290
7.285
7.277
7.272
7.267
7.262
7.212
7.193
7.175
7.106
7.103
7.085
3.126
3.107
3.087
2.687
2.667
2.647
2.142
2.122
2.103
2.083
2.063
-0.000
1.02
3.81
1.03
1.91
2.00
2.01
2.02
f1 (ppm)

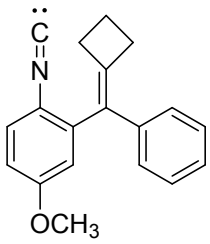

166.935
145.456
139.736
138.085
135.101
131.329
128.364
128.324
128.090
127.539
127.470
126.725
32.697
31.601
17.280
f1 (ppm)



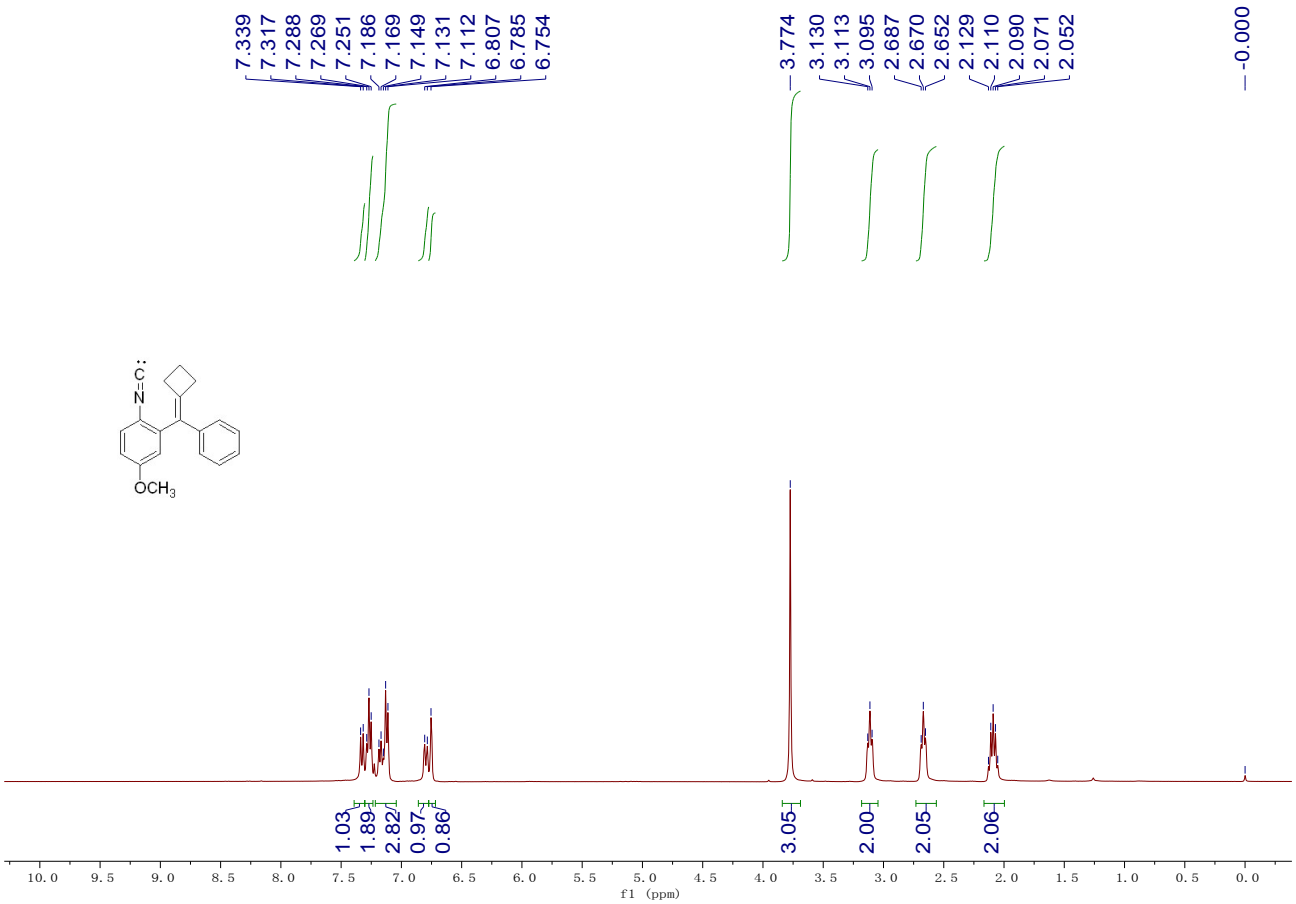
Compound **1s**: Yield: 2.846 g; A brown solid; m.p. 93-95 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.06-2.14 (m, 2H), 2.67 (t, J = 7.8 Hz, 2H), 3.10 (t, J = 7.8 Hz, 2H), 7.08-7.10 (m, 2H), 7.19 (t, J = 7.2 Hz, 1H), 7.26-7.30 (m, 3H), 7.42-7.45 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.3, 31.6, 32.7, 123.2, 126.7, 127.5, 128.3, 128.5, 131.0, 134.2, 138.1, 139.9, 145.5, 167.2; IR (CH_3COCH_3): ν 3056, 2987, 2952, 2911, 2119, 1892, 1712, 1585, 1557, 1493, 1474, 1444, 1410, 1391, 1298, 1266, 1220, 1171, 1105, 1075, 1031, 926, 879, 818, 762 cm^{-1}; MS (ESI) m/z 324.0 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{18}H_{15}NBr$: 324.0382, Found: 324.0379.

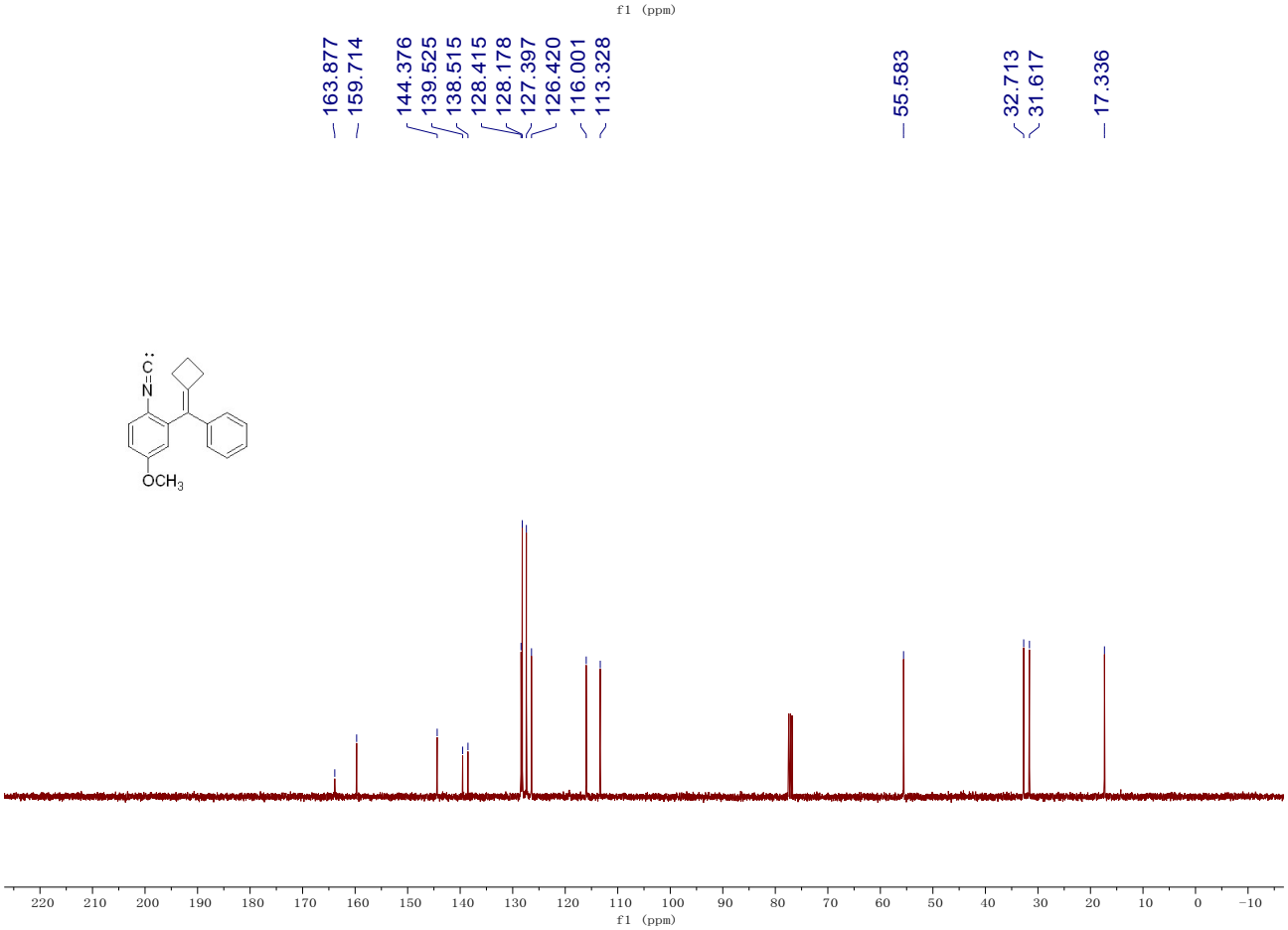


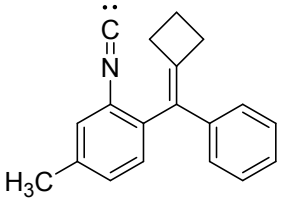




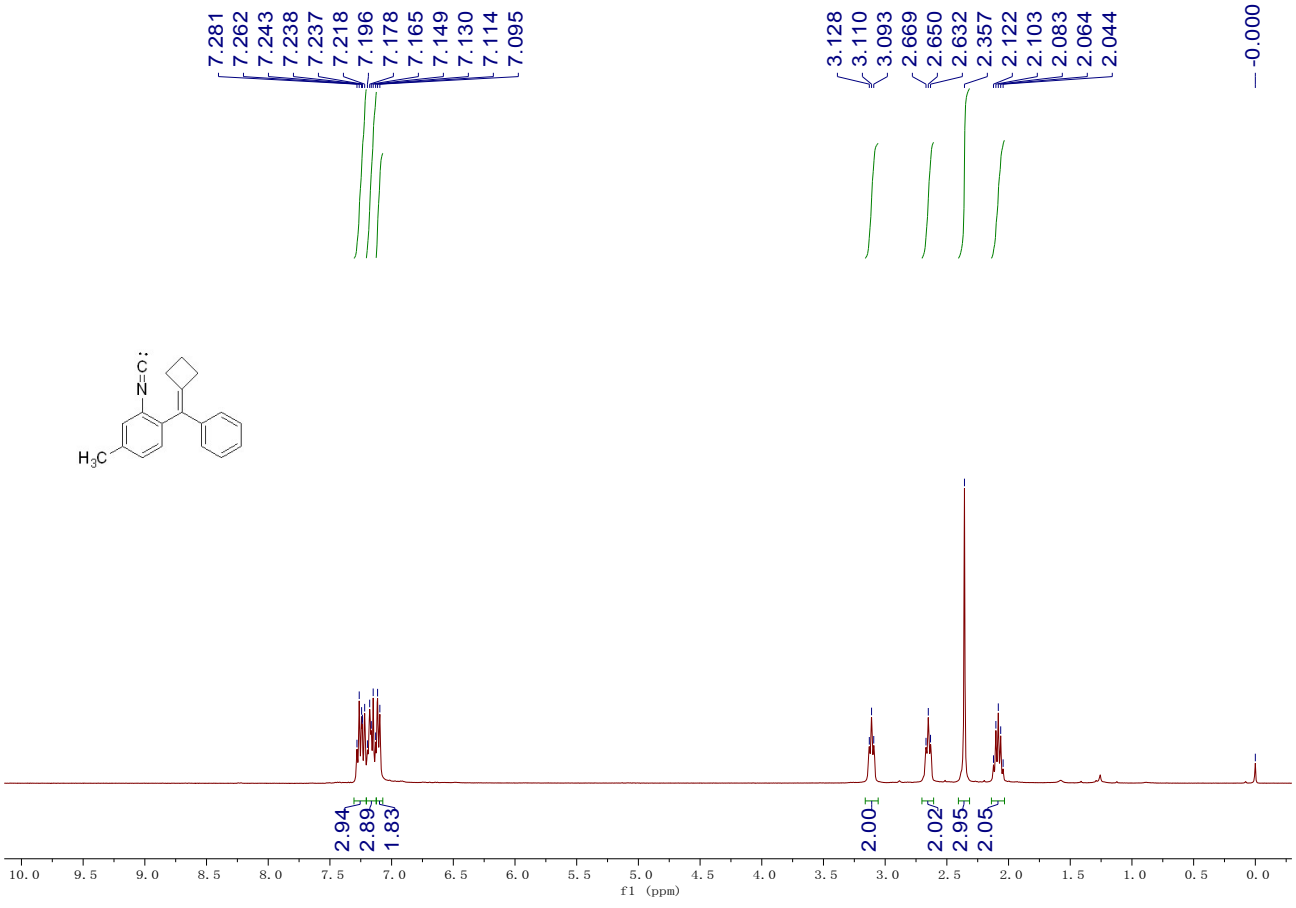
Compound **1t**: Yield: 1.169 g; A brown solid; m.p. 74-76 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.05-2.13 (m, 2H), 2.67 (t, *J* = 7.0 Hz, 2H), 3.11 (t, *J* = 7.0 Hz, 2H), 3.77 (s, 3H), 6.75 (s, 1H), 6.80 (d, J = 8.8 Hz, 1H), 7.11-7.19 (m, 3H), 7.27 (t, *J* = 7.4 Hz, 2H), 7.33 (d, *J* = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.3, 31.6, 32.7, 55.6, 113.3, 116.0, 126.4, 127.4, 128.2, 128.4, 138.5, 139.5, 144.4, 159.7, 163.9; IR (CH_3COCH_3): ν 2982, 2954, 2914, 2835, 2119, 1712, 1599, 1570, 1490, 1444, 1361, 1297, 1245, 1229, 1190, 1159, 1124, 1031, 979, 948, 910, 878, 849, 767, 695 cm^{-1}; MS (ESI) m/z 276.1 $(M+H)^{+}$; HRMS (ESI) Calcd. for $C_{19}H_{18}NO$: 276.13829, Found: 276.13795.

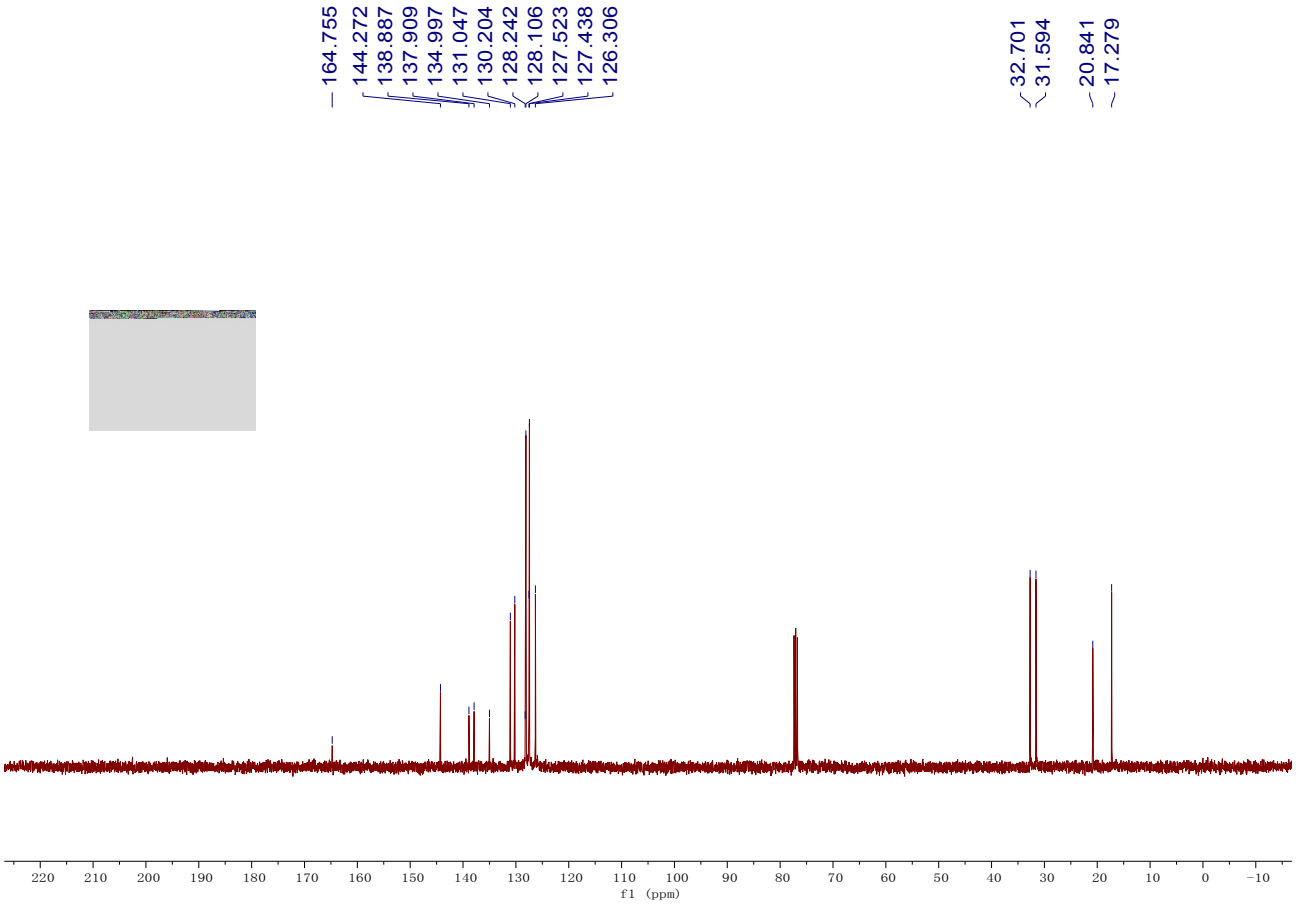

7.339
7.317
7.288
7.269
7.251
7.186
7.169
7.149
7.131
7.112
6.807
6.785
6.754
3.774
3.130
3.113
3.095
2.687
2.670
2.652
2.129
2.110
2.090
2.071
2.052
-0.000
C≡N
OCH3
1.03
1.89
2.82
0.97
0.86
3.05
2.00
2.05
2.06
f1 (ppm)

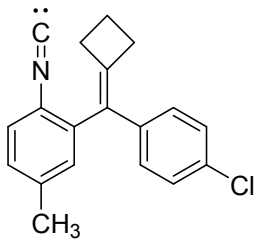

163.877
159.714
144.376
139.525
138.515
128.415
128.178
127.397
126.420
116.001
113.328
55.583
32.713
31.617
17.336
C≡N
OCH3
f1 (ppm)



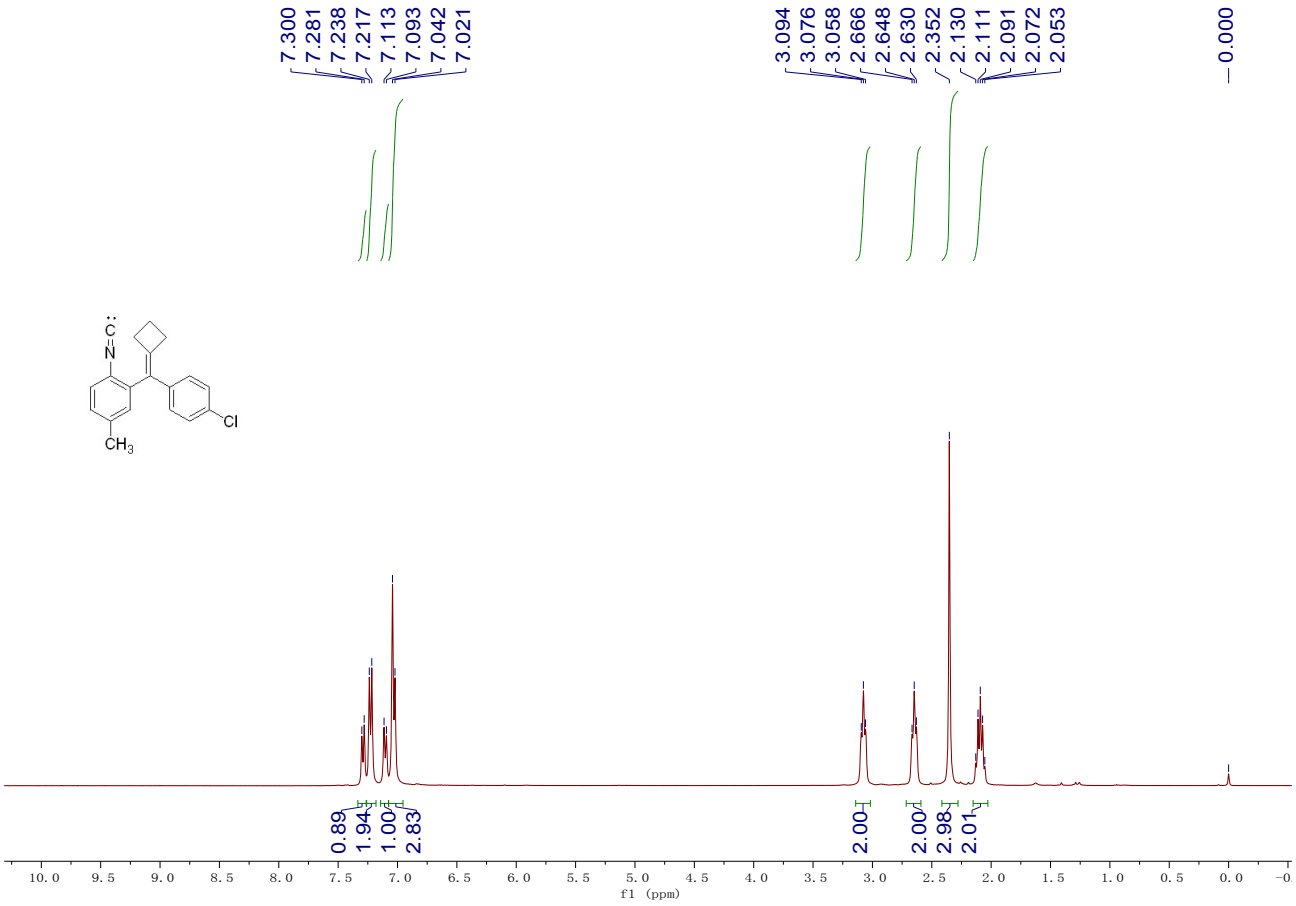
Compound **1u**: Yield: 0.425 g; A brown solid; m.p. 83-85 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.04-2.12 (m, 2H), 2.36 (s, 3H), 2.65 (t, *J* = 7.0 Hz, 2H), 3.11 (t, *J* = 7.4 Hz, 2H), 7.10-7.13 (m, 2H), 7.15-7.20 (m, 3H), 7.22-7.28 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.3, 20.8, 31.6, 32.7, 126.3, 127.4, 127.5, 128.1, 128.2, 130.2, 131.0, 135.0, 137.9, 138.9, 144.3, 164.8; IR (CH_3COCH_3): ν 3055, 2979, 2951, 2914, 2120, 1712, 1597, 1493, 1444, 1411, 1360, 1220, 1100, 1032, 933, 877, 819, 765, 695 cm^{-1}; MS (ESI) m/z 260.1 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{19}H_{18}N$: 260.14338, Found: 260.14349.

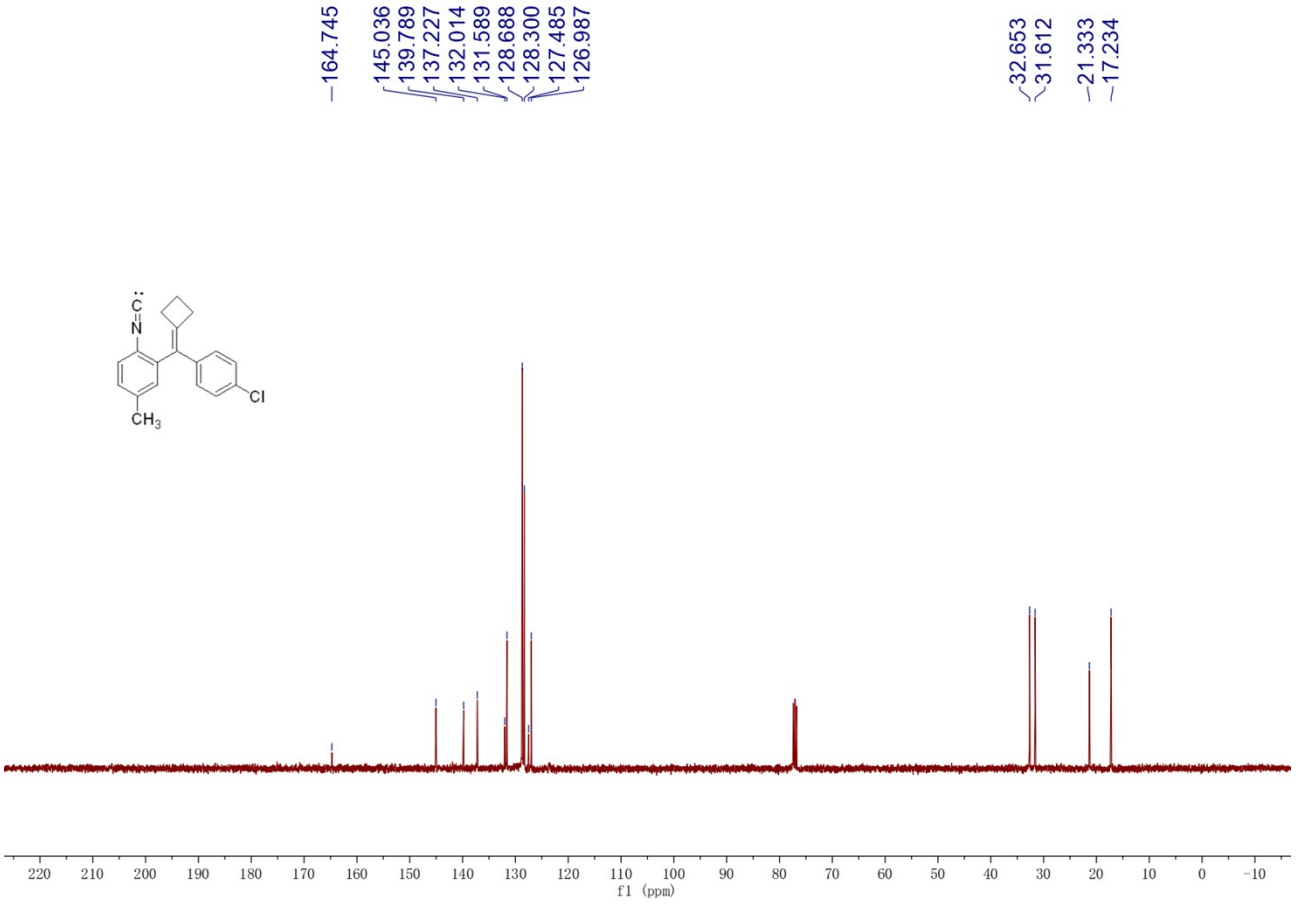


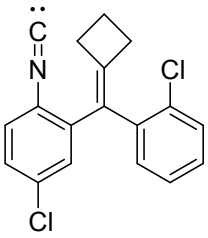




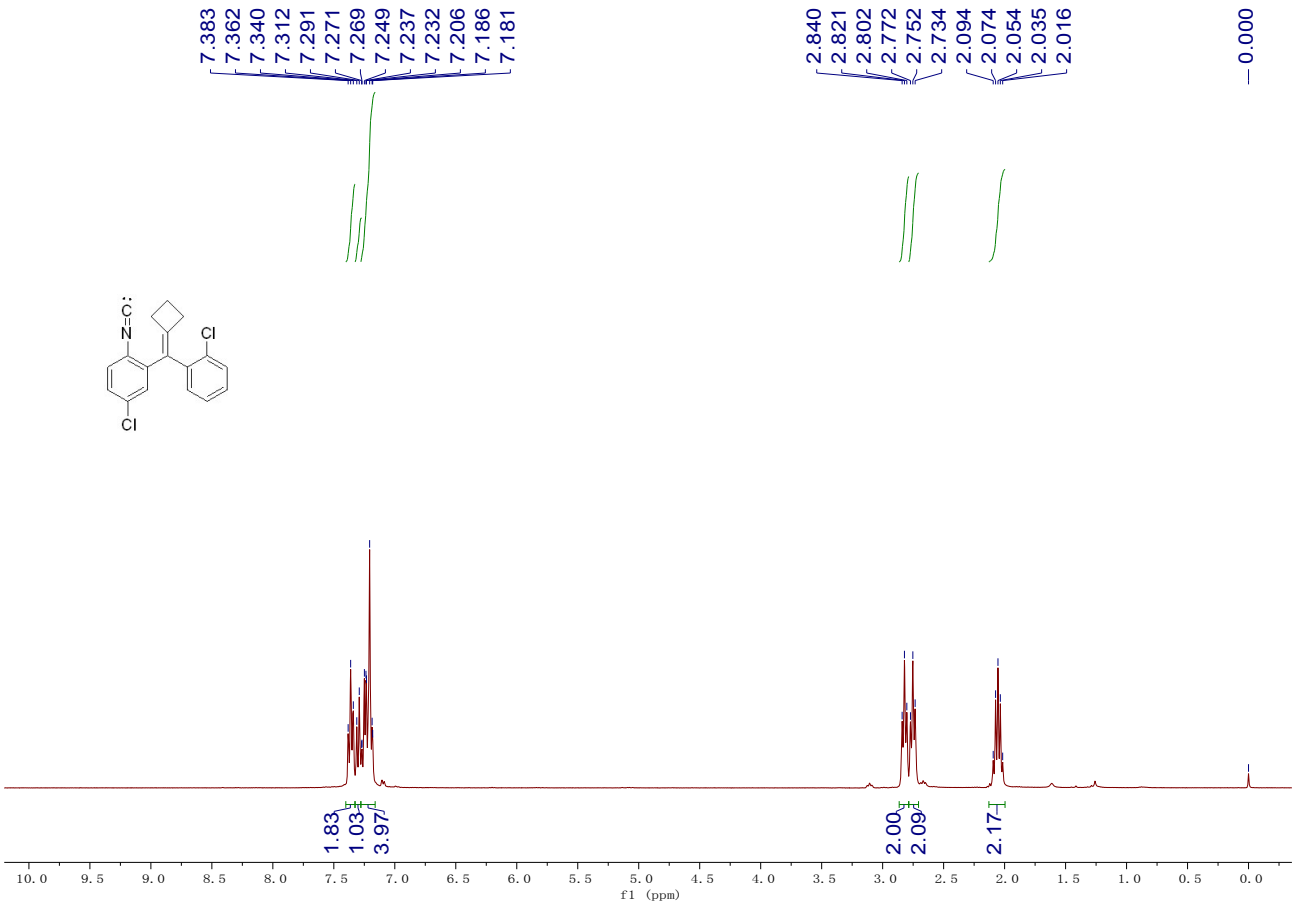
Compound **1v**: Yield: 1.679 g; A brown solid; m.p. 69-71 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.05-2.13 (m, 2H), 2.35 (s, 3H), 2.65 (t, *J* = 7.2 Hz, 2H), 3.08 (t, *J* = 7.2 Hz, 2H), 7.02-7.04 (m, 3H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.23 (d, *J* = 7.4 Hz, 2H), 7.29 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 17.2, 21.3, 31.6, 32.7, 127.0, 127.5, 128.3, 128.7, 131.6, 132.0, 137.2, 139.8, 145.0, 164.7; IR (CH_3COCH_3): ν 2980, 2954, 2915, 2119, 1713, 1657, 1490, 1399, 1360, 1220, 1091, 1012, 950, 832, 732, 696 cm^{-1}; MS (ESI) m/z 294.1 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{19}H_{17}NCl$: 294.10440, Found: 294.10399.

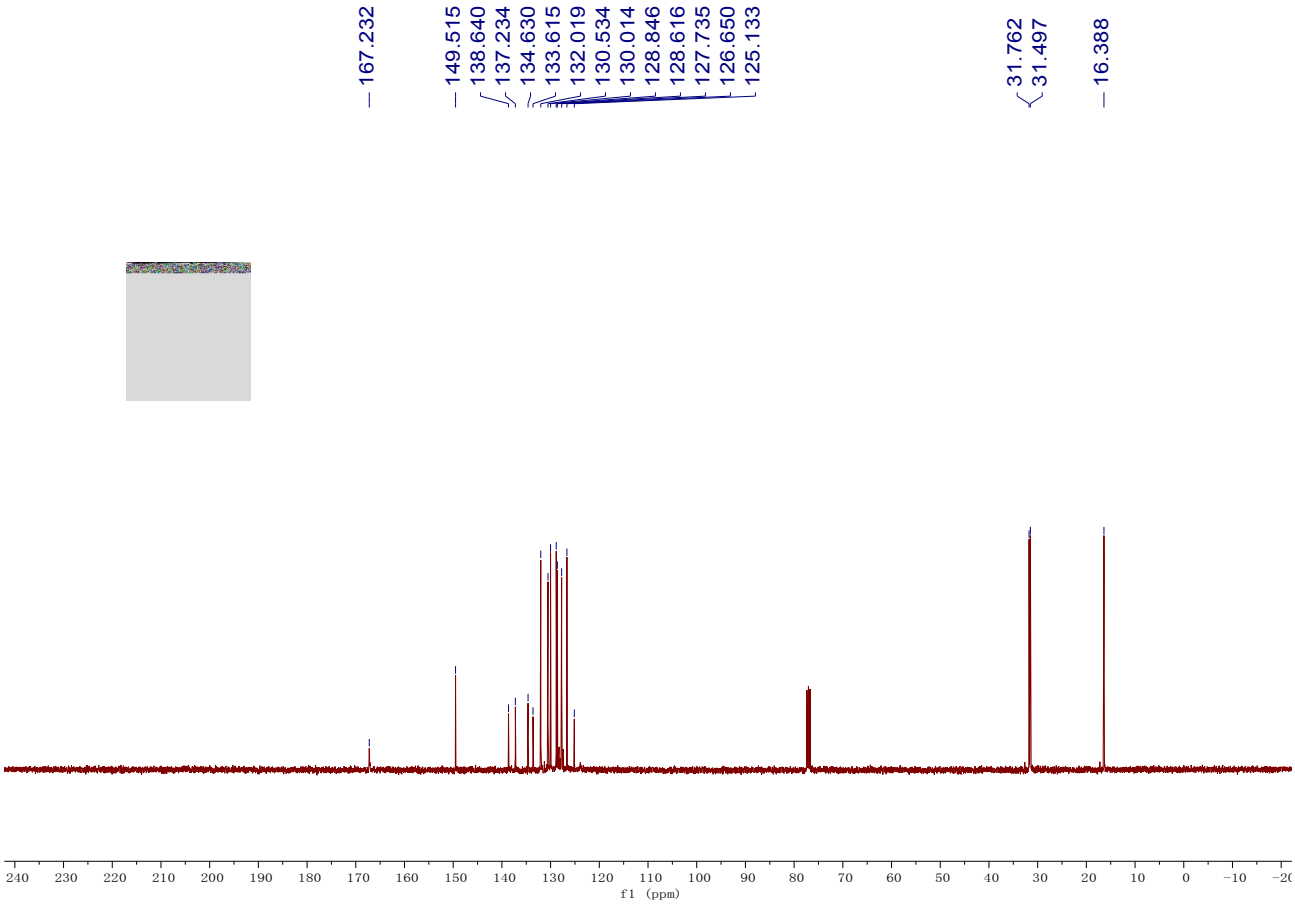

7.300
7.281
7.238
7.217
7.113
7.093
7.042
7.021
3.094
3.076
3.058
2.666
2.648
2.630
2.352
2.130
2.111
2.091
2.072
2.053
0.000
Cl
CH3
0.89
1.94
1.00
2.83
2.00
2.00
2.98
2.01
f1 (ppm)

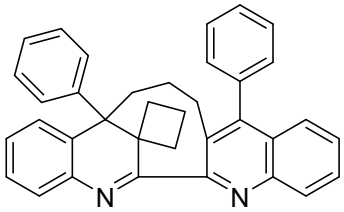

164.745
145.036
139.789
137.227
132.014
131.589
128.688
128.300
127.485
126.987
32.653
31.612
21.333
17.234
Cl
CH3
f1 (ppm)



Compound **1w**: Yield: 0.884 g; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.02-2.09 (m, 2H), 2.75 (t, *J* = 7.6 Hz, 2H), 2.82 (t, *J* = 7.6 Hz, 2H), 7.18-7.27 (m, 4H), 7.30 (d, *J* = 8.4 Hz, 1H), 7.36 (t, *J* = 8.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.4, 31.5, 31.8, 125.1, 126.7, 127.7, 128.6, 128.8, 130.0, 130.5, 132.0, 133.6, 134.6, 137.2, 138.6, 149.5, 167.2; IR (CH_3COCH_3): ν 3060, 2985, 2955, 2917, 2121, 1712, 1590, 1470, 1429, 1360, 1307, 1220, 1173, 1111, 1086, 1056, 1035, 981, 934, 880, 820, 732, 707 cm^{-1}; MS (ESI) m/z 314.1 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{18}H_{14}NCl_2$: 314.04978, Found: 314.05029.

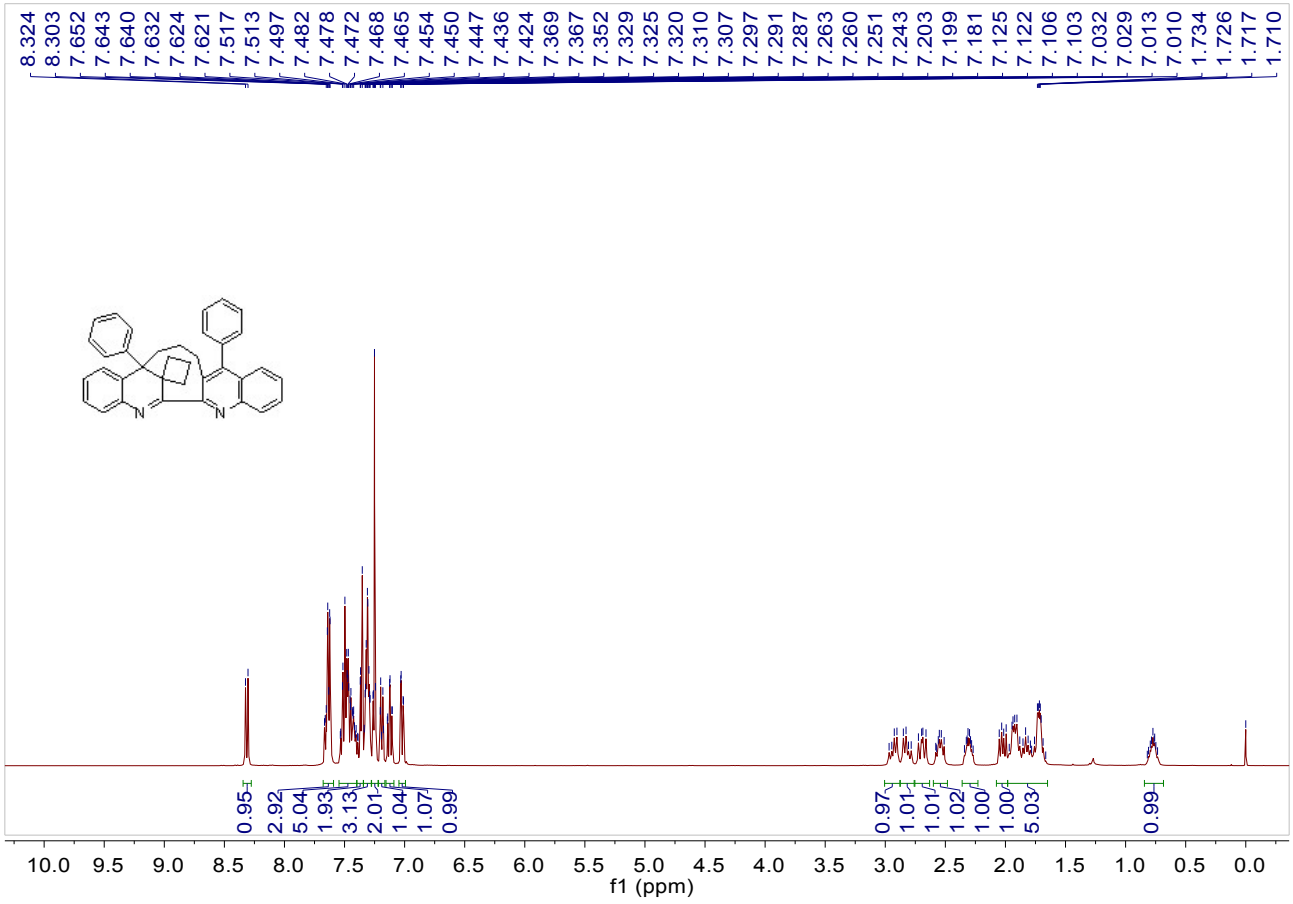


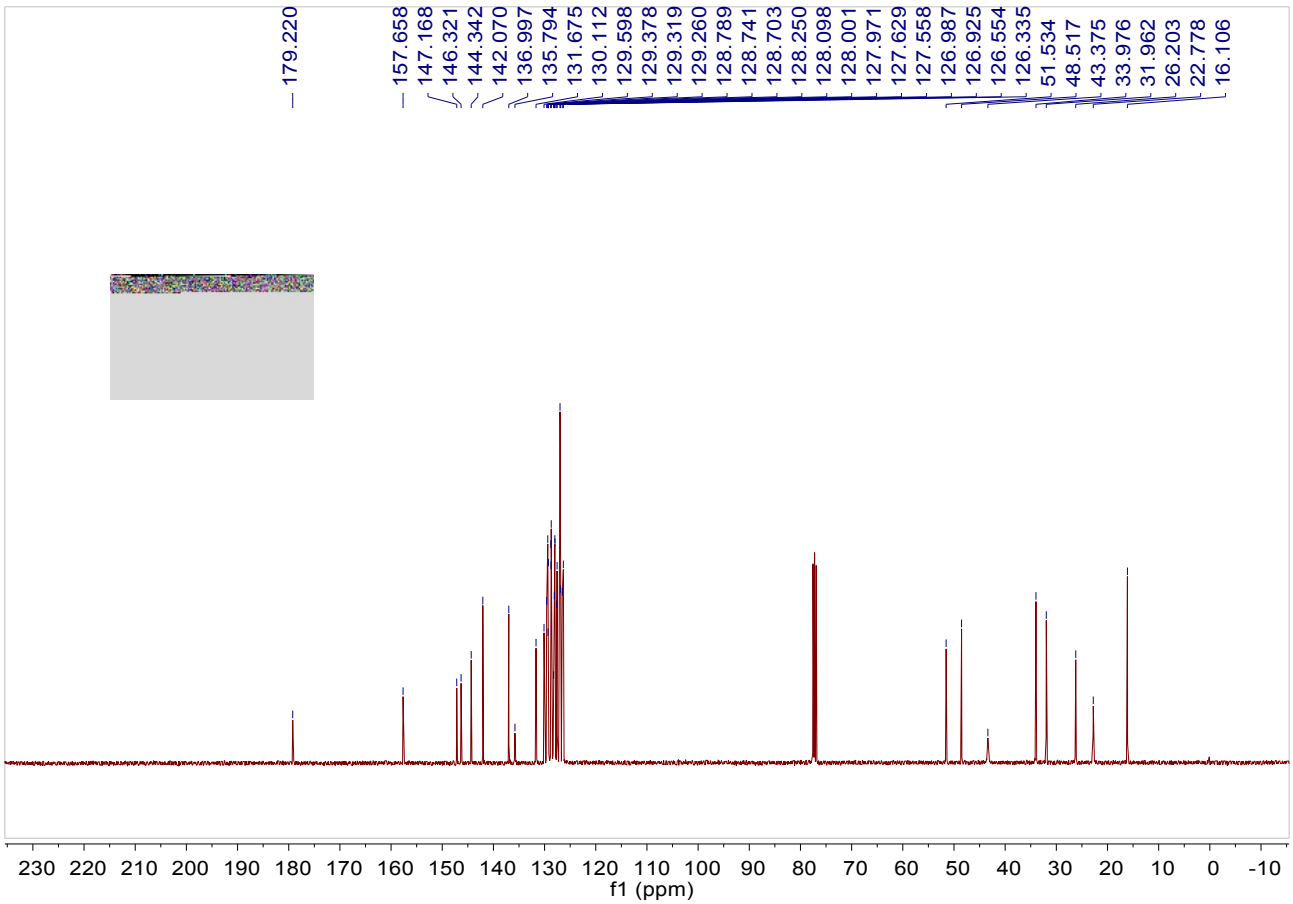


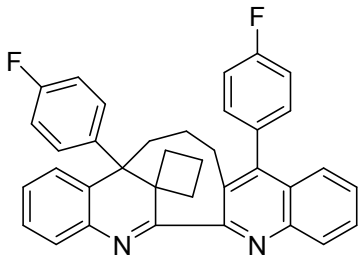


Compound **2a**: Yield: 97 mg, 40%; A brown solid; m.p. 301-303 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.73-0.82 (m, 1H), 1.67-1.97 (m, 5H), 2.02 (dd, *J* = 15.2 Hz, *J* = 8.4 Hz, 1H), 2.27-2.34 (m, 1H), 2.51-2.58 (m, 1H), 2.69 (dd, *J* = 14.8 Hz, *J* = 10.4 Hz, 1H), 2.82 (dd, *J* = 17.2 Hz, *J* = 9.2 Hz, 1H), 2.94 (dd , *J* = 17.2 Hz, *J* = 8.8 Hz, 1H), 7.02 (dd, *J* = 7.6 Hz, *J* = 1.2 Hz, 1H), 7.12 (td, *J* = 7.6 Hz, *J* = 1.2 Hz, 1H), 7.18-7.20 (m, 1H), 7.24-7.26 (m, 1H), 7.29-7.34 (m, 3H), 7.35-7.39 (m, 2H), 7.40-7.54 (m, 5H), 7.62-7.67 (m, 3H), 8.31 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.1, 22.8, 26.2, 32.0, 34.0, 43.4, 48.5, 51.5, 126.3, 126.6, 126.9, 127.0, 127.56, 127.63, 127.97, 128.00, 128.1, 128.2, 128.70, 128.74, 128.8, 129.26, 129.32, 129.4, 129.6, 130.1, 131.7, 135.8, 137.0, 142.1, 144.3, 146.3, 147.2, 157.7, 179.2; IR (CH_3COCH_3): ν 3050, 2987, 2950, 1712, 1624 1594, 1565, 1487, 1440, 1396, 1360, 1221, 1182, 1158, 1089, 1076, 1034, 992, 907, 847, 761,

748, 703 cm^{-1}; MS (ESI) m/z 491.2 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{36}H_{31}N_2$: 491.2482, Found: 491.2481.

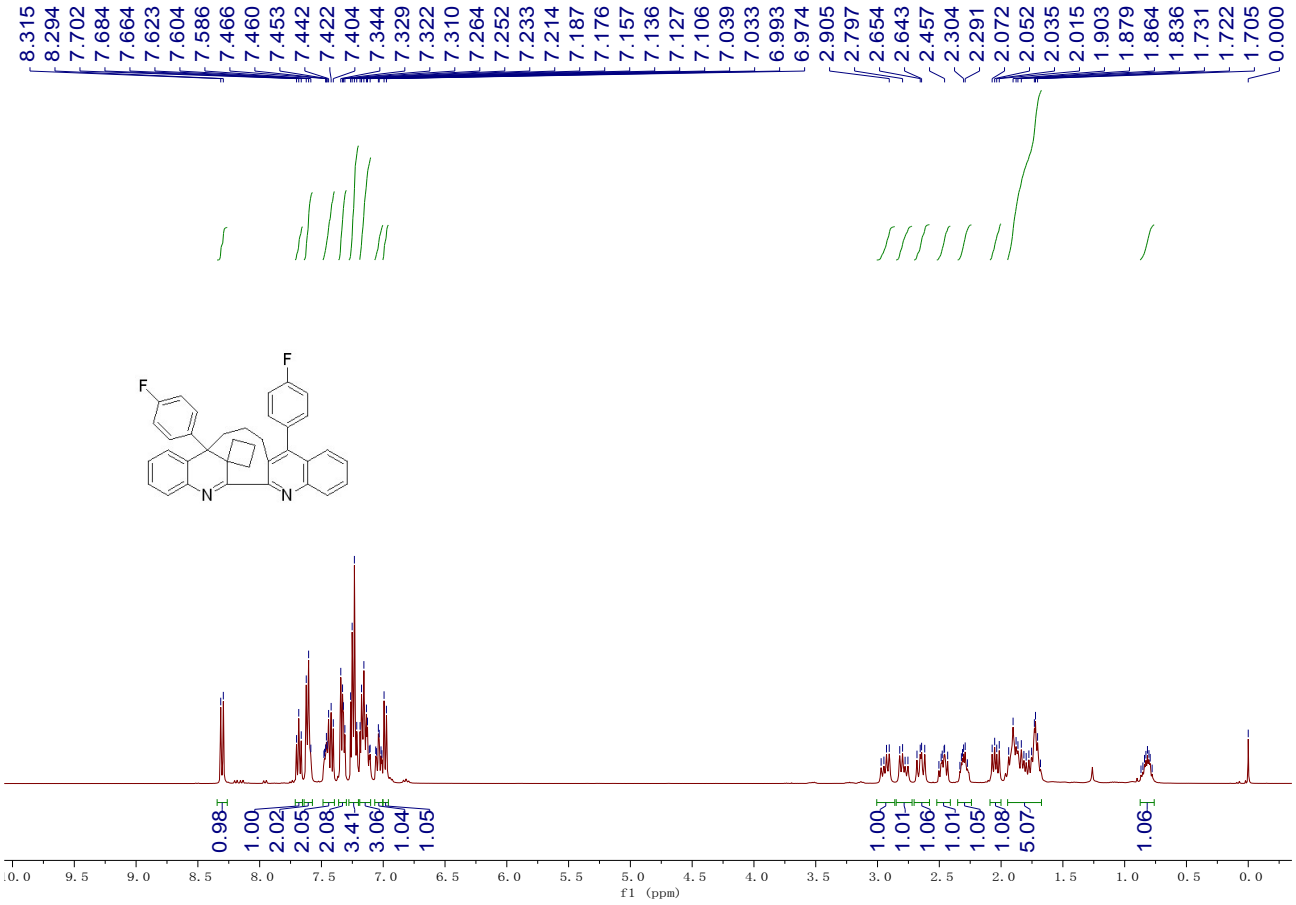


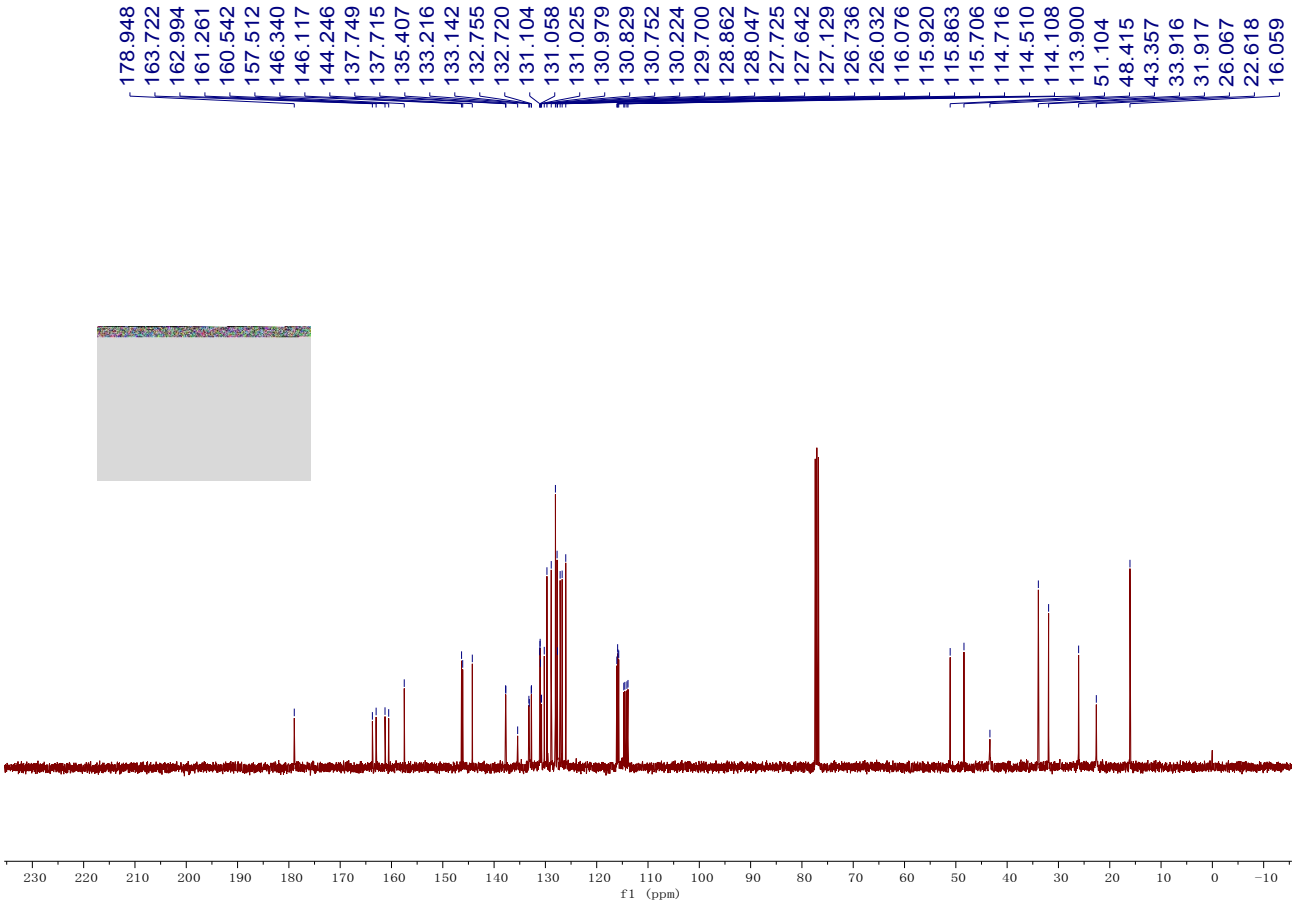


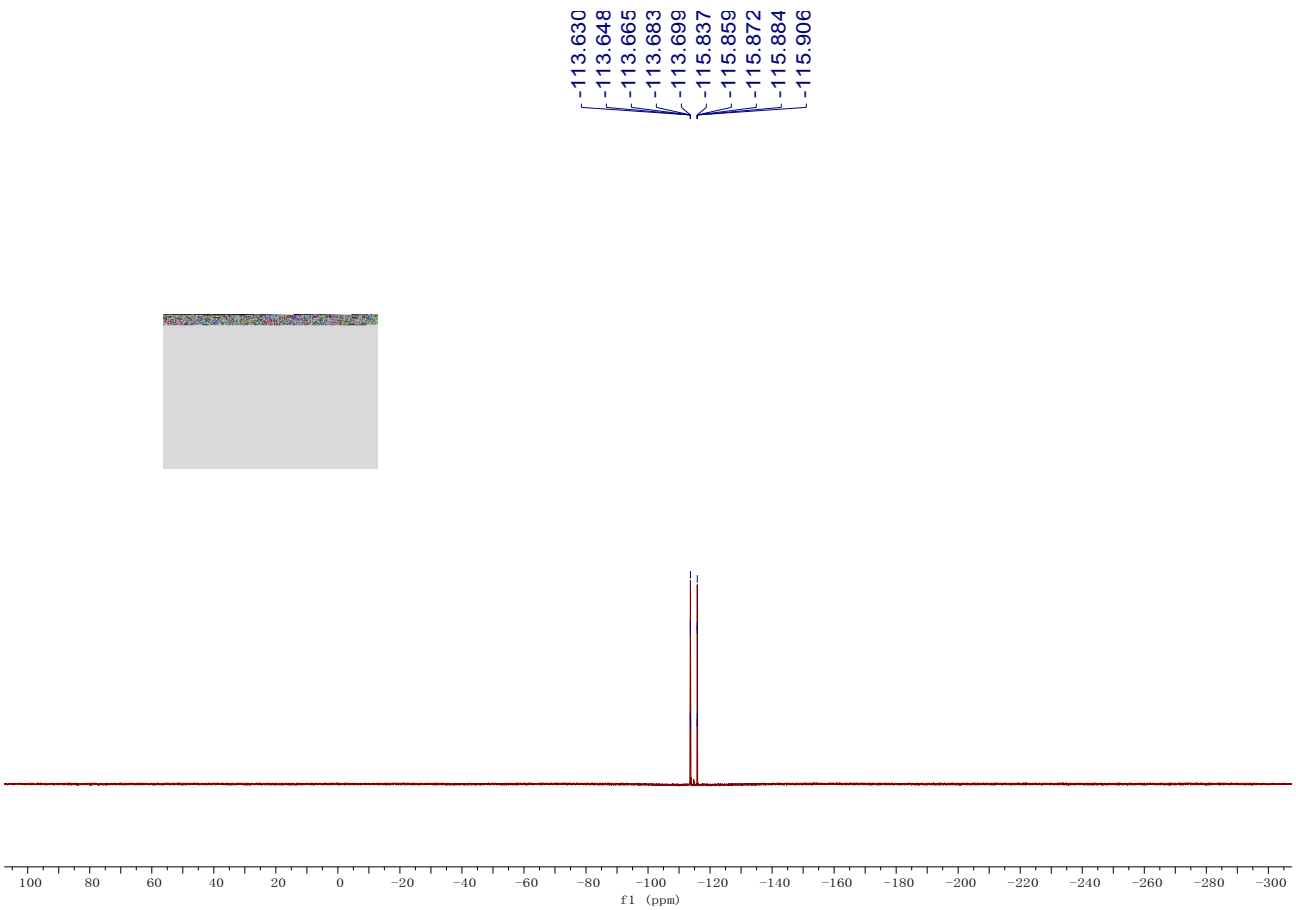


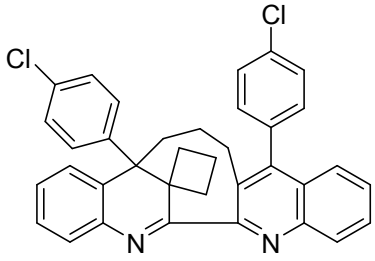
Compound **2b**: Yield: 306 mg, 58%; A brown solid; m.p. 274-276 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.78-0.87 (m, 1H), 1.68-1.94 (m, 5H), 2.04 (dd, J = 14.8 Hz, J = 8.0 Hz, 1H), 2.27-2.33 (m, 1H), 2.43-2.50 (m, 1H), 2.65 (dd, J = 15.2 Hz, J = 10.8 Hz, 1H), 2.79 (dd, J = 17.2 Hz, J = 9.2 Hz, 1H), 2.94 (dd , J = 17.2 Hz, J = 9.2 Hz, 1H), 6.98 (d, J = 7.6 Hz, 1H), 7.04 (td, J = 8.8 Hz, J = 2.8 Hz, 1H), 7.11-7.19 (m, 3H), 7.21-7.26 (m, 3H), 7.31-7.34 (m, 2H), 7.40-7.48 (m, 2H), 7.59-7.62 (m, 2H), 7.68 (t, J = 7.6 Hz, 1H), 8.30 (d, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.1, 22.6, 26.1, 31.9, 33.9, 43.4, 48.4, 51.1, 114.0 (d, $J_{C\text{-}F}$ = 20.8 Hz), 114.6 (d, $J_{C\text{-}F}$ = 20.6 Hz), 115.8 (d, $J_{C\text{-}F}$ = 21.4 Hz), 116.0 (d, $J_{C\text{-}F}$ = 21.3 Hz), 126.0, 126.7, 127.1, 127.6, 127.7, 128.0, 128.9, 129.7, 130.2, 130.8 (d, $J_{C\text{-}F}$ = 7.7 Hz), 131.1 (d, $J_{C\text{-}F}$ = 7.9 Hz), 131.0 (d, $J_{C\text{-}F}$ = 7.9 Hz), 132.7 (d, $J_{C\text{-}}$

$_F$ = 3.5 Hz), 133.2 (d, J_{C-F} = 7.4 Hz), 135.4, 137.7 (d, J_{C-F} = 3.4 Hz), 144.2, 146.1, 146.3, 157.5, 161.2 (d, J_{C-F} = 245.2 Hz), 162.5 (d, J_{C-F} = 246.1 Hz), 178.9; ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$): δ -115.9 (m), -113.7 (m); IR (CH_3COCH_3): ν 3063, 2995, 2944, 2867, 1711, 1603, 1509, 1448, 1360, 1220, 1159, 1093, 1015, 907, 840, 764, 734 cm^{-1}; MS (ESI) m/z 527.2 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{36}H_{29}N_2F_2$: 527.22933, Found: 527.22811.

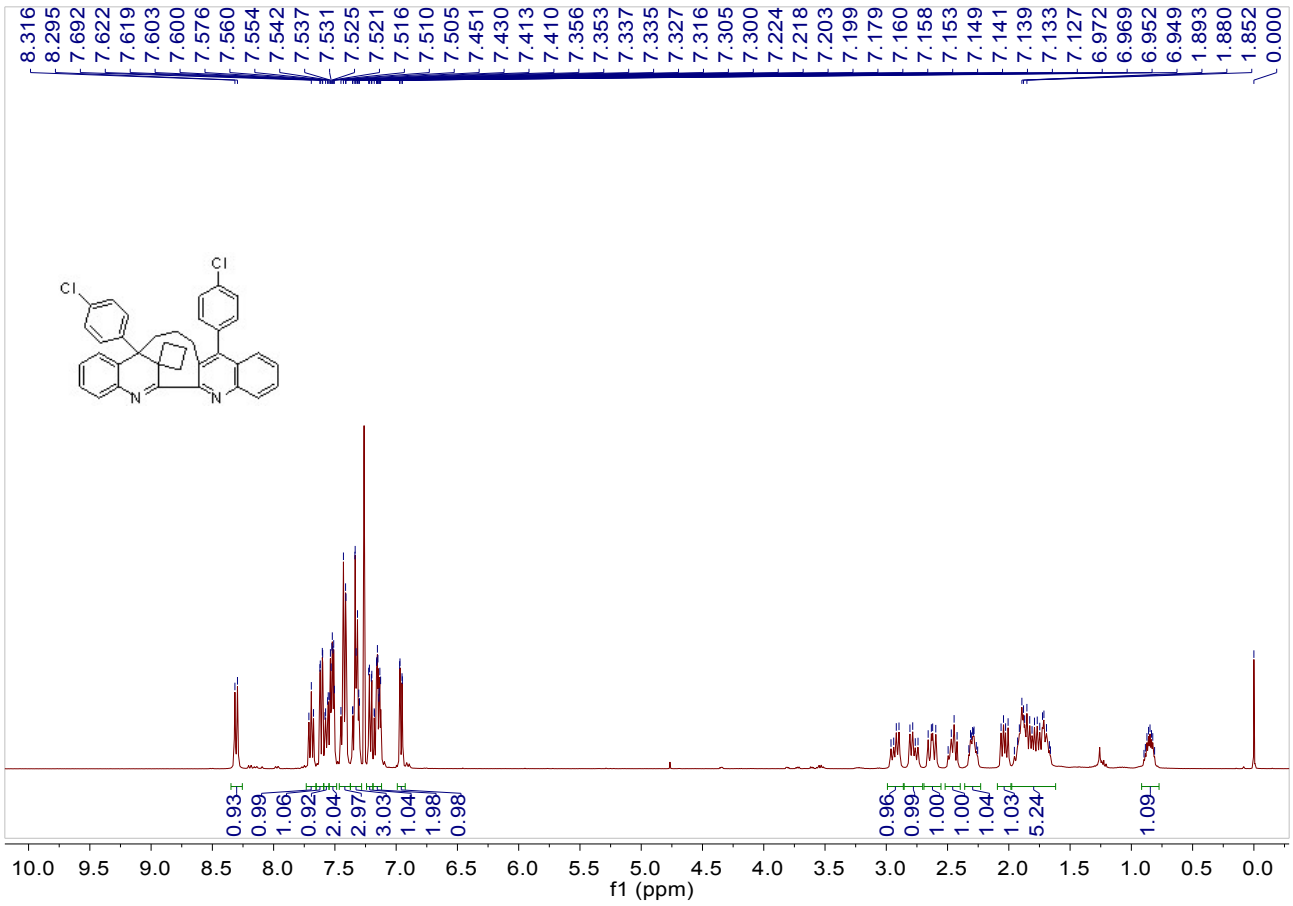


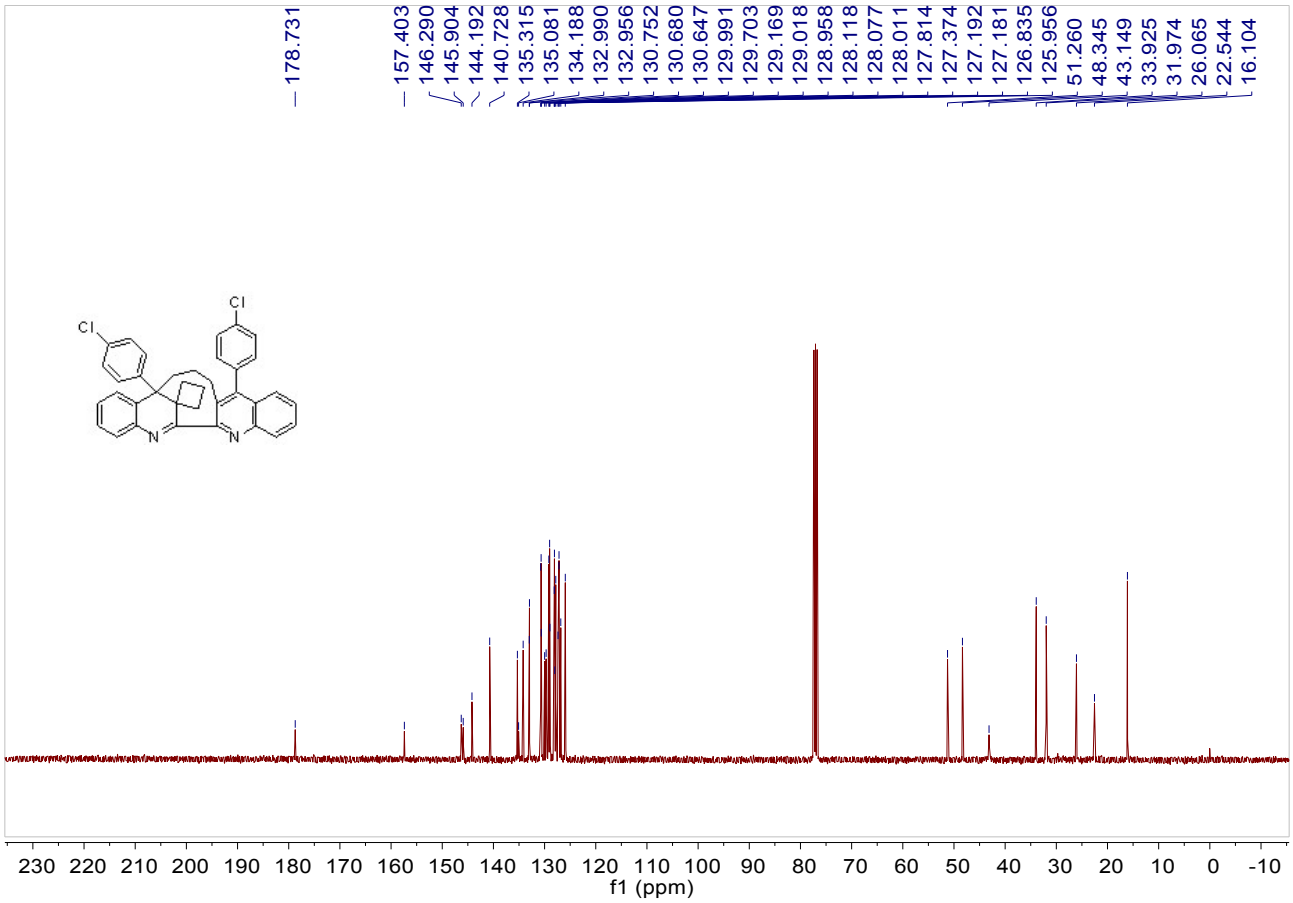

178.948
163.722
162.994
161.261
160.542
157.512
146.340
146.117
144.246
137.749
137.715
135.407
133.216
133.142
132.755
132.720
131.104
131.058
131.025
130.979
130.829
130.752
130.224
129.700
128.862
128.047
127.725
127.642
127.129
126.736
126.032
116.076
115.920
115.863
115.706
114.716
114.510
114.108
113.900
51.104
48.415
43.357
33.916
31.917
26.067
22.618
16.059
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

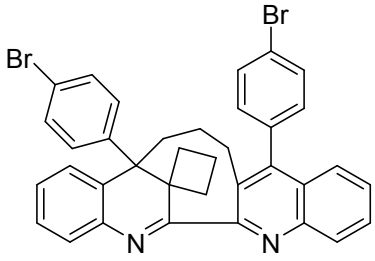

-113.630
-113.648
-113.665
-113.683
-113.699
-115.837
-115.859
-115.872
-115.884
-115.906
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 −180 −200 −220 −240 −260 −280 −300
f1 (ppm)



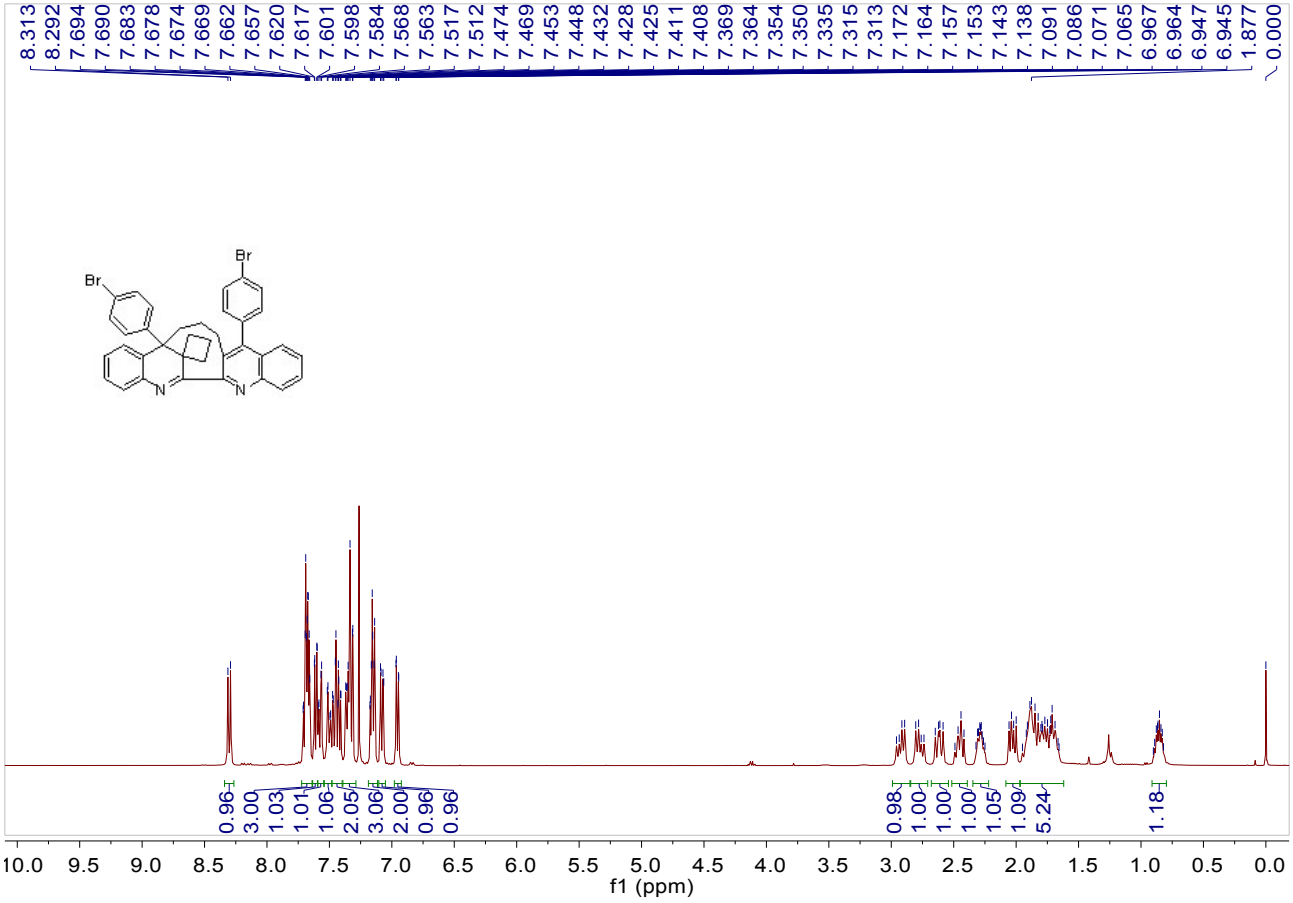
Compound **2c**: Yield: 67 mg, 48%; A brown solid; m.p. 342-344 ^{o}C; ^{1} H NMR (400 MHz, $CDCl_3$, TMS): δ 0.81-0.90 (m, 1H), 1.66-1.93 (m, 5H), 2.03 (dd, *J* = 14.8 Hz, *J* = 8.0 Hz, 1H), 2.25-2.33 (m, 1H), 2.42-2.50 (m, 1H), 2.63 (dd, *J* = 14.4 Hz, *J* = 10.4 Hz, 1H), 2.77 (dd, *J* = 17.6 Hz, *J* = 8.8 Hz, 1H), 2.93 (dd , *J* = 17.6 Hz, *J* = 9.2 Hz, 1H) 6.96 (dd, *J* = 8.0 Hz, *J* = 1.2 Hz, 1H), 7.13-7.18 (m, 2H), 7.21 (dd, *J* = 8.0 Hz, *J* = 2.0 Hz, 1H), 7.30-7.36 (m, 3H), 7.41-7.45 (m, 3H), 7.51-7.54 (m, 2H), 7.57 (dd, *J* = 8.6 Hz, *J* = 1.2 Hz, 1H), 7.61 (dd, *J* = 7.6 Hz, *J* = 1.2 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 8.31 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.1, 22.5, 26.1, 32.0, 33.9, 43.1, 48.3, 51.3, 126.0, 126.8, 127.18, 127.19, 127.4, 127.8, 128.0, 128.08, 128.12, 128.96, 129.02, 129.2, 129.7, 130.0, 130.6, 130.7, 130.8, 132.96, 132.99, 134.2, 135.1, 135.3, 140.7, 144.2, 145.9, 146.3, 157.4, 178.7; IR (CH_3COCH_3): ν 3061, 2943, 2869, 1712, 1621, 1594, 1559, 1485, 1449, 1396, 1359, 1219, 1117, 1088, 1034, 1014, 993, 907, 833, 814, 763, 748, 684 cm^{-1}; MS (ESI) m/z 559.2 $(M+H)^{+}$; HRMS (ESI) Calcd. for $C_{36}H_{29}N_2Cl_2$: 559.1702, Found: 559.1702.

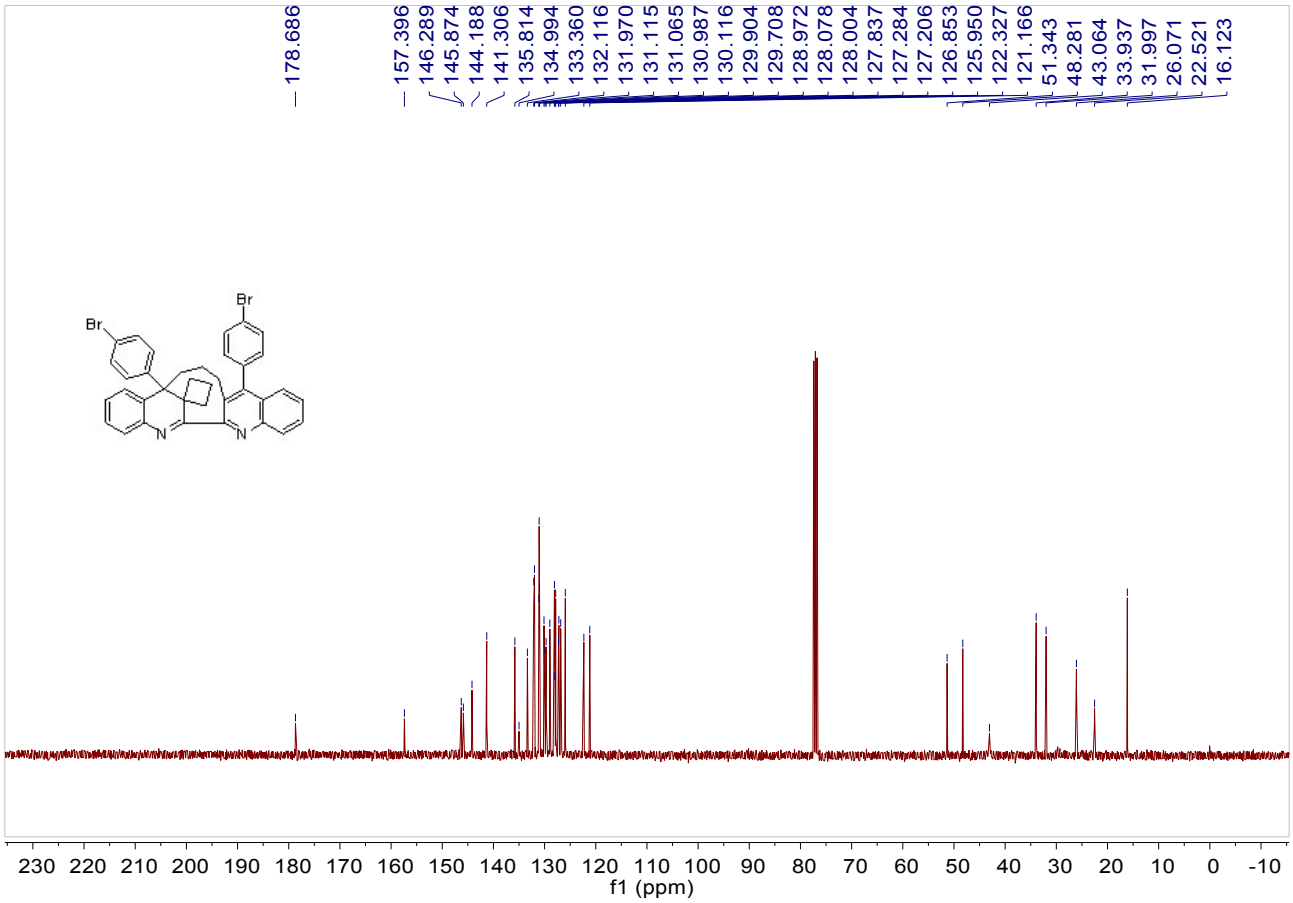

8.316
8.295
7.692
7.622
7.619
7.603
7.600
7.576
7.560
7.554
7.542
7.537
7.531
7.525
7.521
7.516
7.510
7.505
7.451
7.430
7.413
7.410
7.356
7.353
7.337
7.335
7.327
7.316
7.305
7.300
7.224
7.218
7.203
7.199
7.179
7.160
7.158
7.153
7.149
7.141
7.139
7.133
7.127
6.972
6.969
6.952
6.949
1.893
1.880
1.852
0.000
Cl
Cl
N
N
0.93
0.99
1.06
0.92
2.04
2.97
3.03
1.04
1.98
0.98
0.96
0.99
1.00
1.00
1.04
1.03
5.24
1.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

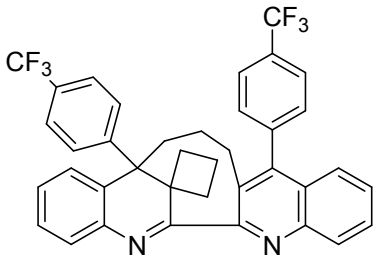

178.731
157.403
146.290
145.904
144.192
140.728
135.315
135.081
134.188
132.990
132.956
130.752
130.680
130.647
129.991
129.703
129.169
129.018
128.958
128.118
128.077
128.011
127.814
127.374
127.192
127.181
126.835
125.956
51.260
48.345
43.149
33.925
31.974
26.065
22.544
16.104
Cl
Cl
N
N
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



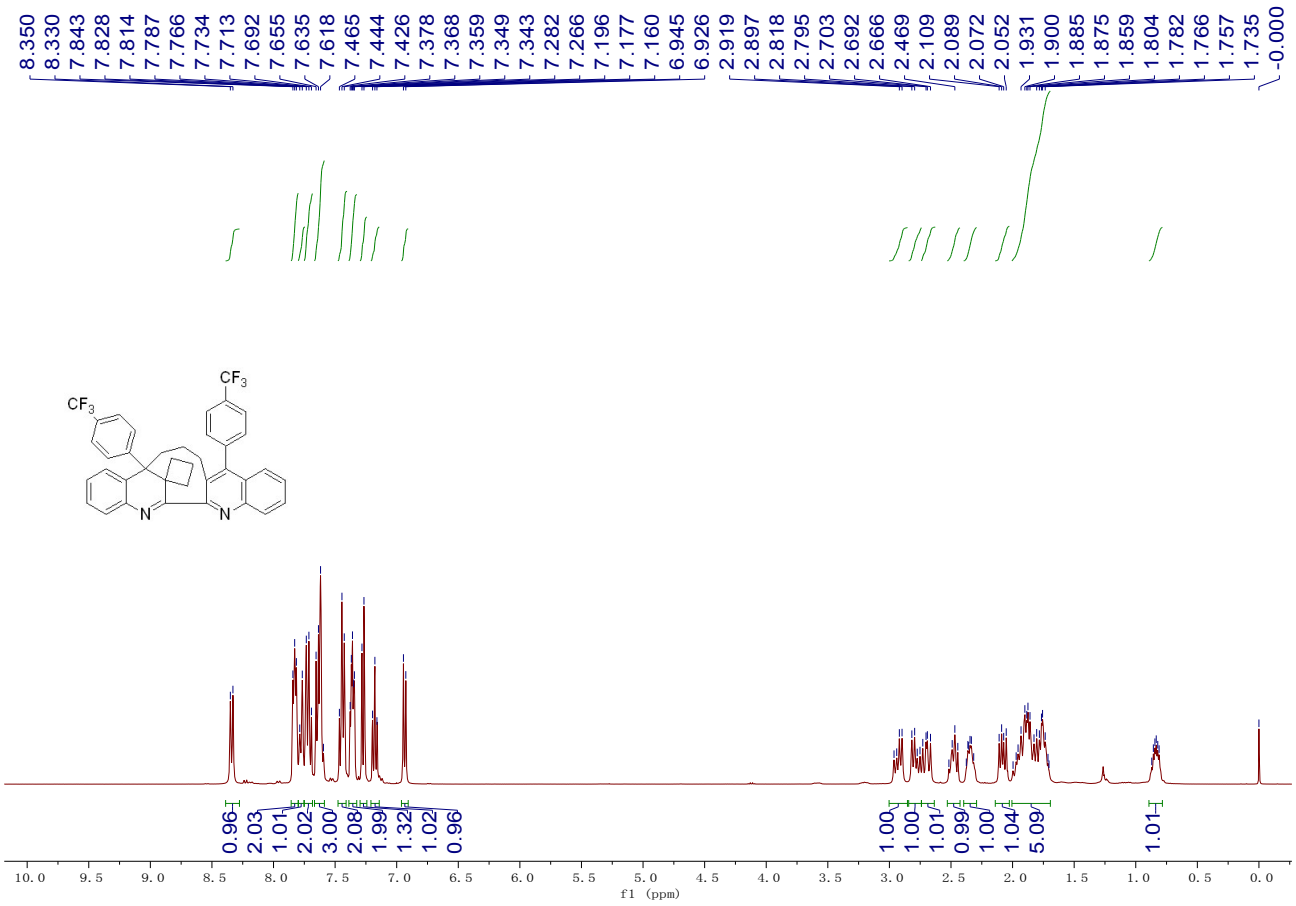
Compound **2d**: Yield: 151 mg, 47%; A brown solid; m.p. 366-368 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.82-0.90 (m, 1H), 1.66-1.92 (m, 5H), 2.03 (dd, *J* = 14.8 Hz, *J* = 8.0 Hz, 1H), 2.25-2.32 (m, 1H), 2.42-2.49 (m, 1H), 2.62 (dd, *J* = 14.8 Hz, *J* = 10.8 Hz, 1H), 2.77 (dd, *J* = 17.6 Hz, *J* = 9.2 Hz, 1H), 2.93 (dd , *J* = 17.2 Hz, *J* = 8.8 Hz, 1H), 6.96 (dd, *J* = 7.8 Hz, *J* = 1.0 Hz, 1H), 7.08 (dd, *J* = 8.2 Hz, *J* = 2.2 Hz, 2H), 7.14-7.18 (m, 2H), 7.31-7.37 (m, 3H), 7.41-7.47 (m, 2H), 7.50 (dd, *J* = 8.8 Hz, *J* = 2.0 Hz, 1H), 7.58 (dd, *J* = 8.4 Hz, *J* = 2.0 Hz, 1H), 7.61 (dd, *J* = 7.8 Hz, *J* = 1.2 Hz, 1H), 7.66-7.71 (m, 3H), 8.30 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.1, 22.5, 26.1, 32.0, 33.9, 43.1, 48.3, 51.3, 121.2, 122.3, 125.9, 126.9, 127.2, 127.3, 127.8, 128.0, 128.1, 129.0, 129.7, 129.9, 130.1, 131.0, 131.07, 131.12, 132.0, 132.1, 133.4, 135.0, 135.8, 141.3, 144.2, 145.9, 146.3, 157.4, 178.7; IR (CH_3COCH_3): ν 3061, 2943, 2864, 1712, 1622, 1591, 1567, 1484, 1449, 1390, 1360, 1268, 1220, 1187, 1117, 1070, 1010, 907, 829, 813, 763, 748, 716 cm^{-1}; MS (ESI) m/z 647.1 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{36}H_{29}N_2Br_2$: 647.0692, Found: 647.0689.

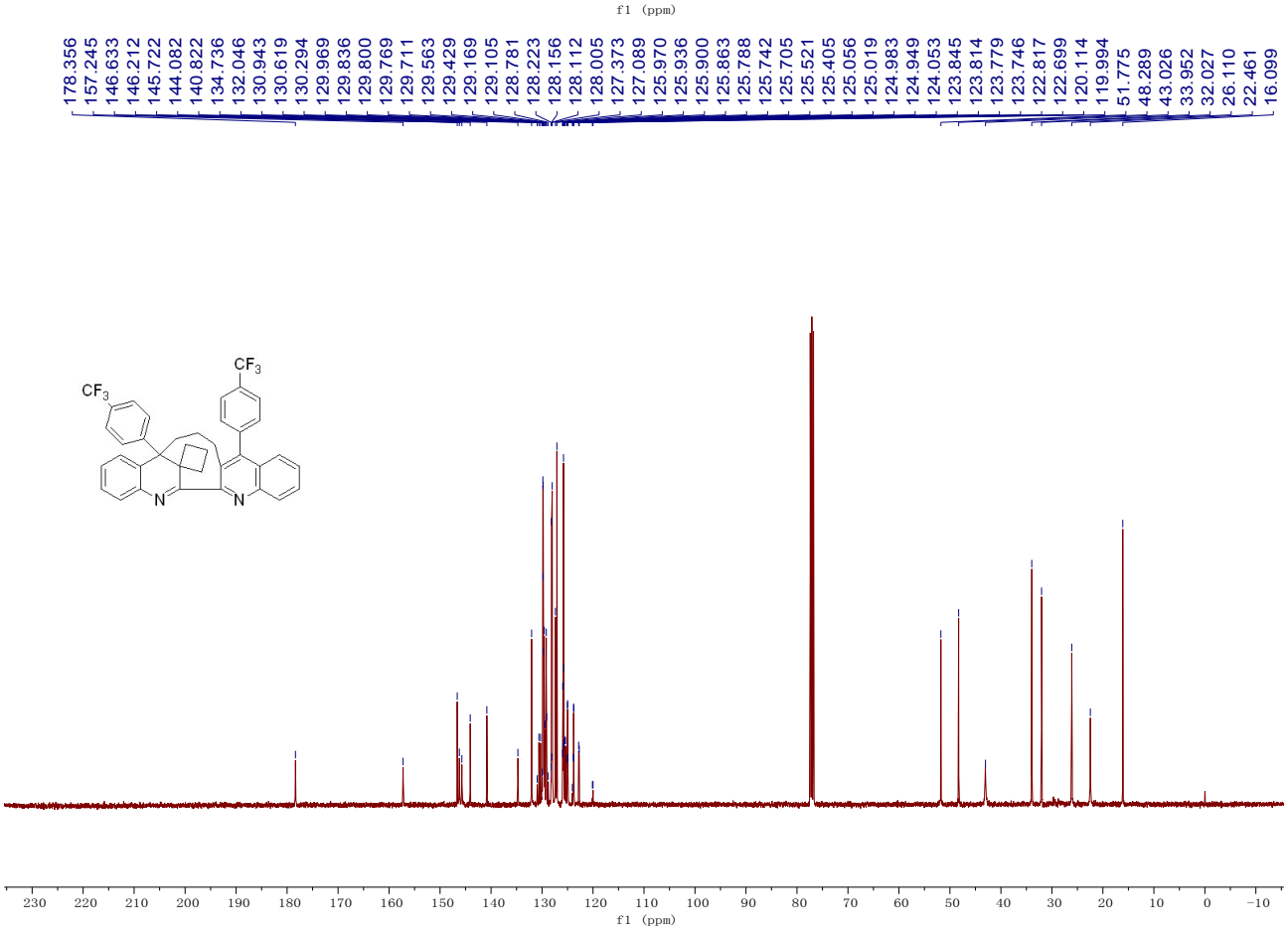

8.313
8.292
7.694
7.690
7.683
7.678
7.674
7.669
7.662
7.657
7.620
7.617
7.601
7.598
7.584
7.568
7.563
7.517
7.512
7.474
7.469
7.453
7.448
7.432
7.428
7.425
7.411
7.408
7.369
7.364
7.354
7.350
7.335
7.315
7.313
7.172
7.164
7.157
7.153
7.143
7.138
7.091
7.086
7.071
7.065
6.967
6.964
6.947
6.945
1.877
0.000
Br
Br
N
N
0.96
3.00
1.03
1.01
1.06
2.05
3.06
2.00
0.96
0.96
0.98
1.00
1.00
1.00
1.05
1.09
5.24
1.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

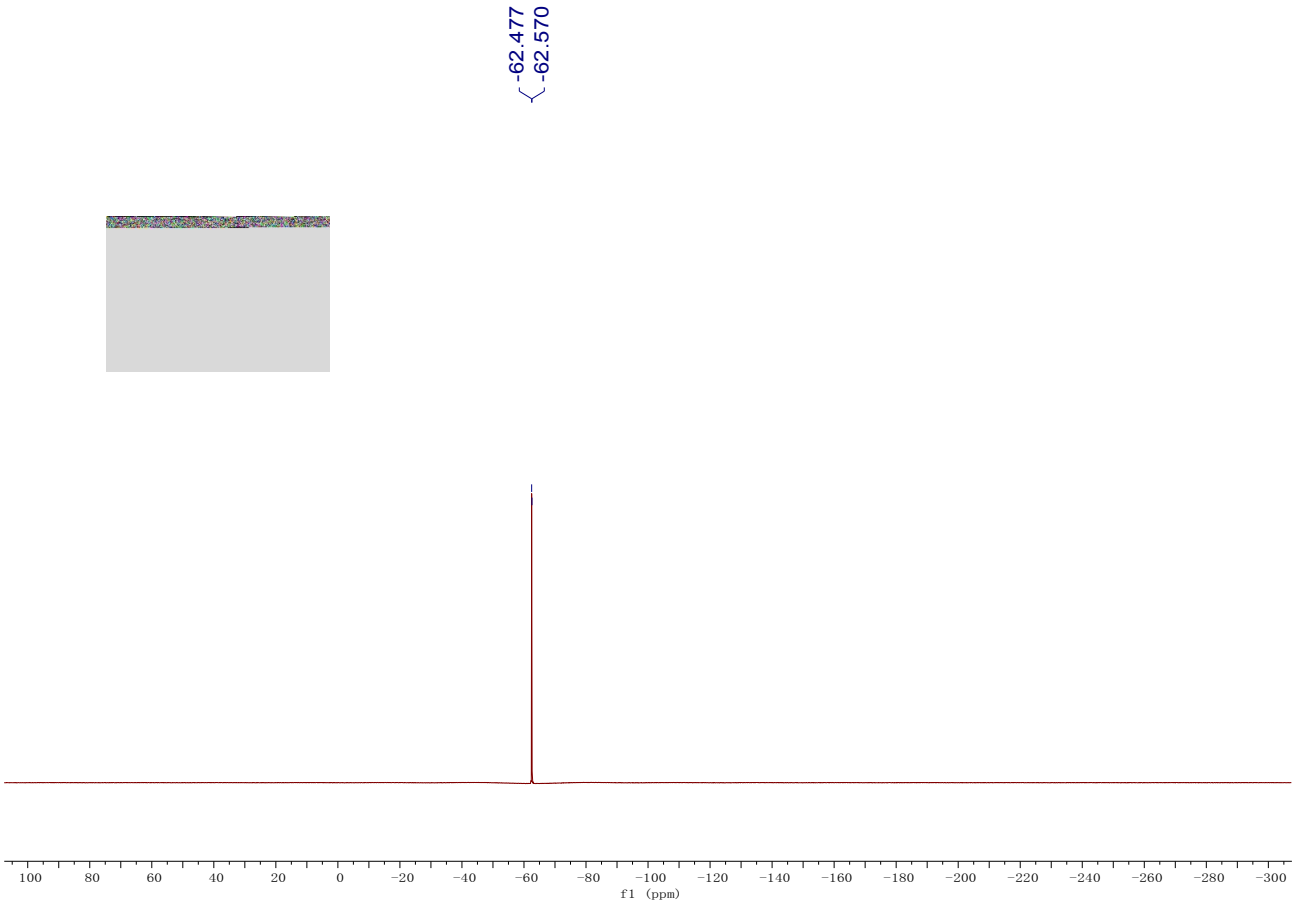

178.686
157.396
146.289
145.874
144.188
141.306
135.814
134.994
133.360
132.116
131.970
131.115
131.065
130.987
130.116
129.904
129.708
128.972
128.078
128.004
127.837
127.284
127.206
126.853
125.950
122.327
121.166
51.343
48.281
43.064
33.937
31.997
26.071
22.521
16.123
Br
Br
N
N
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

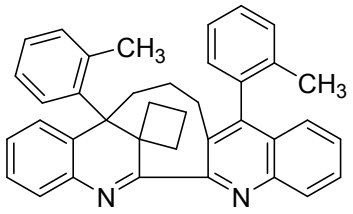


Compound **2e**: Yield: 278 mg, 44%; A brown solid; m.p. 348-350 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.81-0.87 (m, 1H), 1.70-2.00 (m, 5H), 2.08 (dd, *J* = 14.8 Hz, *J* = 8.0 Hz, 1H), 2.32-2.38 (m, 1H), 2.45-2.52 (m, 1H), 2.70 (dd, *J* = 14.8 Hz, *J* = 10.4 Hz, 1H), 2.78 (dd, *J* = 17.6 Hz, *J* = 9.2 Hz, 1H), 2.93 (dd , *J* = 17.6 Hz, *J* = 9.2 Hz, 1H), 6.94 (d, *J* = 7.6 Hz, 1H), 7.18 (t, *J* = 7.2 Hz, 1H), 7.27 (d, *J* = 6.4 Hz, 1H), 7.34-7.38 (m, 2H), 7.74 (t, *J* = 7.8 Hz, 1H), 7.60-7.66 (m, 3H), 7.69-7.73 (m, 2H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.81-7.84 (m, 2H), 8.34 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.1, 22.5, 26.1, 32.0, 34.0, 43.0, 48.3, 51.8, 123.8 (q, $J_{C\text{-}F}$ = 3.5 Hz), 124.052 (q, $J_{C\text{-}F}$ = 270.6 Hz), 124.053, 124.2 (q, $J_{C\text{-}F}$ = 270.4 Hz), 125.0 (q, $J_{C\text{-}F}$ = 3.6 Hz), 125.76 (q, $J_{C\text{-}F}$ = 3.7 Hz), 125.79, 125.9 (q, $J_{C\text{-}F}$ = 3.6 Hz), 127.1, 127.4, 128.0, 128.2, 129.2, 129.3 (q, $J_{C\text{-}F}$ = 32.4 Hz), 129.6, 129.7, 129.77, 129.80, 129.84, 130.5 (q, $J_{C\text{-}F}$ = 32.5 Hz), 132.0, 134.7, 140.8, 144.1, 145.7, 146.2, 146.6, 157.2, 178.4; ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$): δ -62.6 (s), -62.5 (s); IR (CH_3COCH_3): ν 3068, 2935, 2854, 1713, 1617, 1491, 1408, 1361, 1324, 1221, 1164, 1119, 1067, 1018, 842, 766 cm^{-1}; MS (ESI) m/z 627.2 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{38}H_{29}N_2F_6$: 627.22294, Found: 627.22156.


8.350
8.330
7.843
7.828
7.814
7.787
7.766
7.734
7.713
7.692
7.655
7.635
7.618
7.465
7.444
7.426
7.378
7.368
7.359
7.349
7.343
7.282
7.266
7.196
7.177
7.160
6.945
6.926
2.919
2.897
2.818
2.795
2.703
2.692
2.666
2.469
2.109
2.089
2.072
2.052
1.931
1.900
1.885
1.875
1.859
1.804
1.782
1.766
1.757
1.735
-0.000
CF3
CF3
N
N
0.96
2.03
1.01
2.02
3.00
2.08
1.99
1.32
1.02
0.96
1.00
1.00
1.01
0.99
1.00
1.04
5.09
1.01
f1 (ppm)

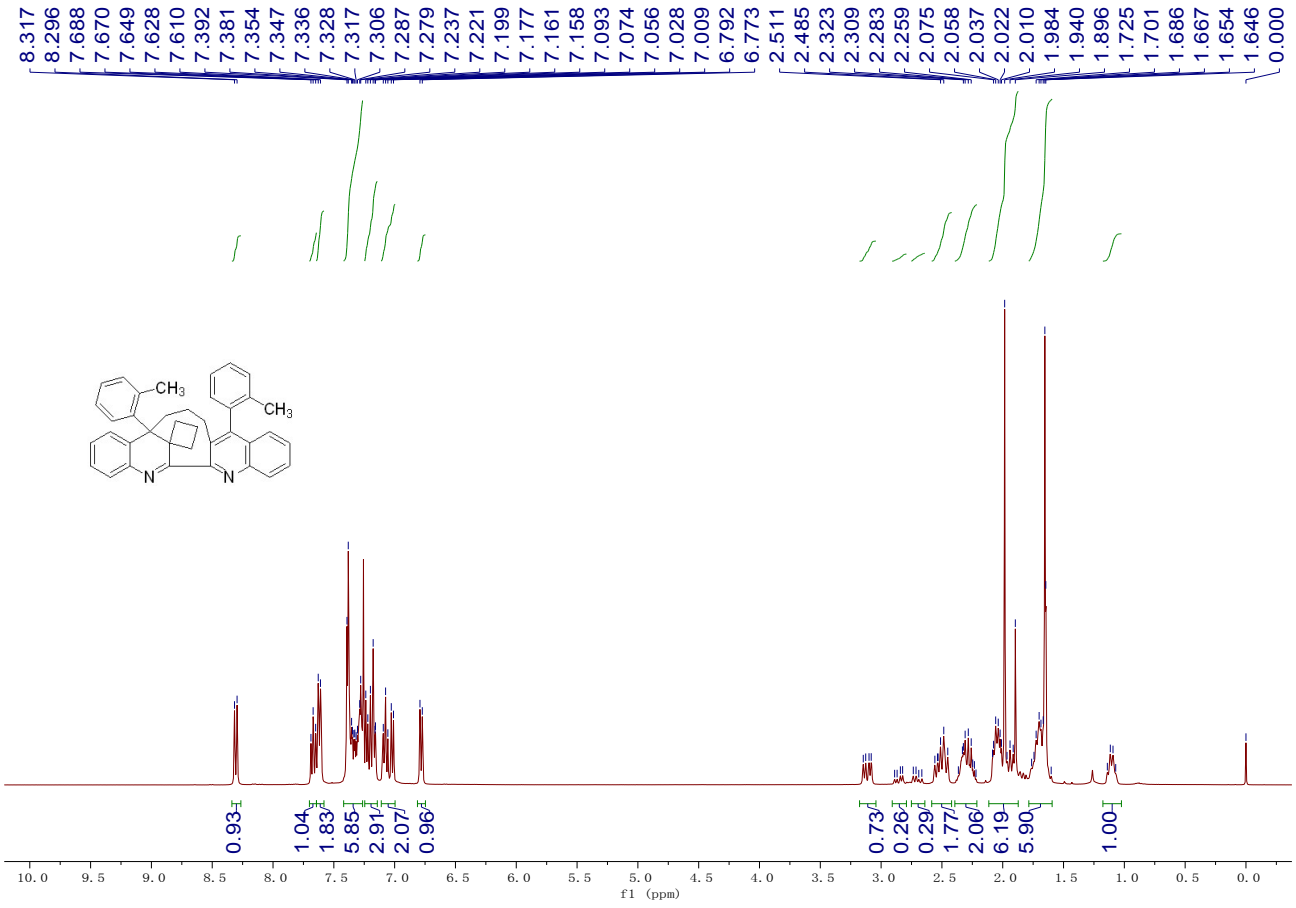

178.356
157.245
146.633
146.212
145.722
144.082
140.822
134.736
132.046
130.943
130.619
130.294
129.969
129.836
129.800
129.769
129.711
129.563
129.429
129.169
129.105
128.781
128.223
128.156
128.112
128.005
127.373
127.089
125.970
125.936
125.900
125.863
125.788
125.742
125.705
125.521
125.405
125.056
125.019
124.983
124.949
124.053
123.845
123.814
123.779
123.746
122.817
122.699
120.114
119.994
51.775
48.289
43.026
33.952
32.027
26.110
22.461
16.099
CF3
CF3
N
N
f1 (ppm)

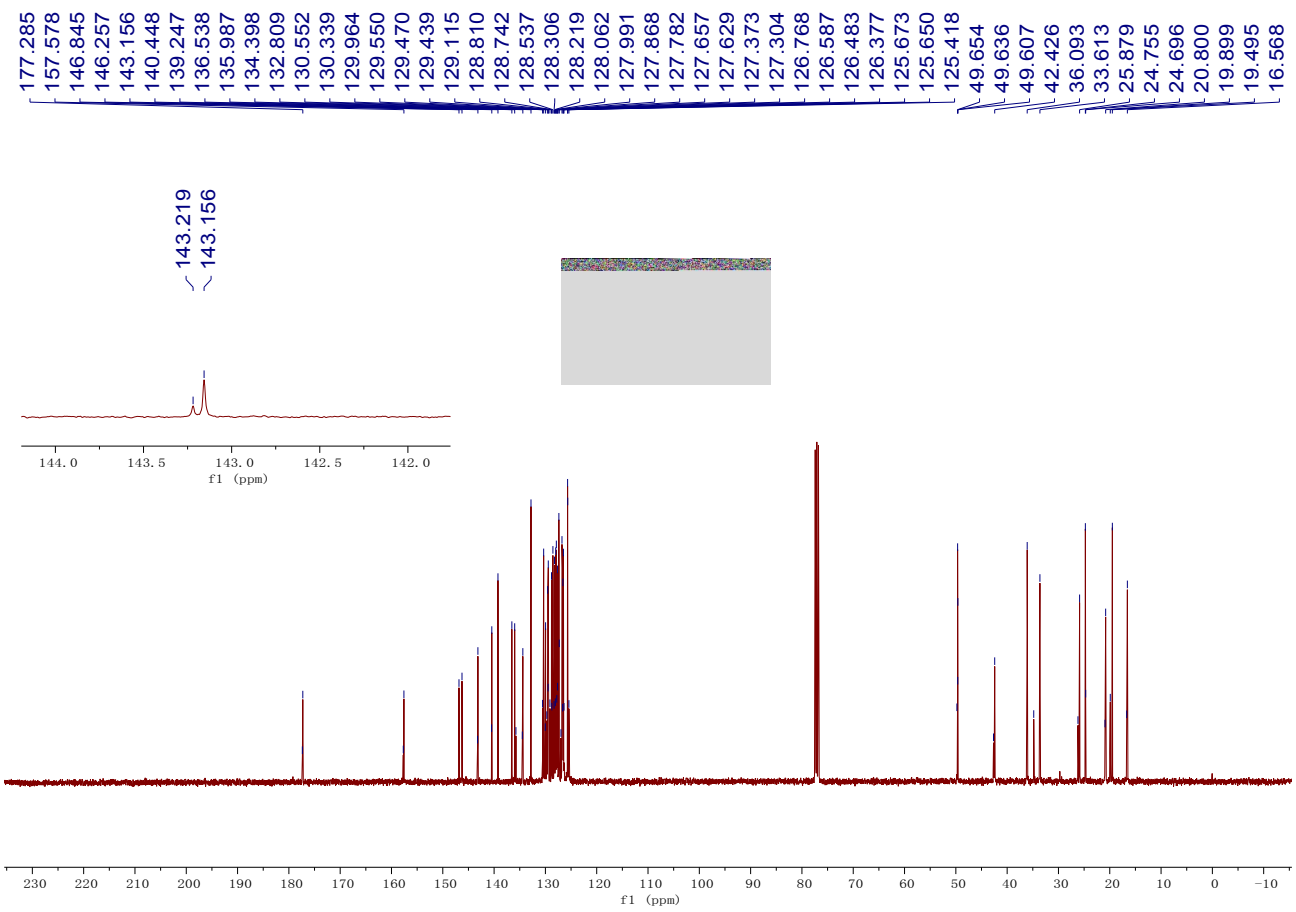


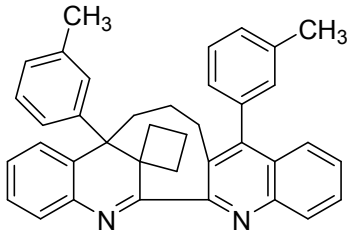


Compound **2f** (atropisomers: 2.7:1): Yield: 142 mg, 27%; A brown solid; m.p. 204-206 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.07-1.14 (m, 1H), 1.60-1.76 (m, 6H), 1.90-2.08 (m, 6H), 2.22-2.37 (m, 2H), 2.45-2.56 (m, 1.77 H), 2.70 (dd, *J* = 18.0 Hz, *J* = 8.8 Hz, 0.29 H), 2.86 (dd, *J* = 18.4 Hz, *J* = 8.0 Hz, 0.26 H), 3.11 (dd, *J* = 18.4 Hz, *J* = 8.0 Hz, 0.73 H), 6.78 (d, *J* = 7.6 Hz, 1H), 7.01-7.09 (m, 2H), 7.16-7.24 (m, 3H), 7.28-7.39 (m, 6H), 7.62 (d, *J* = 7.2 Hz, 2H), 7.67 (t, *J* = 7.8 Hz,, 1H), 8.31 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.6, 16.7, 19.5, 19.9, 20.8, 20.9, 24.7, 24.8, 25.9, 26.2, 33.6, 34.8, 36.1, 42.4, 42.7, 49.61, 49.64, 49.7, 49.8, 125.4, 125.65, 125.67, 126.4, 126.5, 126.6, 126.7, 126.8, 127.0, 127.3, 127.4, 127.6, 127.7, 127.8, 127.9, 128.0, 128.1, 128.2, 128.3, 128.5, 128.7, 128.8, 129.1, 129.4, 129.5, 129.6, 129.7, 129.96, 130.3, 130.3, 130.6, 132.8, 134.4, 134.5, 135.7, 136.0, 136.5, 139.2, 140.4, 140.5, 143.16, 143.22, 146.3, 146.8,

157.6, 157.7, 177.3, 177.4; IR (CH_3COCH_3): ν 3063, 2995, 2925, 1711, 1566, 1449, 1359, 1220, 1091, 993, 906, 766, 750, 733, 683 cm^{-1}; MS (ESI) m/z 519.3 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{38}H_{35}N_2$: 519.27948, Found: 519.27820.

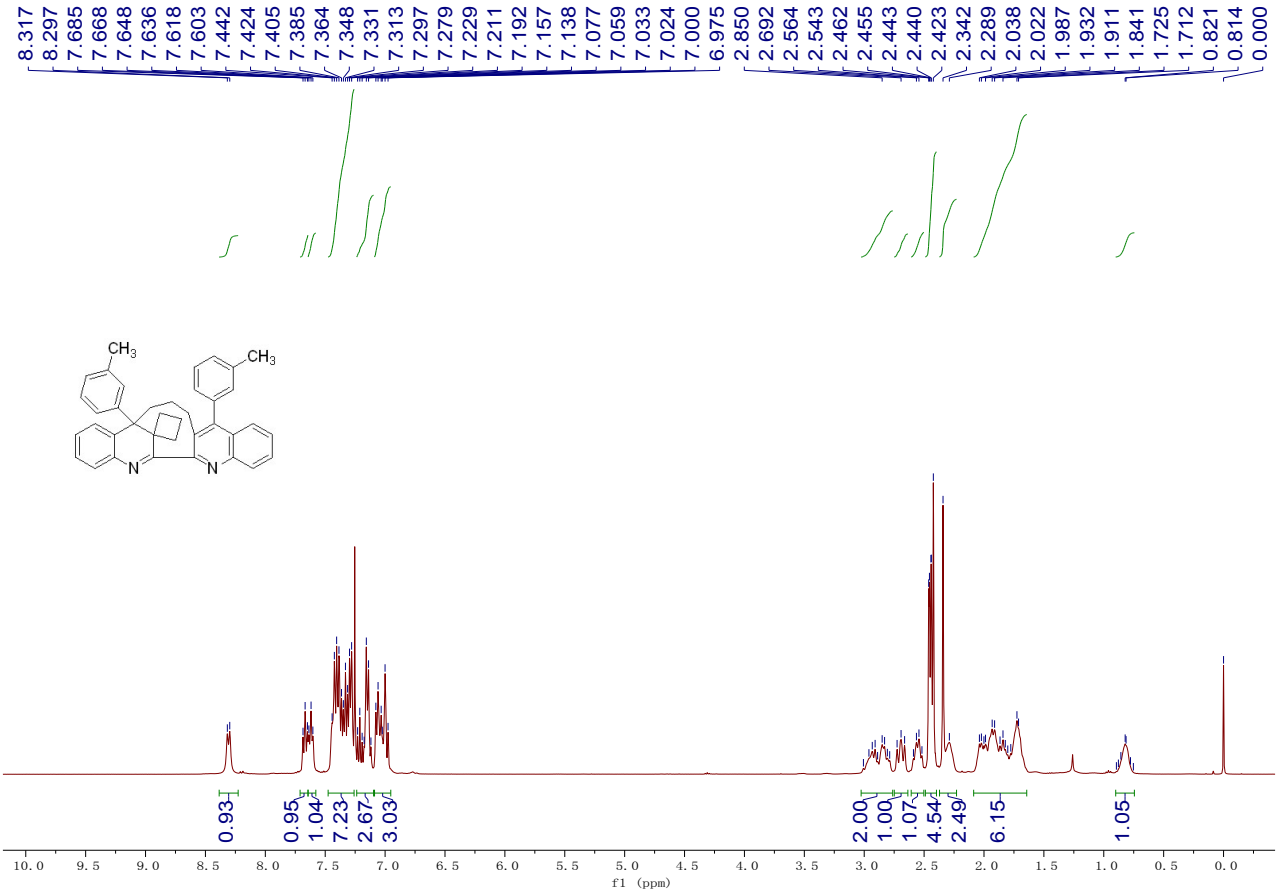


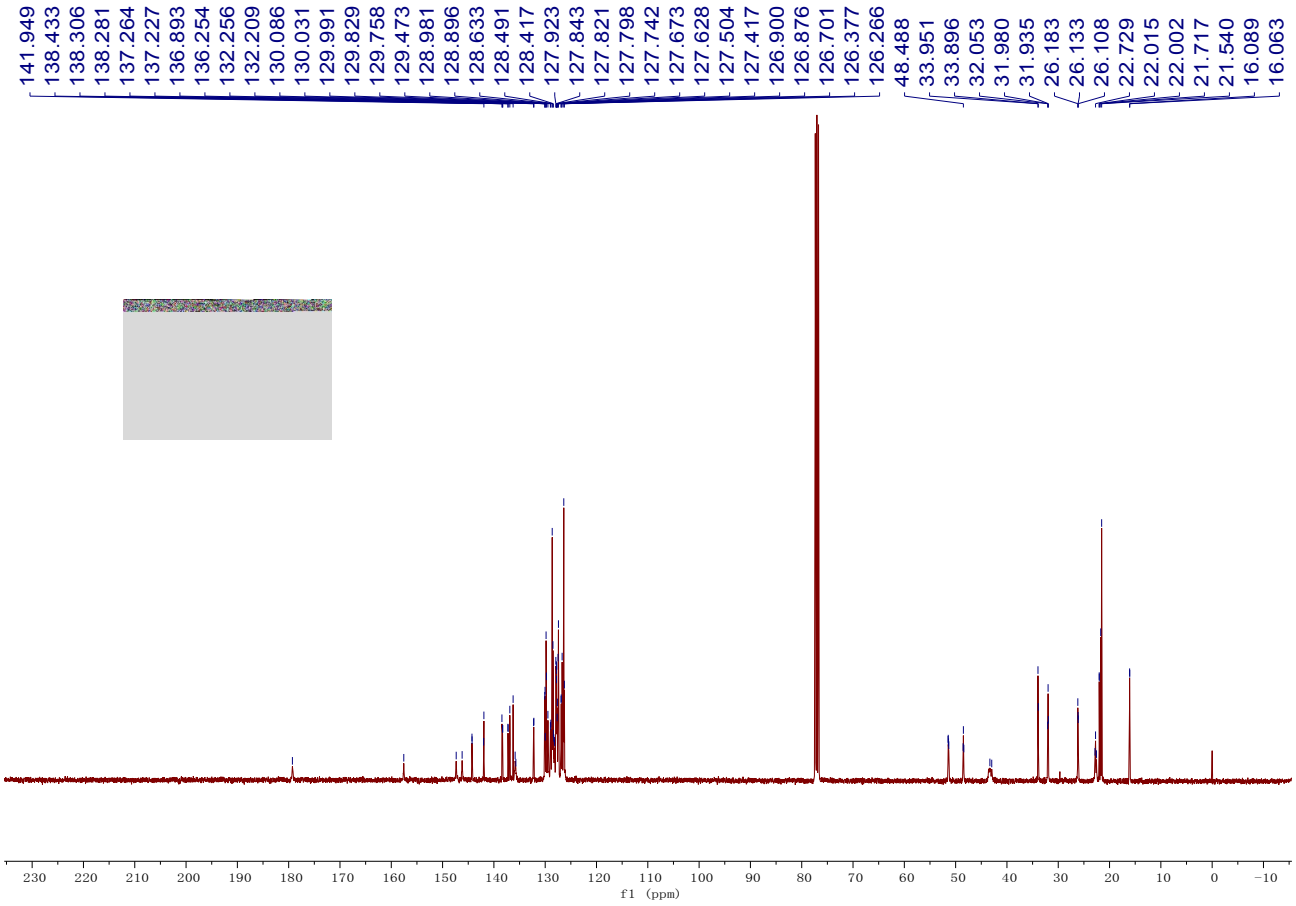


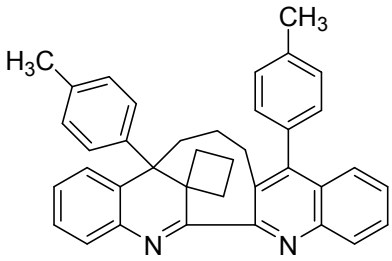


Compound **2g** (atropisomers): Yield: 291 mg, 56%; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.75-0.90 (m, 1H), 1.71-2.04 (m, 6H), 2.29-2.34 (m, 2.49H), 2.42-2.46 (m, 4.54H), 2.52-2.59 (m, 1H), 2.66-2.73 (m, 1H), 2.79-3.01 (m, 2H), 6.98-7.08 (m, 3H), 7.12-7.23 (m, 2.67H), 7.28-7.44 (m, 7.23H), 7.62 (t, *J* = 6.6 Hz, 1H), 7.67 (t, *J* = 7.4 Hz, 1H), 8.31 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.06, 16.09, 21.5, 21.7, 22.00, 22.02, 22.6, 22.7, 22.8, 26.11, 26.13, 26.2, 31.9, 32.0, 32.1, 33.9, 34.0, 43.0, 43.3, 48.4, 48.49, 48.54, 51.3, 51.38, 51.45, 51.5, 126.3, 126.4, 126.7, 126.88, 126.90, 127.4, 127.5, 127.6, 127.67, 127.74, 127.80, 127.82, 127.84, 127.9, 128.16, 128.20, 128.3, 128.4, 128.5, 128.6, 128.9, 129.0, 129.5, 129.76, 129.83, 129.99, 130.03, 130.1, 132.2, 132.3, 135.7, 135.9, 136.3, 136.9, 137.2, 137.3, 138.28, 138.31, 138.4, 141.9, 142.0, 144.25, 144.27, 146.2, 147.3, 157.6, 179.3; IR (CH_3COCH_3): ν 3055, 2943, 2851, 1712, 1603, 1566, 1450,

1360, 1263, 1220, 1116, 1091, 1034, 1009, 919, 791, 766, 720, 707 cm^{-1}; MS (ESI) m/z 519.3 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{38}H_{35}N_2$: 519.27948, Found: 519.27864.

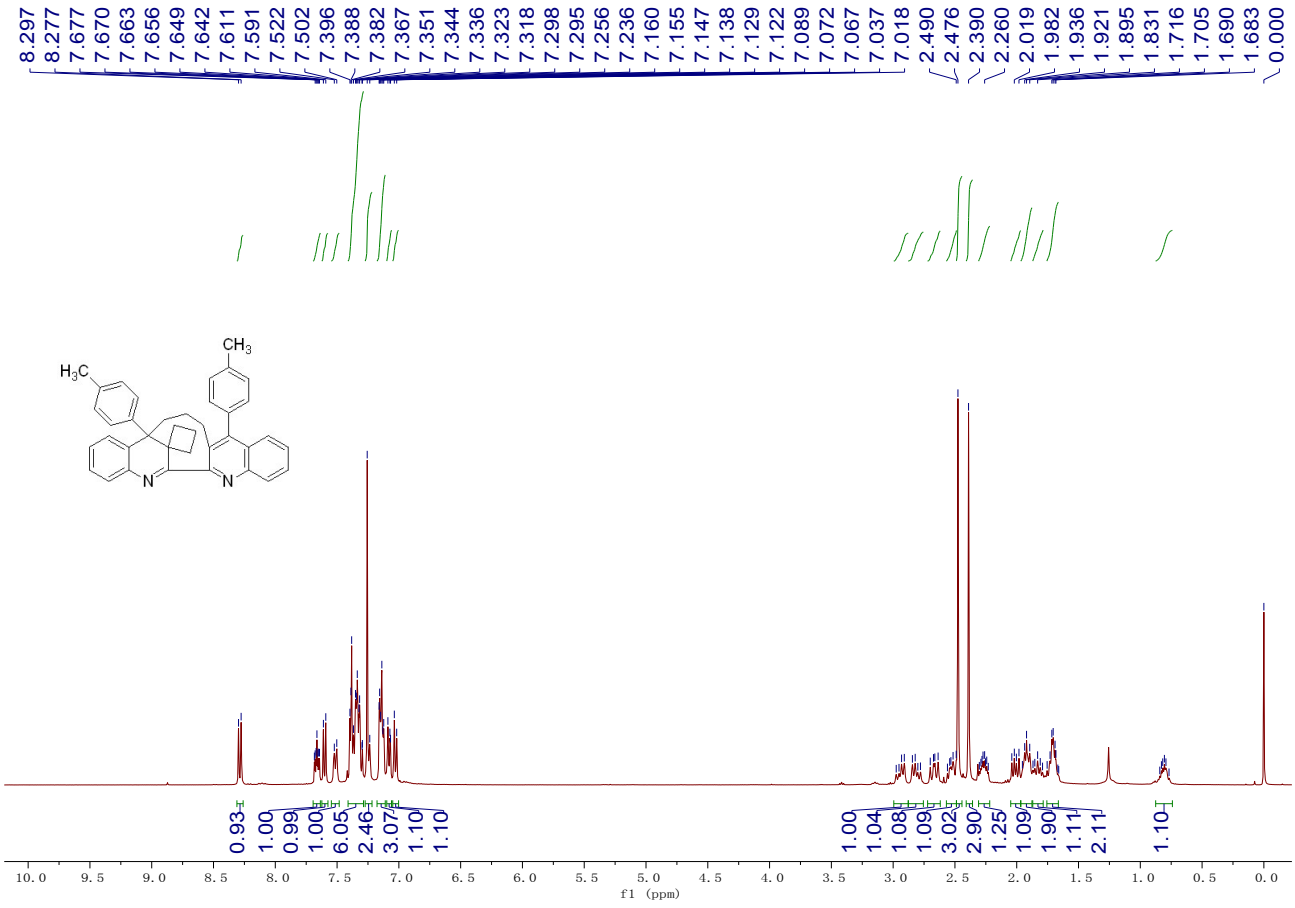


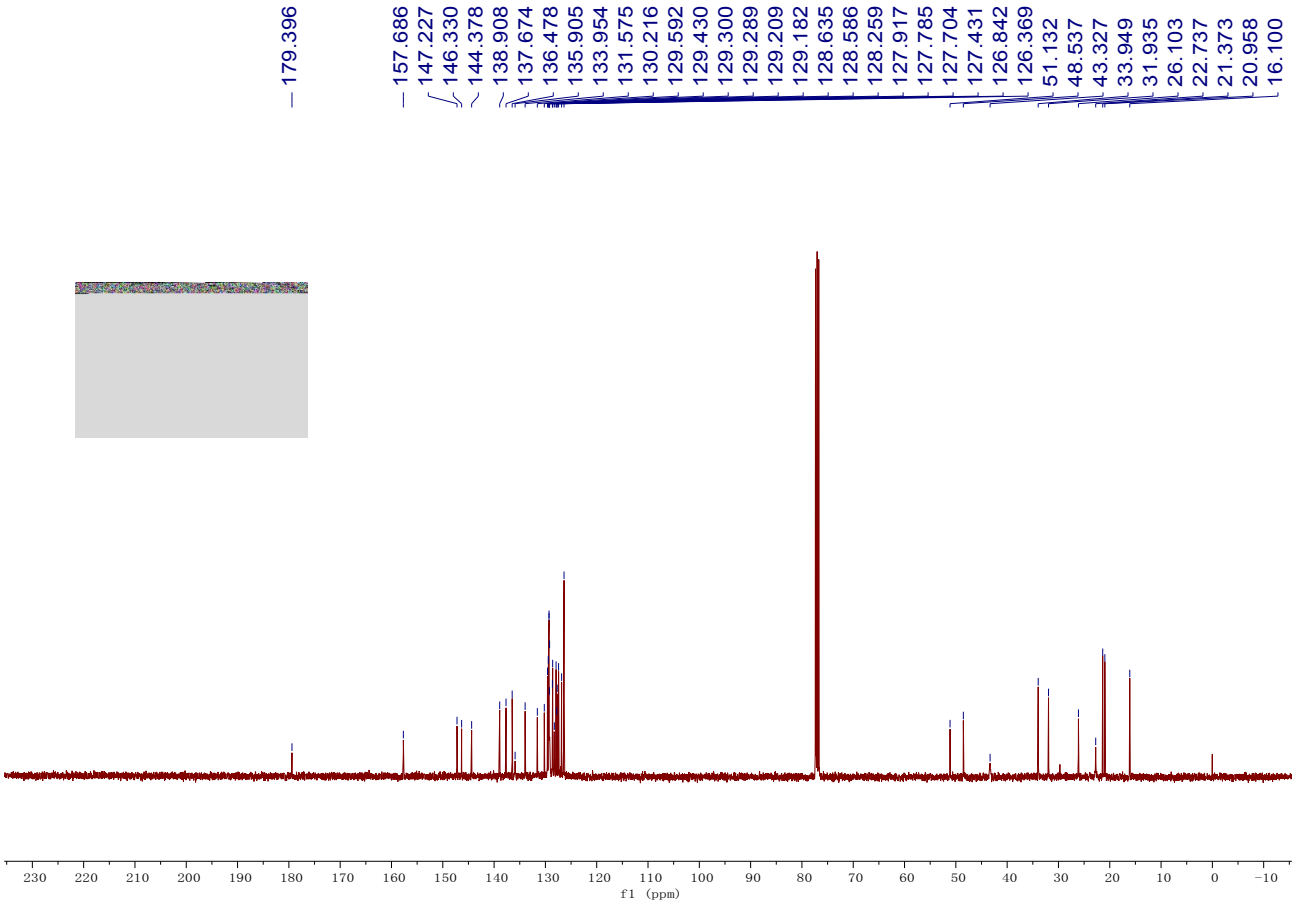


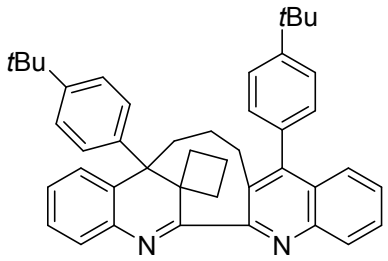


Compound **2h**: Yield: 134 mg, 26%; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.77-0.84 (m, 1H), 1.66-1.75 (m, 2H), 1.79-1.87 (m, 1H), 1.90-1.95 (m, 2H), 2.01 (dd, *J* = 14.8 Hz, *J* = 8.4 Hz, 1H), 2.23-2.30 (m, 1H), 2.39 (s, 3H), 2.48 (s, 3H), 2.49-2.56 (m, 1H), 2.67 (dd, *J* = 14.8 Hz, *J* = 10.8 Hz, 1H), 2.81 (dd, *J* = 17.6 Hz, *J* = 8.8 Hz, 1H), 2.94 (dd, *J* = 17.6 Hz, *J* = 8.8 Hz, 1H), 7.03 (d, *J* = 7.6 Hz, 1H), 7.07-7.09 (m, 1H), 7.12-7.16 (m, 3H), 7.24-7.26 (m, 1H), 7.30-7.40 (m, 6H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.64-7.68 (m, 1H), 8.29 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.1, 21.0, 21.4, 22.7, 26.1, 31.9, 33.9, 43.3, 48.5, 51.1, 126.4, 126.8, 127.4, 127.7, 127.8, 127.9, 128.3, 128.59, 128.64, 129.18, 129.21, 129.29, 129.30, 129.4, 129.6, 130.2, 131.6, 134.0, 135.9, 136.5, 137.7, 138.9, 144.4, 146.3, 147.2, 157.7, 179.4; IR

(CH_3COCH_3): ν 3002, 2945, 2919, 1711, 1624, 1567, 1514, 1421, 1360, 1220, 1091. 1022, 994, 907, 825. 768, 733 cm^{-1}; MS (ESI) m/z 519.3 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{38}H_{35}N_2$: 519.27948, Found: 519.27907.

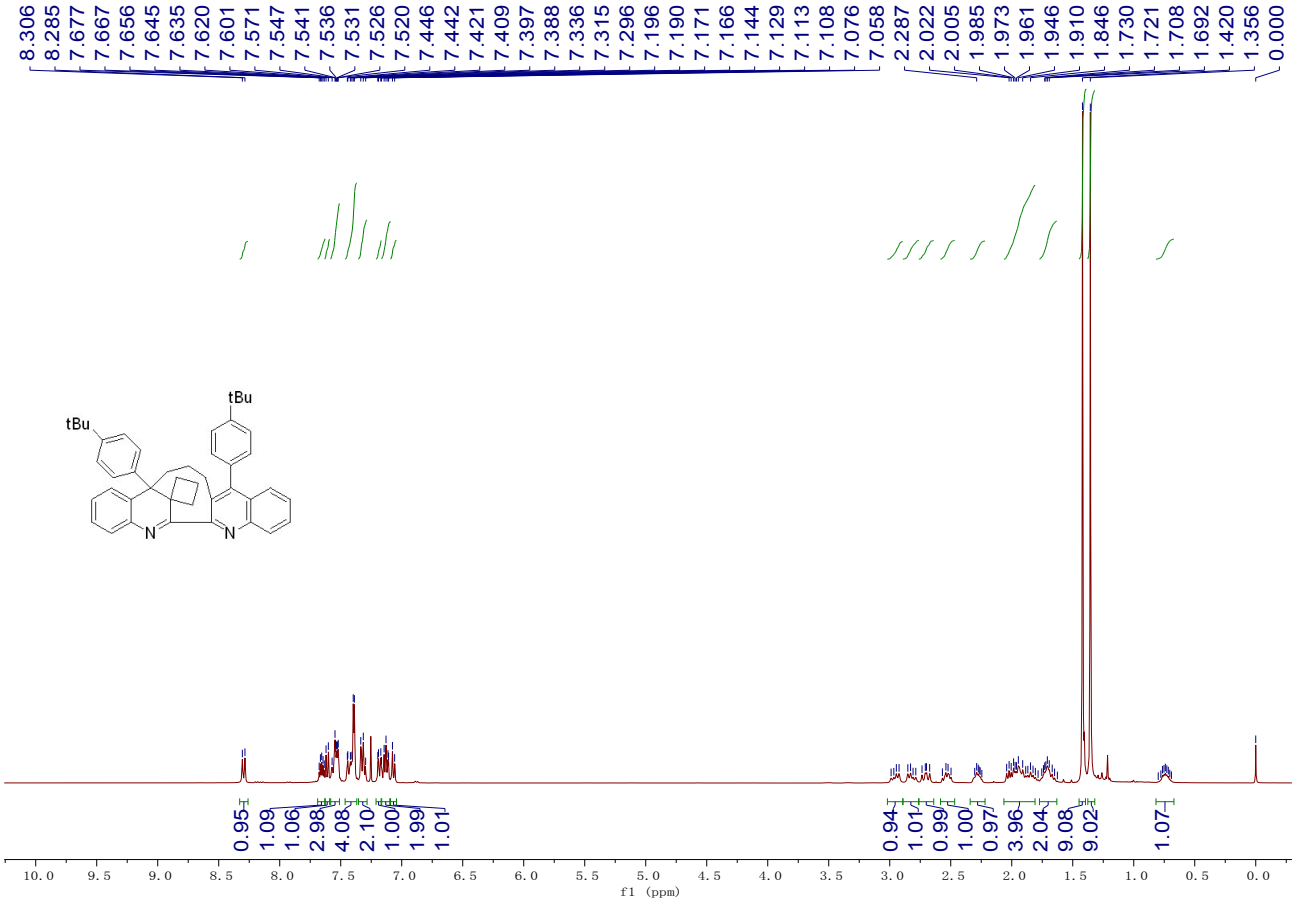


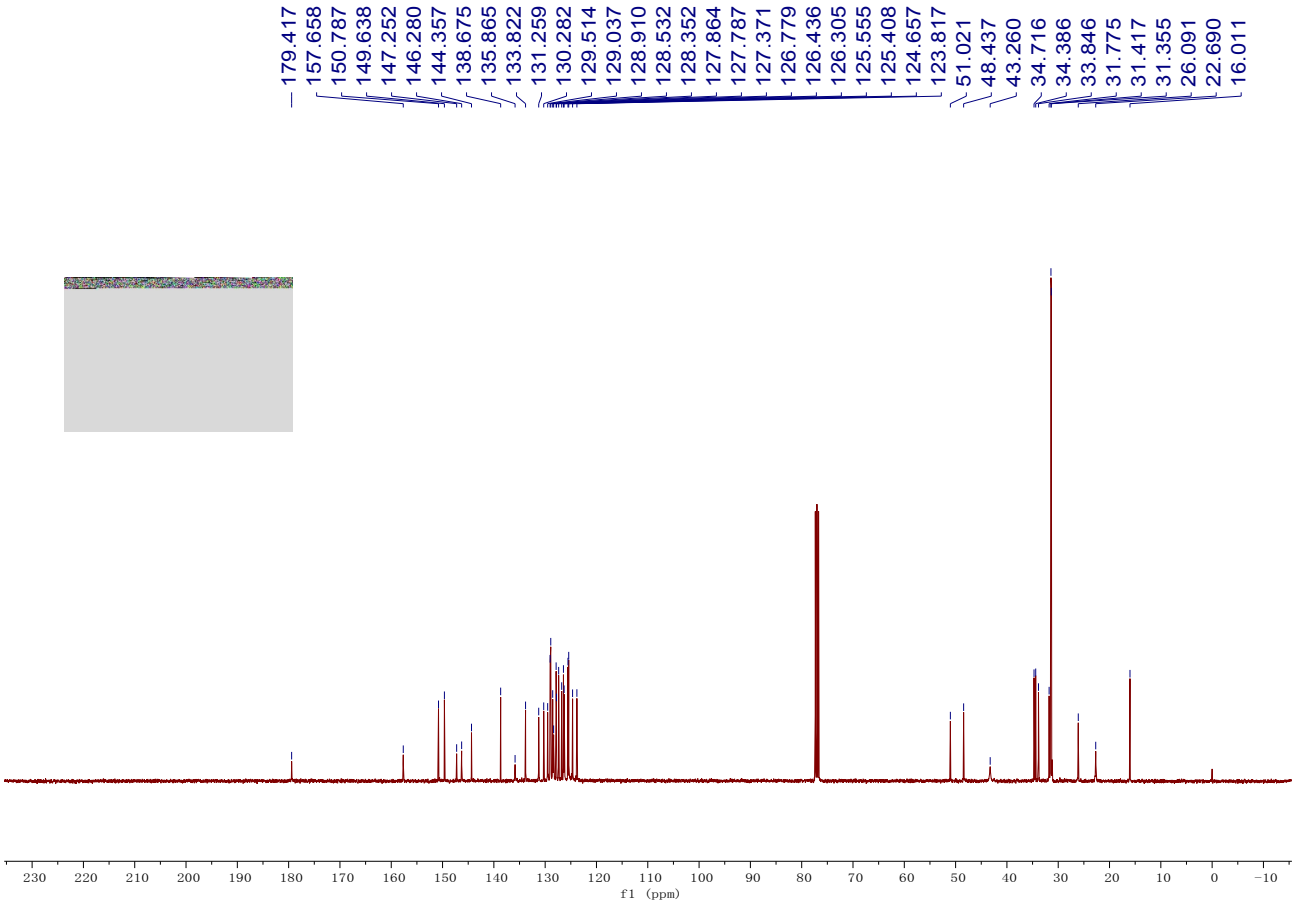


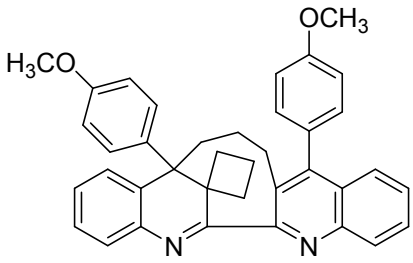


Compound **2i**: Yield: 207 mg, 34%; A brown solid; m.p. 256-258 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.69-0.80 (m, 1H), 1.36 (s, 9H), 1.42 (s, 9H), 1.63-1.75 (m, 2H), 1.78-2.04 (m, 4H), 2.25-2.30 (m, 1H), 2.50-2.57 (m, 1H), 2.70 (dd, *J* = 14.4 Hz, *J* = 10.4 Hz, 1H), 2.82 (dd, *J* = 17.2 Hz, *J* = 9.2 Hz, 1H), 2.96 (dd, *J* = 17.2 Hz, *J* = 9.2 Hz, 1H), 7.07 (d, *J* = 7.2 Hz, 1H), 7.11-7.14 (m, 2H), 7.18 (dd, *J* = 10.0 Hz, *J* = 2.2 Hz, 1H), 7.32 (t, *J* = 8.4 Hz, 1H), 7.39-7.45 (m, 4H), 7.52-7.57 (m, 3H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.64-7.68 (m, 1H), 8.30 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.0, 22.7, 26.1, 31.4, 31.4, 31.8, 33.8, 34.4, 34.7, 43.3, 48.4, 51.0, 123.8, 124.7, 125.4, 125.6, 126.3, 126.4, 126.8, 127.4, 127.8, 127.9, 128.4, 128.5, 128.9, 129.0, 129.5, 130.3, 131.3, 133.8, 135.9, 138.7, 144.4, 146.3, 147.3, 149.6, 150.8, 157.7, 179.4; IR (CH_3COCH_3): ν

3063, 2961, 2868, 1712, 1567, 1511, 1448, 1361, 1268, 1219, 1109, 1020, 908, 833, 766, 747, 728 cm^{-1}; MS (ESI) m/z 603.4 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{44}H_{47}N_2$: 603.37338, Found: 603.37243.

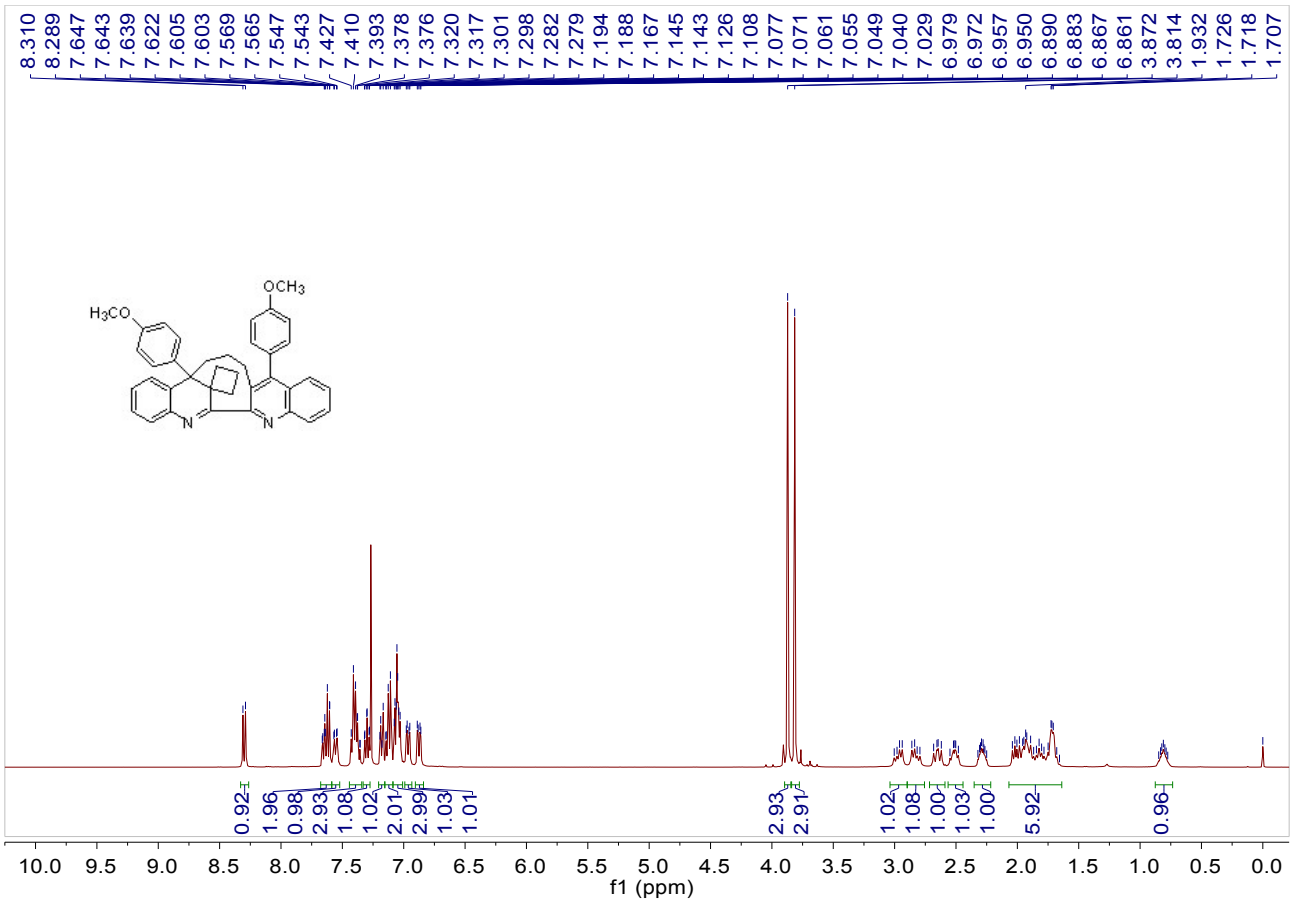


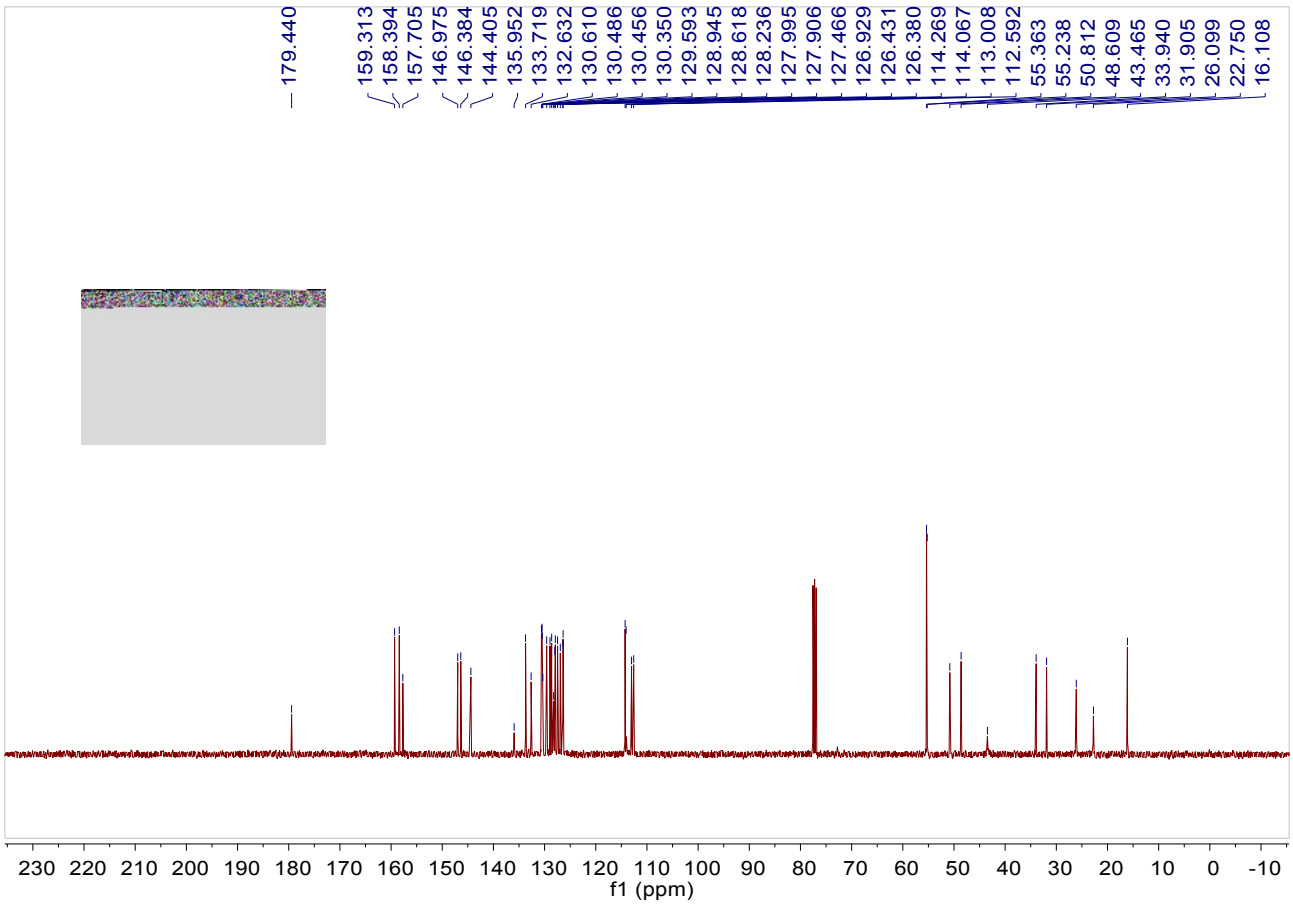


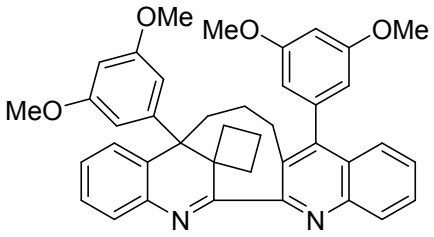


Compound **2j**: Yield: 310 mg, 28%; A brown solid; m.p. 247-249; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.78-0.85 (m, 1H), 1.66-2.04 (m, 6H), 2.25-2.32 (m, 1H), 2.48-2.55 (m, 1H), 2.65 (dd, *J* = 14.4 Hz, *J* = 10.8 Hz, 1H), 2.83 (dd, *J* = 17.2 Hz, *J* = 9.2 Hz, 1H), 2.97 (dd , *J* = 17.2 Hz, *J* = 8.8 Hz, 1H), 3.81 (s, 3H), 3.87 (s, 3H), 6.88 (dd, *J* = 9.2 Hz, *J* = 2.8 Hz, 1H), 6.96 (dd, *J* = 8.8 Hz, *J* = 2.8 Hz, 1H), 7.03-7.08 (m, 3H), 7.11-7.15 (m, 2H), 7.17-7.19 (m, 1H), 7.30 (td, *J* = 7.6 Hz, *J* = 1.2 Hz, 1H), 7.36-7.43 (m, 3H), 7.56 (dd, *J* = 8.8 Hz, *J* = 1.6 Hz, 1H), 7.60-7.66 (m, 2H), 8.30 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.1, 22.7, 26.1, 31.9, 33.9, 43.5, 48.6, 50.8, 55.2, 55.4, 112.6, 113.0, 114.1, 114.3, 126.38, 126.43, 126.9, 127.5, 127.9, 128.0, 128.2, 128.6, 128.9, 129.6, 130.4, 130.46, 130.49, 130.6, 132.6, 133.7, 136.0, 144.4, 146.4, 147.0, 157.7, 158.4,

159.3, 179.4; IR (CH_3COCH_3): ν 3066, 2935, 2833, 1711, 1609, 1513, 1489, 1443, 1360, 1288, 1246, 1220, 1177, 1109, 1031, 992, 908, 835, 765 cm^{-1}; MS (ESI) m/z 551.3 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{38}H_{35}N_2O_2$: 551.2693, Found: 551.2693.

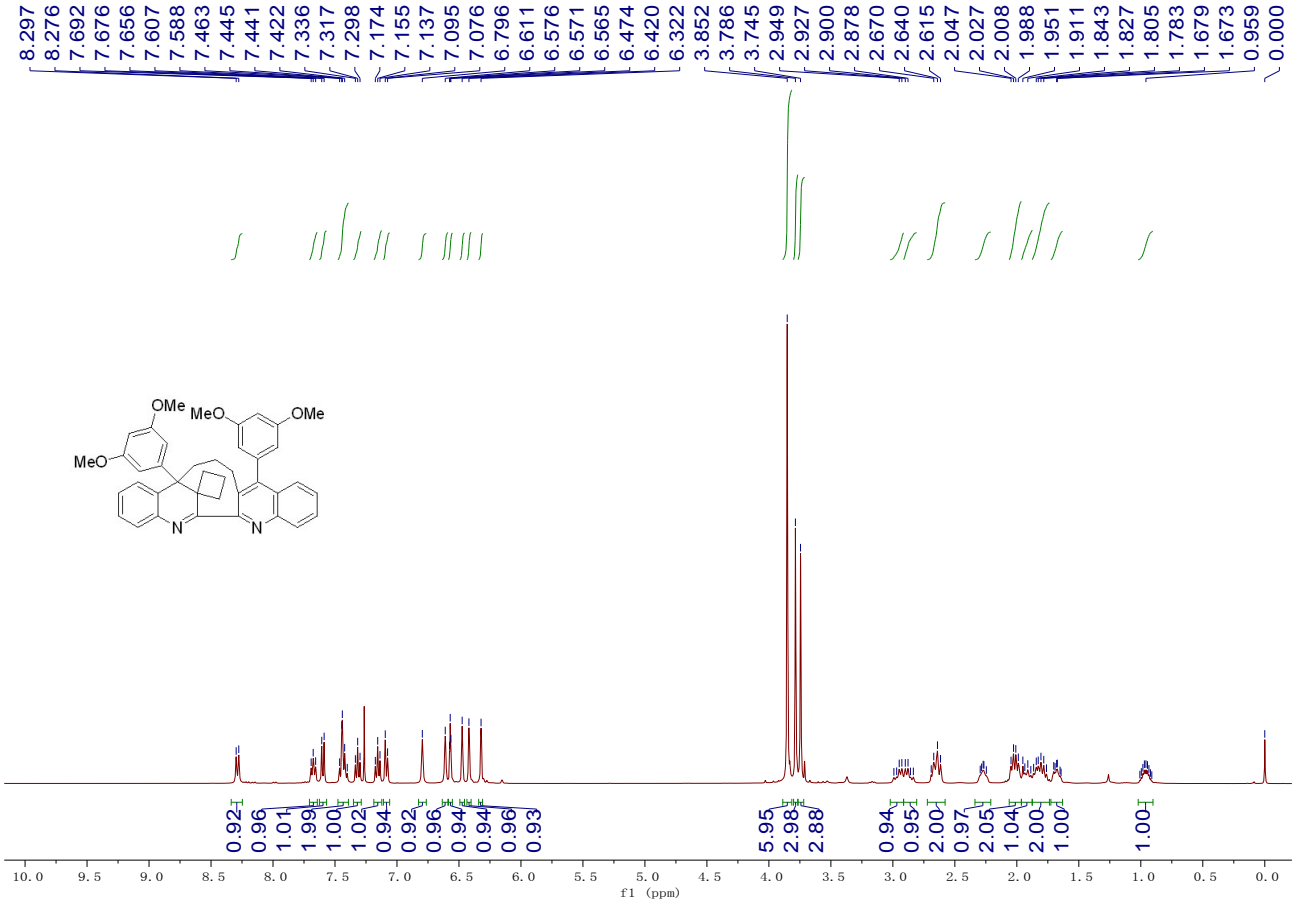


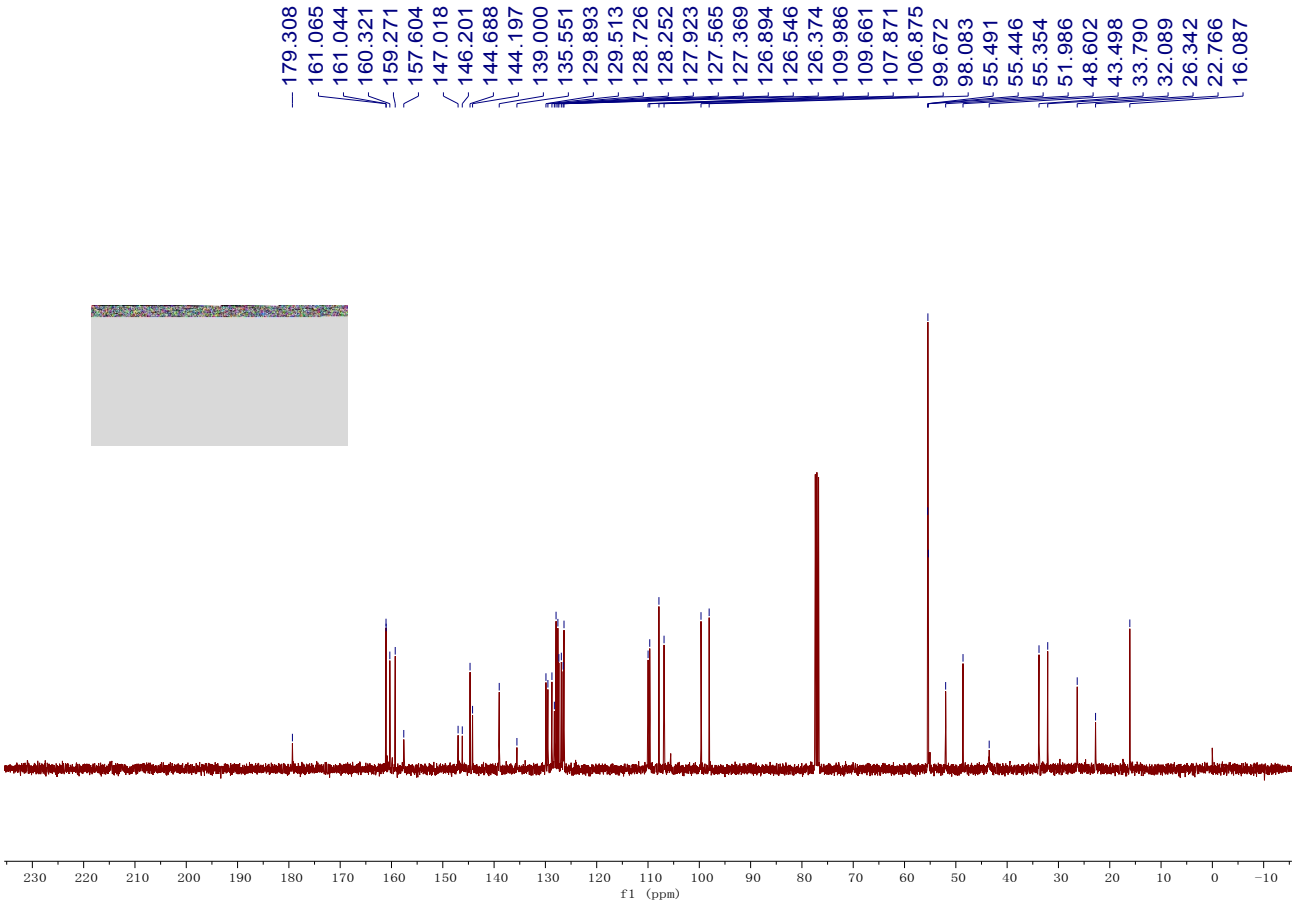


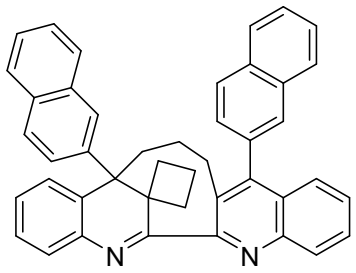


Compound **2k**: Yield: 295 mg, 48%; A brown solid; m.p. 243-245 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.91-1.01 (m, 1H), 1.64-1.70 (m, 1H), 1.76-1.86 (m, 2H), 1.89-1.95 (m, 1H), 1.99-2.05 (m, 2H), 2.25-2.30 (m, 1H), 2.62-2.69 (m, 2H), 2.87 (dd, *J* = 16.8 Hz, *J* = 8.8 Hz, 1H), 2.96 (dd, *J* = 16.8 Hz, *J* = 8.8 Hz, 1H), 3.75 (s, 3H), 3.79 (s, 3H), 3.85 (s, 6H), 6.32 (s, 1H), 6.42 (s, 1H), 6.47 (s, 1H), 6.57 (t, *J* = 2.0 Hz, 1H), 6.61 (s, 1H), 6.80 (s, 1H), 7.09 (d, *J* = 7.6 Hz, 1H), 7.16 (t, *J* = 7.6 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.41-7.46 (m, 2H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.68 (t, *J* = 7.2 Hz, 1H), 8.29 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.1, 22.8, 26.3, 32.1, 33.8, 43.5, 48.6, 52.0, 55.35, 55.45, 55.5, 98.1, 99.7, 106.9, 107.9, 109.7, 110.0, 126.4, 126.5, 126.9, 127.4, 127.6, 127.9, 128.3, 128.7, 129.5, 129.9, 135.6, 139.0, 144.2, 144.7, 146.2, 147.0, 157.6, 159.3, 160.3, 161.0, 161.1, 179.3; IR (CH_3COCH_3): ν 3003, 2956, 2927, 2856, 1710, 1591, 1453, 1422,

1360, 1220, 1205, 1155, 1064, 928, 844, 765, 702 cm^{-1}; MS (ESI) m/z 611.3 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{40}H_{39}N_2O_4$: 611.29043, Found: 611.28901.

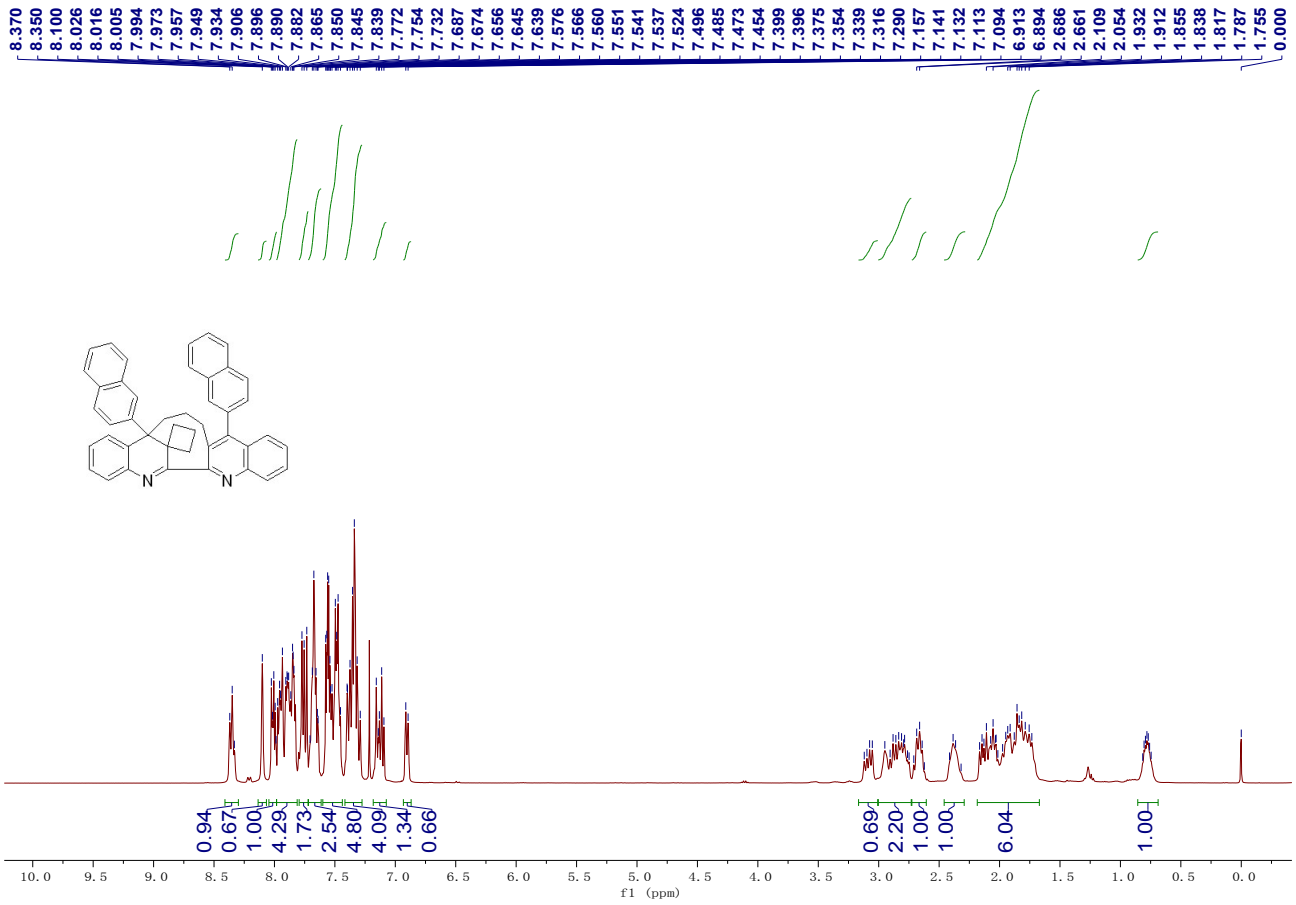


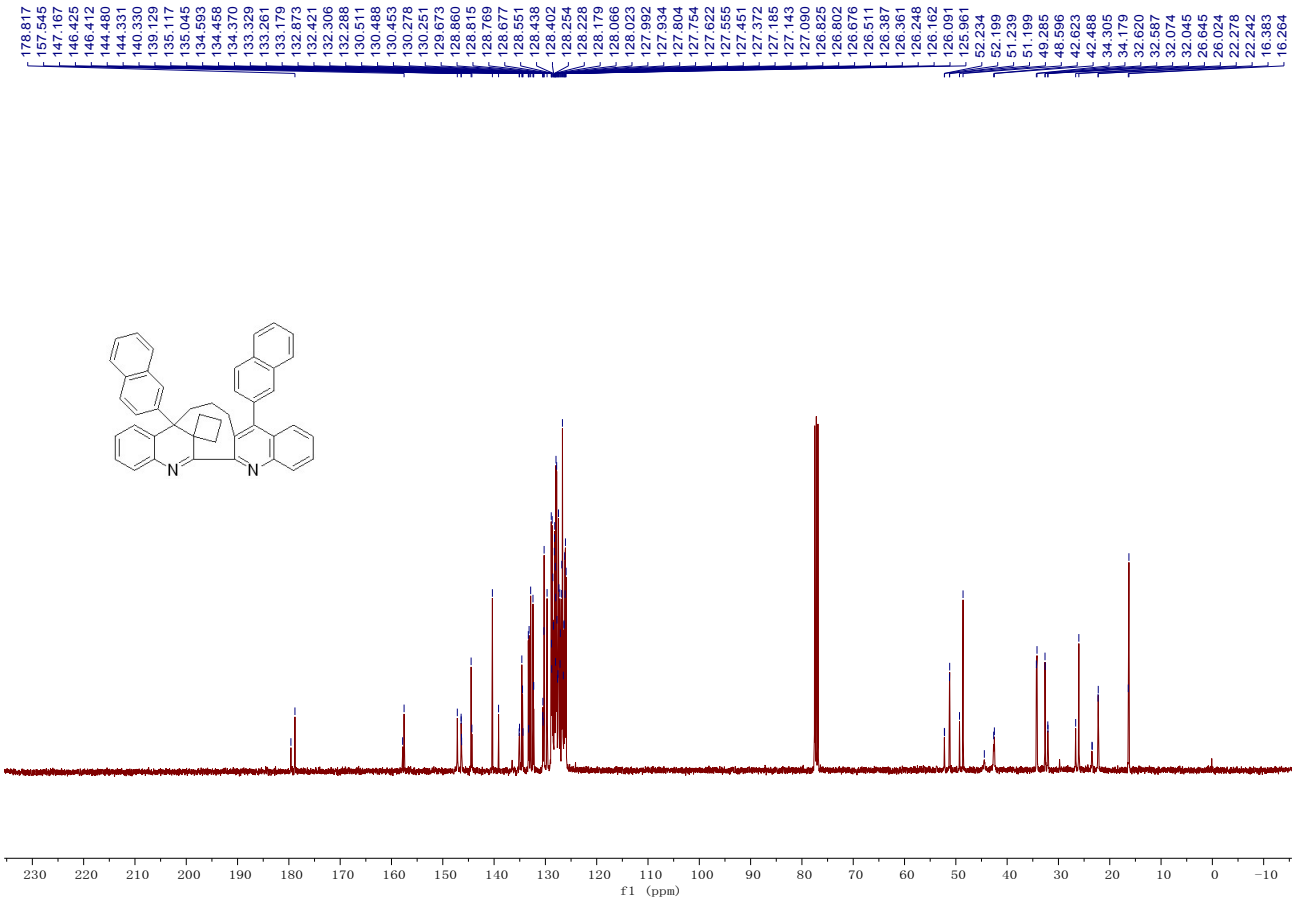


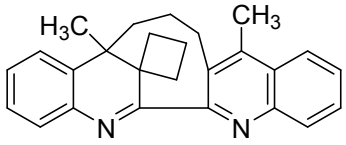


Compound **2l** (atropisomers): Yield: 227 mg, 38%; A brown solid; m.p. 250-252 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.75-0.82 (m, 1H), 1.73-2.17 (m, 6H), 2.32-2.41 (m, 1H), 2.62-2.71 (m, 1H), 2.75-2.95 (m, 2.2 H), 3.09 (dd, *J* = 18.0 Hz, *J* = 9.2 Hz, 6.9H), 6.90 (d, *J* = 7.6 Hz, 0.66H), 7.09-7.16 (m, 1.34H), 7.29-7.40 (m, 4H), 7.45-7.58 (m, 4.80H), 7.64-7.71 (m, 2.54H), 7.73-7.77 (m, 1.73H), 7.84-7.97 (m, 4.29H), 7.99-8.03 (m, 1H), 8.10 (s, 0.67 H), 8.35 (t, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.3, 16.4, 22.2, 22.3, 23.4, 23.5, 26.0, 26.6, 32.0, 32.1, 32.59, 32.62, 34.2, 34.3, 42.5, 42.6, 44.4, 48.6, 49.3, 51.20, 51.24, 52.20, 52.23, 126.0, 126.1, 126.16, 126.25, 126.36, 126.39, 126.5, 126.7, 126.80, 126.83, 127.09, 127.14, 127.2, 127.4, 127.5, 127.56, 127.62, 127.75, 127.80, 127.9, 127.99, 128.02, 128.1, 128.18, 128.23, 128.3, 128.40, 128.44, 128.6,

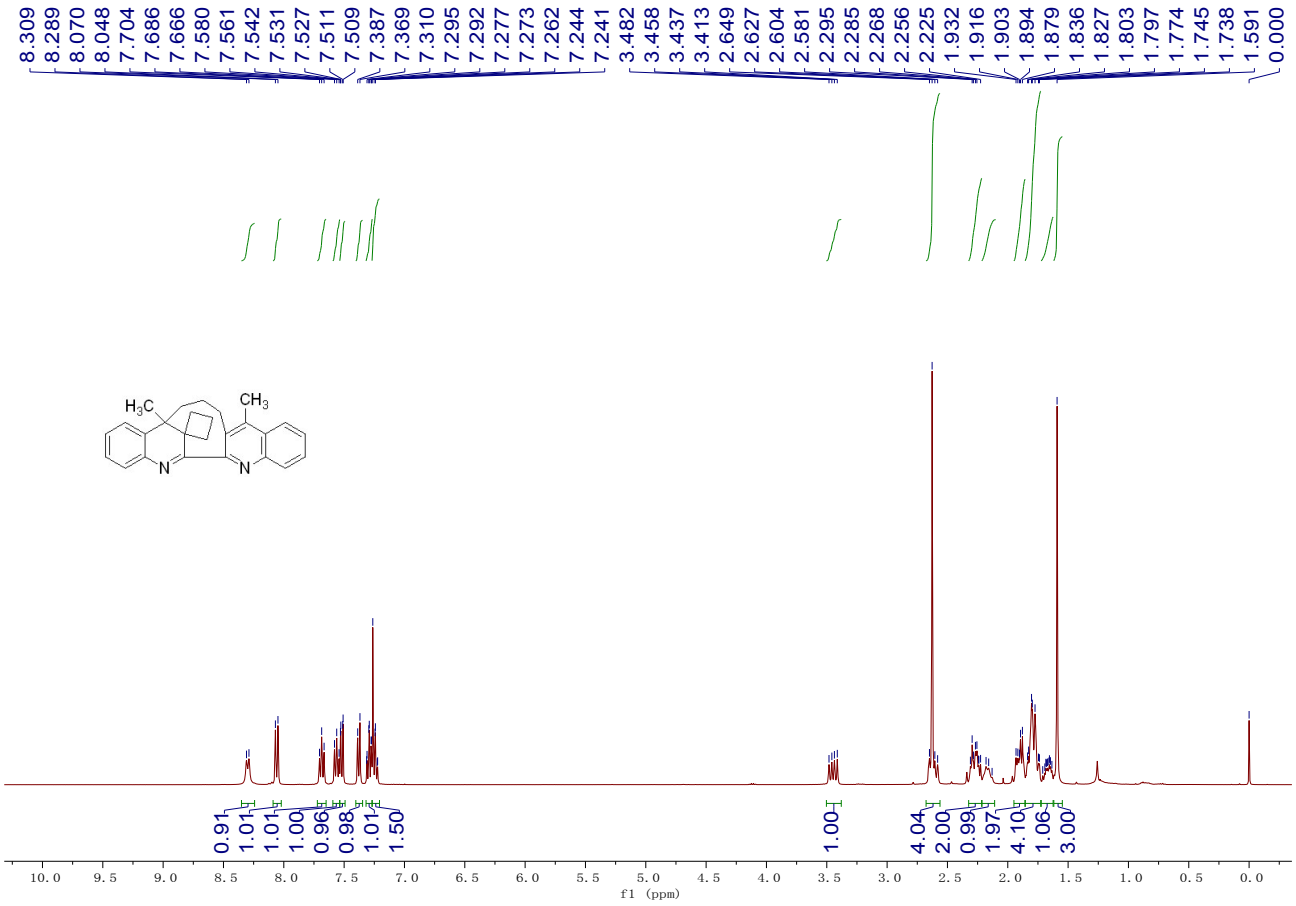
128.7, 128.77, 128.82, 128.9, 129.7, 130.25, 130.28, 130.45, 130.49, 130.51, 132.3, 132.3, 132.4, 132.9, 133.2, 133.29, 133.31, 134.4, 134.5, 134.6, 135.0, 135.1, 139.1, 140.3, 144.3, 144.5, 146.3, 146.36, 146.41, 146.43, 147.2, 157.5, 157.8, 178.8, 179.6; IR (CH_3COCH_3): ν 3058, 3003, 2956, 1710, 1569, 1421, 1359, 1220, 1091, 999, 904, 826, 755, 735 cm^{-1}; MS (ESI) m/z 591.3 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{44}H_{35}N_2$: 591.27948, Found: 591.27901.

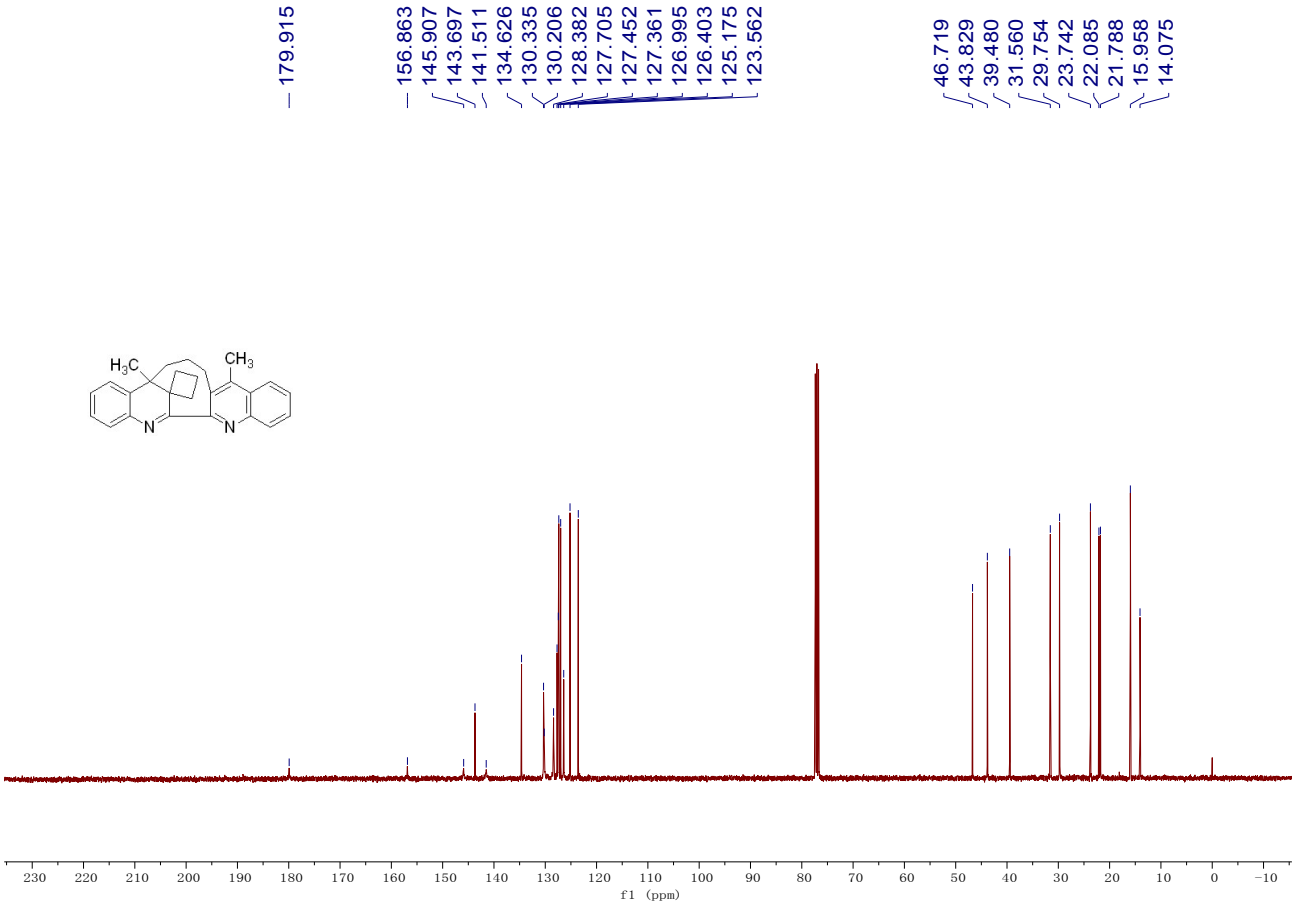


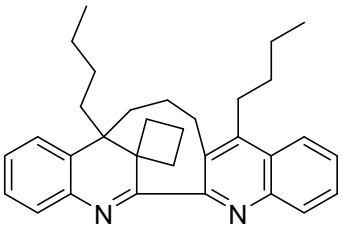




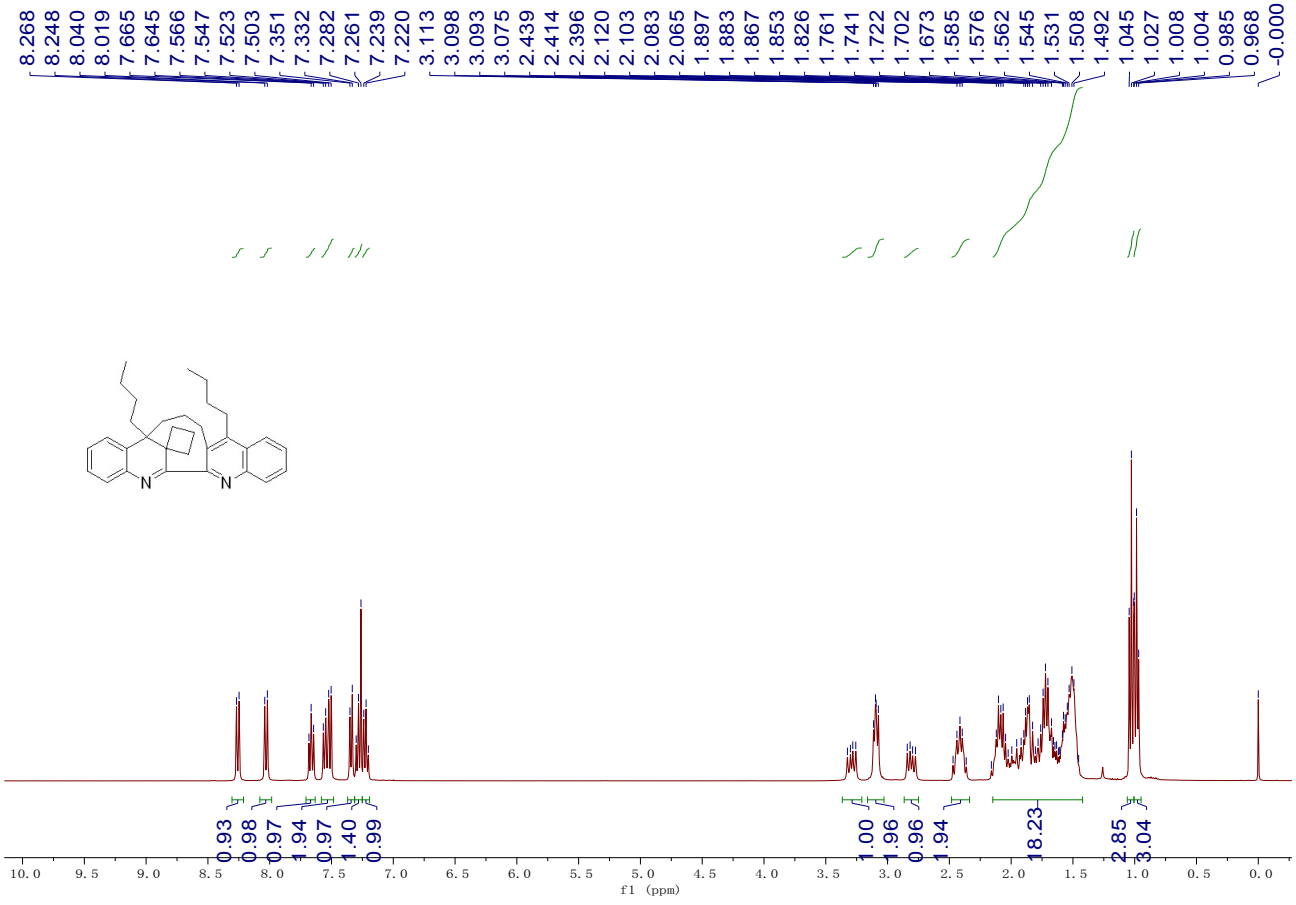
Compound **2n**: Yield:170 mg, 46%; A brown solid; m.p. 205-207 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.59 (s, 3H), 1.63-1.71 (m, 1H), 1.74-1.84 (m, 4H), 1.88-1.93 (m, 2H), 2.13-2.18 (m, 1H), 2.23-2.31 (m, 2H), 2.58-2.65 (m, 4H), 3.45 (dd, *J* = 18.0 Hz, *J* = 9.6 Hz, 1H), 7.22-7.26 (m, 1H), 7.29 (td, *J* = 7.2 Hz, *J* = 1.2 Hz, 1H), 7.38 (d, *J* = 7.2 Hz, 1H), 7.52 (dd, *J* = 7.6 Hz, *J* = 1.2 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 8.06 (d, *J* = 8.8 Hz, 1H), 8.30 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 14.1, 16.0, 21.8, 22.1, 23.7, 29.8, 31.6, 39.5, 43.8, 46.7, 123.6, 125.2, 126.4, 127.0, 127.4, 127.5, 127.7, 128.4, 130.2, 130.3, 134.6, 141.5, 143.7, 145.9, 156.9, 179.9; IR (CH_3COCH_3): ν 2958, 2922, 2856, 1711, 1436, 1359, 1220, 1092, 1011, 909, 762, 746, 661 cm^{-1}; MS (ESI) m/z 367.2 $(M+H)^{+}$; HRMS (ESI) Calcd. for $C_{26}H_{27}N_2$: 367.21688, Found: 367.21697.

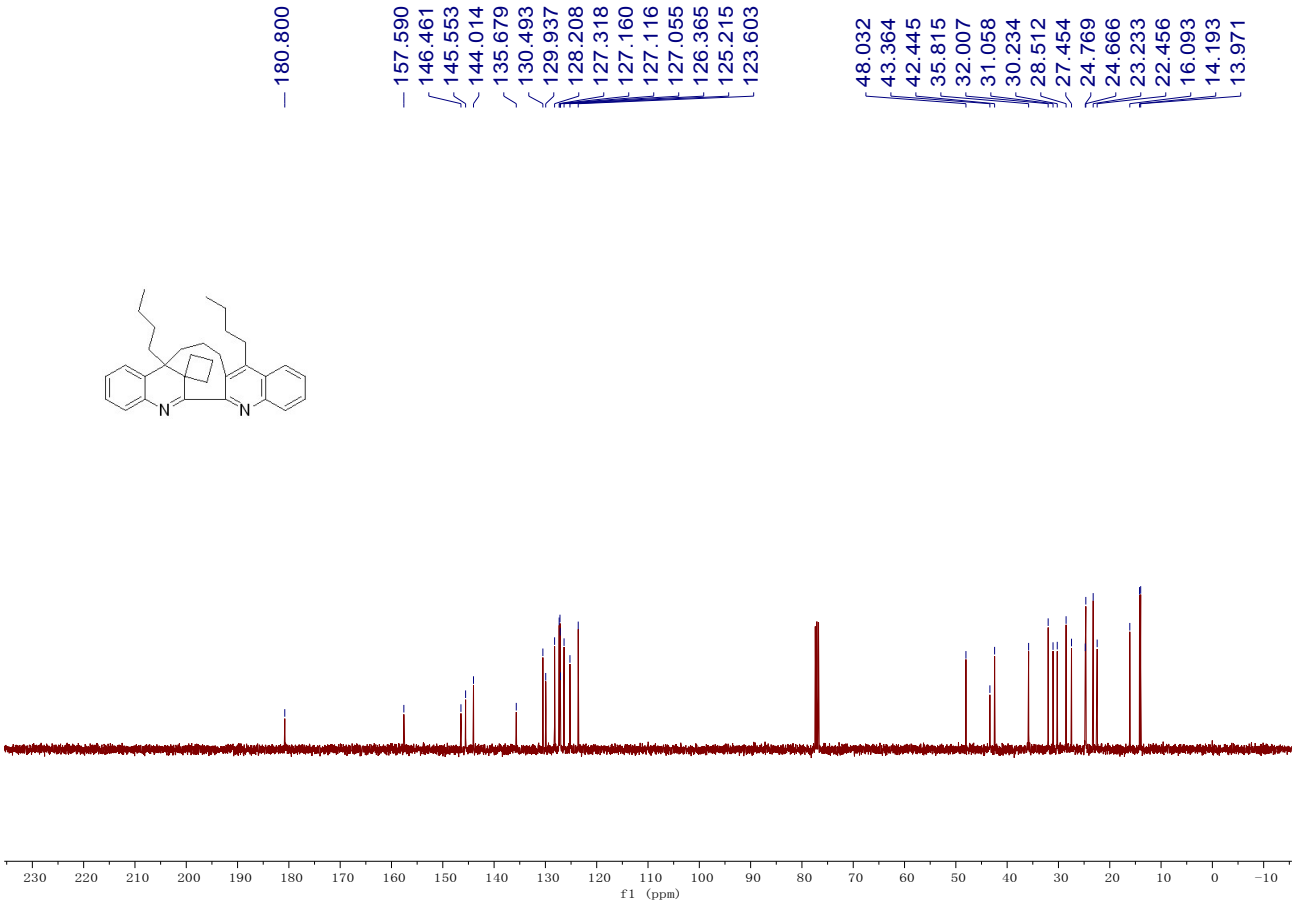

8.309
8.289
8.070
8.048
7.704
7.686
7.666
7.580
7.561
7.542
7.531
7.527
7.511
7.509
7.387
7.369
7.310
7.295
7.292
7.277
7.273
7.262
7.244
7.241
3.482
3.458
3.437
3.413
2.649
2.627
2.604
2.581
2.295
2.285
2.268
2.256
2.225
1.932
1.916
1.903
1.894
1.879
1.836
1.827
1.803
1.797
1.774
1.745
1.738
1.591
0.000
H3C
CH3
N
N
0.91
1.01
1.01
1.00
0.96
0.98
1.01
1.50
1.00
4.04
2.00
0.99
1.97
4.10
1.06
3.00
f1 (ppm)

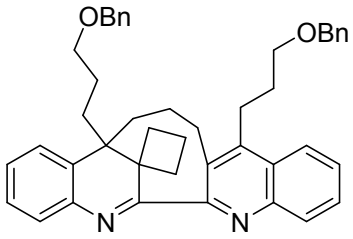

179.915
156.863
145.907
143.697
141.511
134.626
130.335
130.206
128.382
127.705
127.452
127.361
126.995
126.403
125.175
123.562
46.719
43.829
39.480
31.560
29.754
23.742
22.085
21.788
15.958
14.075
H3C
CH3
N
N
f1 (ppm)



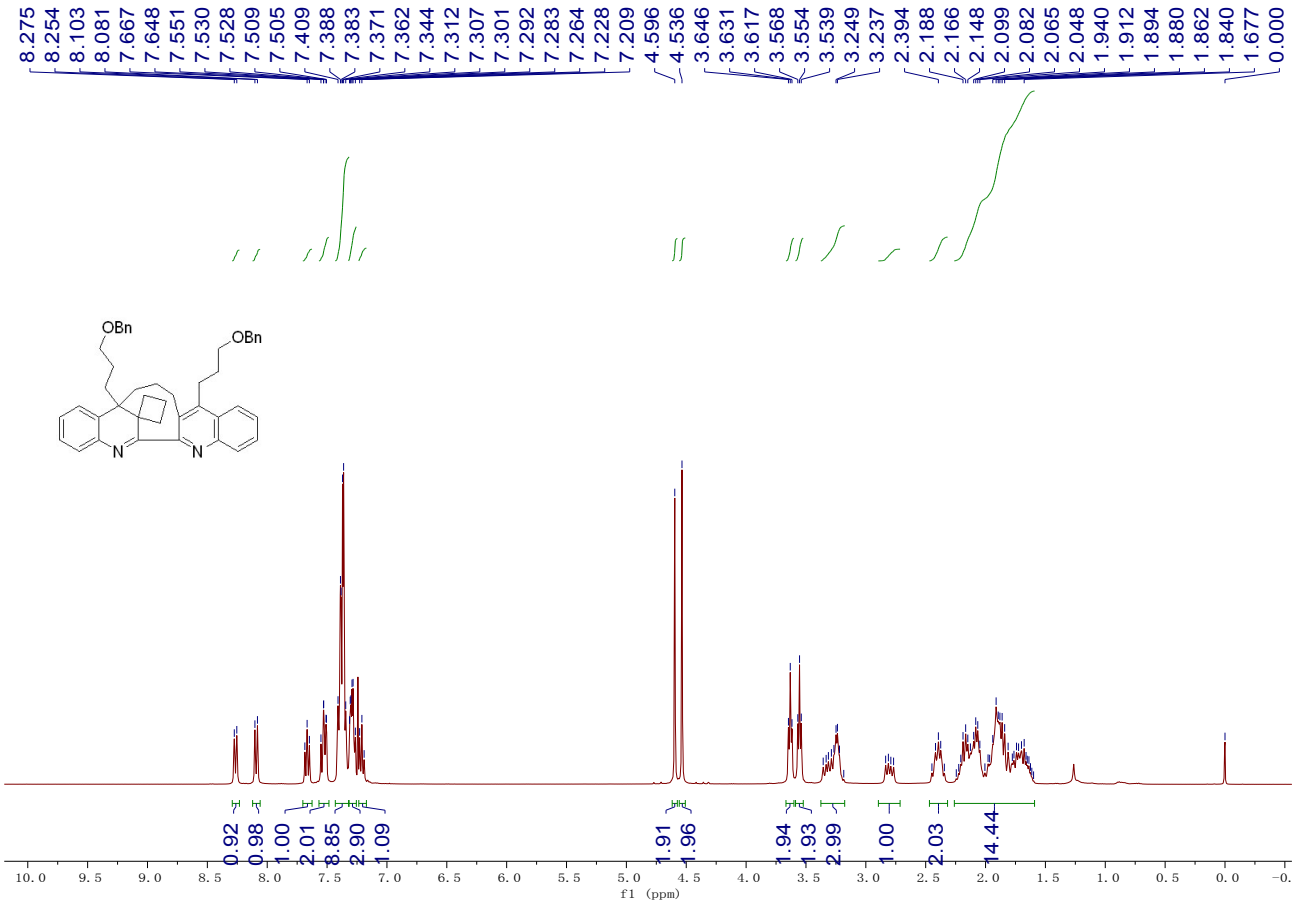
Compound **2o**: Yield: 205 mg, 45%; A brown solid; m.p. 139-141 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.99 (t, *J* = 7.2 Hz, 3H), 1.03 (t, *J* = 7.4 Hz, 3H), 1.45-2.16 (m, 18H), 2.36-2.47 (m, 2H), 2.81 (dd, *J* = 17.6 Hz, *J* = 9.2 Hz, 1H), 3.08-3.11 (m, 2H), 3.29 (dd, *J* = 17.6 Hz, *J* = 9.2 Hz, 1H), 7.22 (t, *J* = 7.4 Hz, 1H), 7.29 (d, *J* = 7.2 Hz, 1H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.50-7.57 (m, 2H), 7.67 (t, *J* = 7.4 Hz, 1H), 8.03 (d, *J* = 8.4 Hz, 1H), 8.26 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 14.0, 14.2, 16.1, 22.5, 23.2, 24.7, 24.8, 27.5, 28.5, 30.2, 31.1, 32.0, 35.8, 42.4, 43.4, 48.0, 123.6, 125.2, 126.4, 127.06, 127.12, 127.2, 127.3, 128.2, 129.9, 130.5, 135.7, 144.0, 145.6, 146.5, 157.6, 180.8; IR (CH_3COCH_3): ν 3066, 2954, 2870, 1712, 1620, 1596, 1569, 1500, 1450, 1360, 1219, 1127, 1090, 1025, 927, 761 cm^{-1}; MS (ESI) m/z 451.3 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{32}H_{39}N_2$: 451.31078, Found: 451.31131.

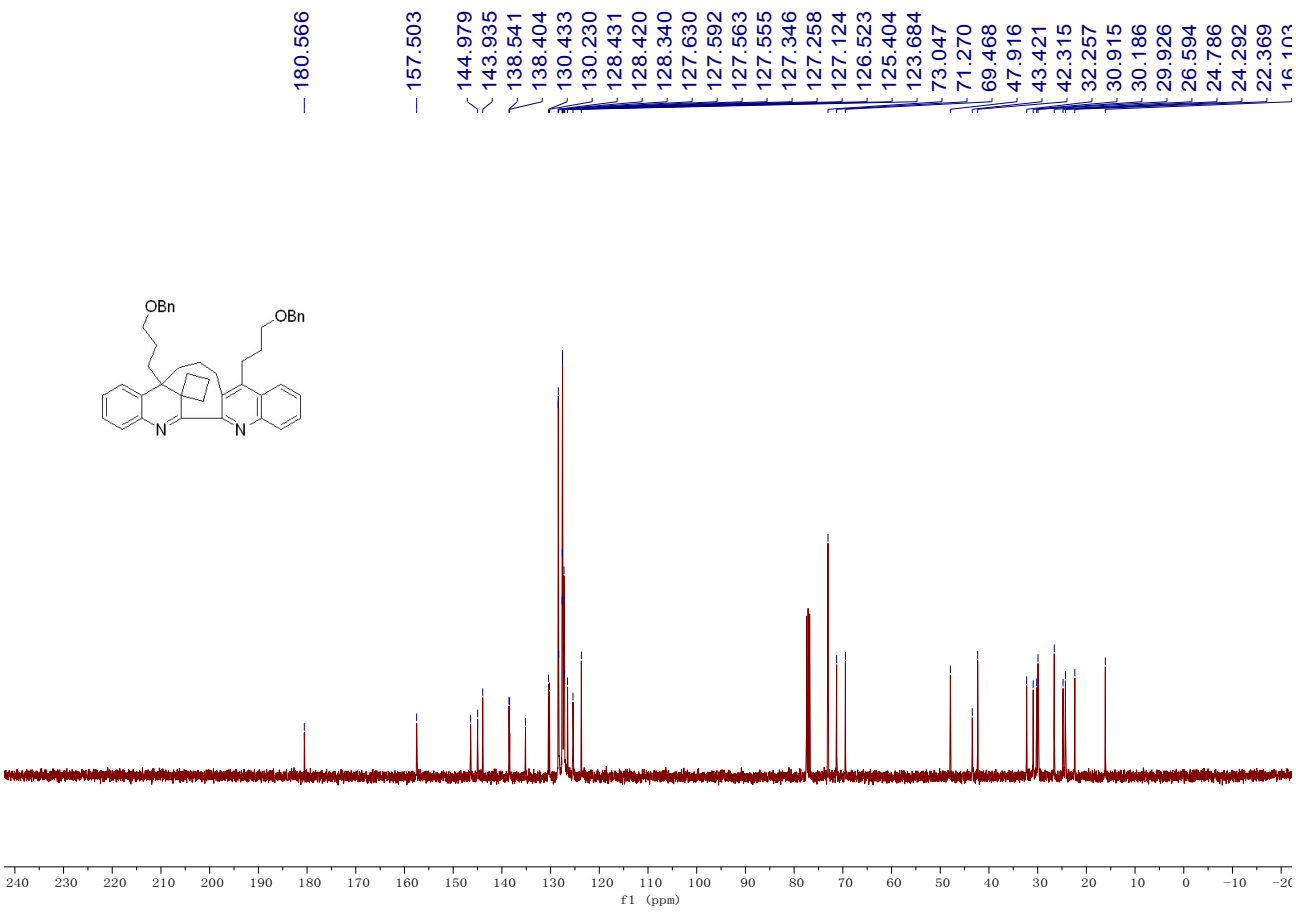


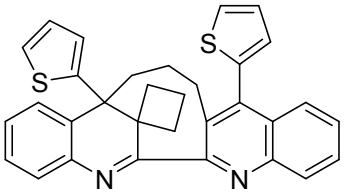




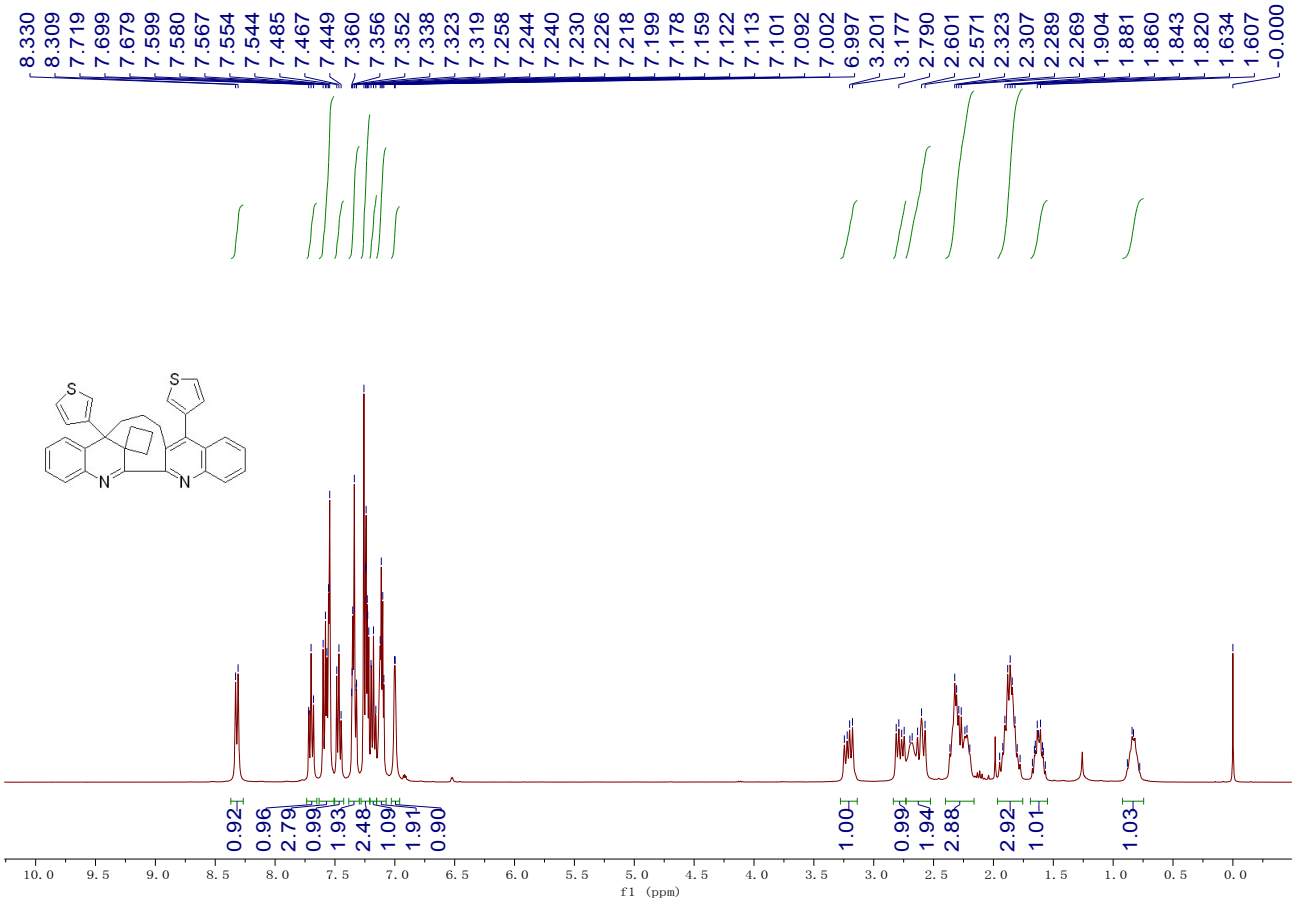
Compound **2p**: Yield: 346 mg, 54%; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.60-2.24 (m, 14H), 2.34-2.45 (m, 2H), 2.80 (dd, *J* = 17.2 Hz, *J* = 8.4 Hz, 1H), 3.18-3.36 (m, 3H), 3.55 (t, *J* = 5.8 Hz, 2H), 3.63 (t, *J* = 5.8 Hz, 2H), 4.54 (s, 2H), 4.60 (s, 2H), 7.21 (t, *J* = 7.4 Hz, 1H), 7.26-7.31 (m, 3H), 7.34-7.41 (m, 9H), 7.51-7.55 (m, 2H), 7.67 (t, *J* = 7.6 Hz, 1H), 8.09 (d, *J* = 8.8 Hz, 1H), 8.26 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.1, 22.4, 24.3, 24.8, 26.6, 29.9, 30.2, 30.9, 32.3, 42.3, 43.4, 47.9, 69.5, 71.3, 73.0, 123.7, 125.4, 126.5, 127.1, 127.26, 127.35, 127.555, 127.563, 127.592, 127.63, 128.3, 128.42, 128.43, 130.2, 130.4, 135.1, 138.4, 138.5, 143.9, 145.0, 146.4, 157.5, 180.6; IR (CH_3COCH_3): ν 3066, 3026, 2947, 2859, 1711, 1620, 1569, 1497, 1453, 1360, 1220, 1100, 1027, 908, 763, 737, 698 cm^{-1}; MS (ESI) m/z 635.4 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{44}H_{47}N_2O_2$: 635.36321, Found: 635.36341.

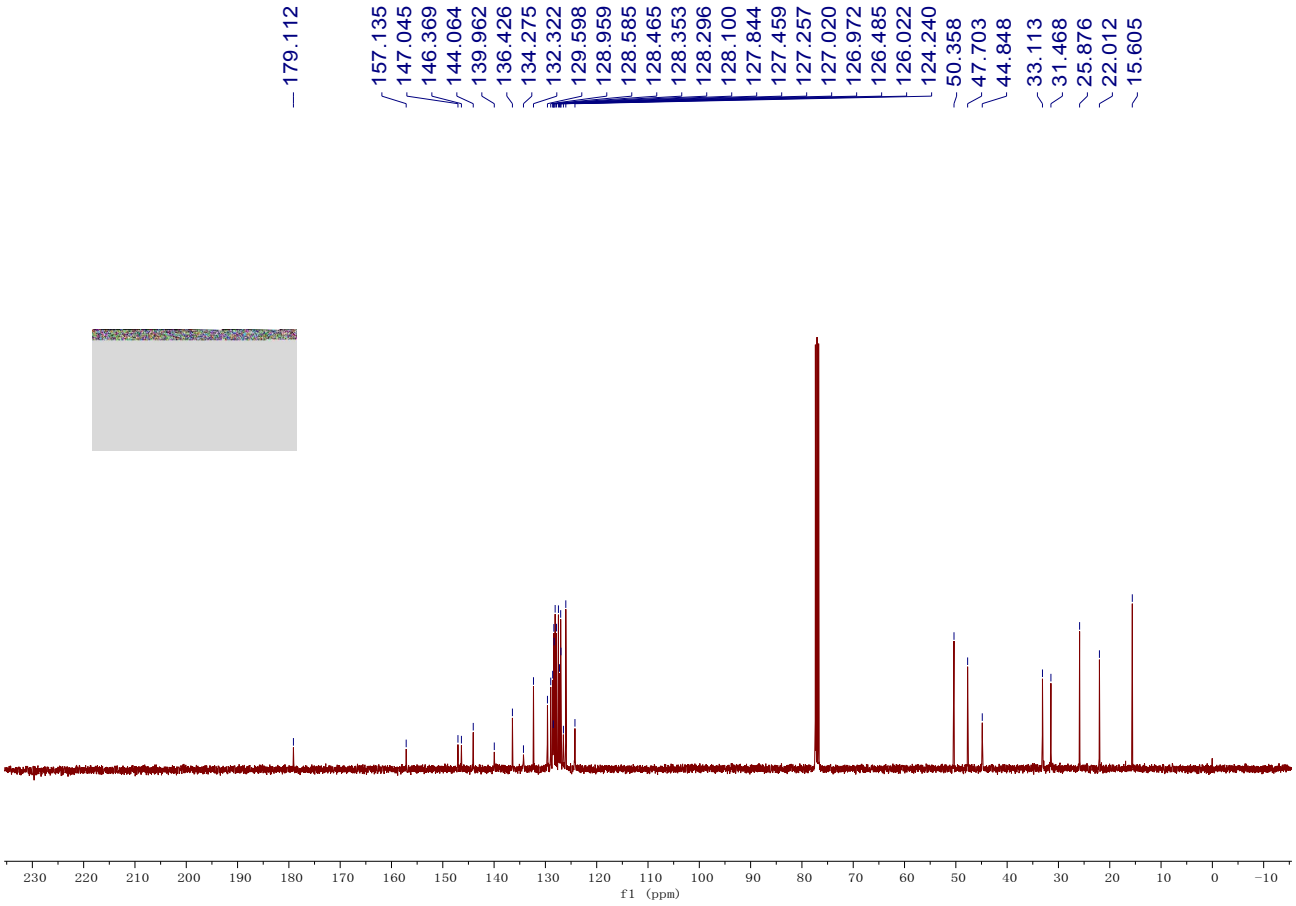

8.275
8.254
8.103
8.081
7.667
7.648
7.551
7.530
7.528
7.509
7.505
7.409
7.388
7.383
7.371
7.362
7.344
7.312
7.307
7.301
7.292
7.283
7.264
7.228
7.209
4.596
4.536
3.646
3.631
3.617
3.568
3.554
3.539
3.249
3.237
2.394
2.188
2.166
2.148
2.099
2.082
2.065
2.048
1.940
1.912
1.894
1.880
1.862
1.840
1.677
0.000
OBn
OBn
N
N
0.92
0.98
1.00
2.01
8.85
2.90
1.09
1.91
1.96
1.94
1.93
2.99
1.00
2.03
14.44
f1 (ppm)

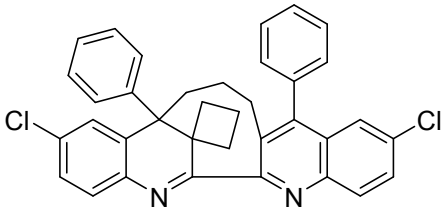

180.566
157.503
144.979
143.935
138.541
138.404
130.433
130.230
128.431
128.420
128.340
127.630
127.592
127.563
127.555
127.346
127.258
127.124
126.523
125.404
123.684
73.047
71.270
69.468
47.916
43.421
42.315
32.257
30.915
30.186
29.926
26.594
24.786
24.292
22.369
OBn
OBn
N
N
f1 (ppm)



Compound **2q**: Yield: 331 mg, 66%; A brown solid; m.p. 230-232 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.78-0.88 (m, 1H), 1.57-1.67 (m, 1H), 1.78-1.95 (m, 3H), 2.20-2.36 (m, 3H), 2.57-2.70 (m, 2H), 2.78 (dd, *J* = 18.4 Hz, *J* = 8.8 Hz, 1H), 3.21 (dd, *J* = 18.4 Hz, *J* = 8.8 Hz, 1H), 7.00 (d, *J* = 2.0 Hz, 1H), 7.09-7.12 (m, 2H), 7.18 (t, *J* = 8.0 Hz, 1H), 7.22-7.26 (m, 2H), 7.32-7.36 (m, 2H), 7.47 (t, *J* = 7.2 Hz, 1H), 7.54-7.60 (m, 3H), 7.70 (t, *J* = 8.0 Hz, 1H), 8.32 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 15.6, 22.0, 25.9, 31.5, 33.1, 44.8, 47.7, 50.4, 124.2, 126.0, 126.5, 127.0, 127.0, 127.3, 127.5, 127.8, 128.1, 128.3, 128.4, 128.5, 128.6, 129.0, 129.6, 132.3, 134.3, 136.4, 140.0, 144.1, 146.4, 147.0, 157.1, 179.1; IR (CH_3COCH_3): ν 3000, 2961, 2927, 1711, 1571, 1422, 1359, 1220, 1092, 988, 903, 849, 763, 726, 708, 699 cm^{-1}; MS (ESI) m/z 503.2 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{32}H_{27}N_2S_2$: 503.16102, Found: 503.16101.

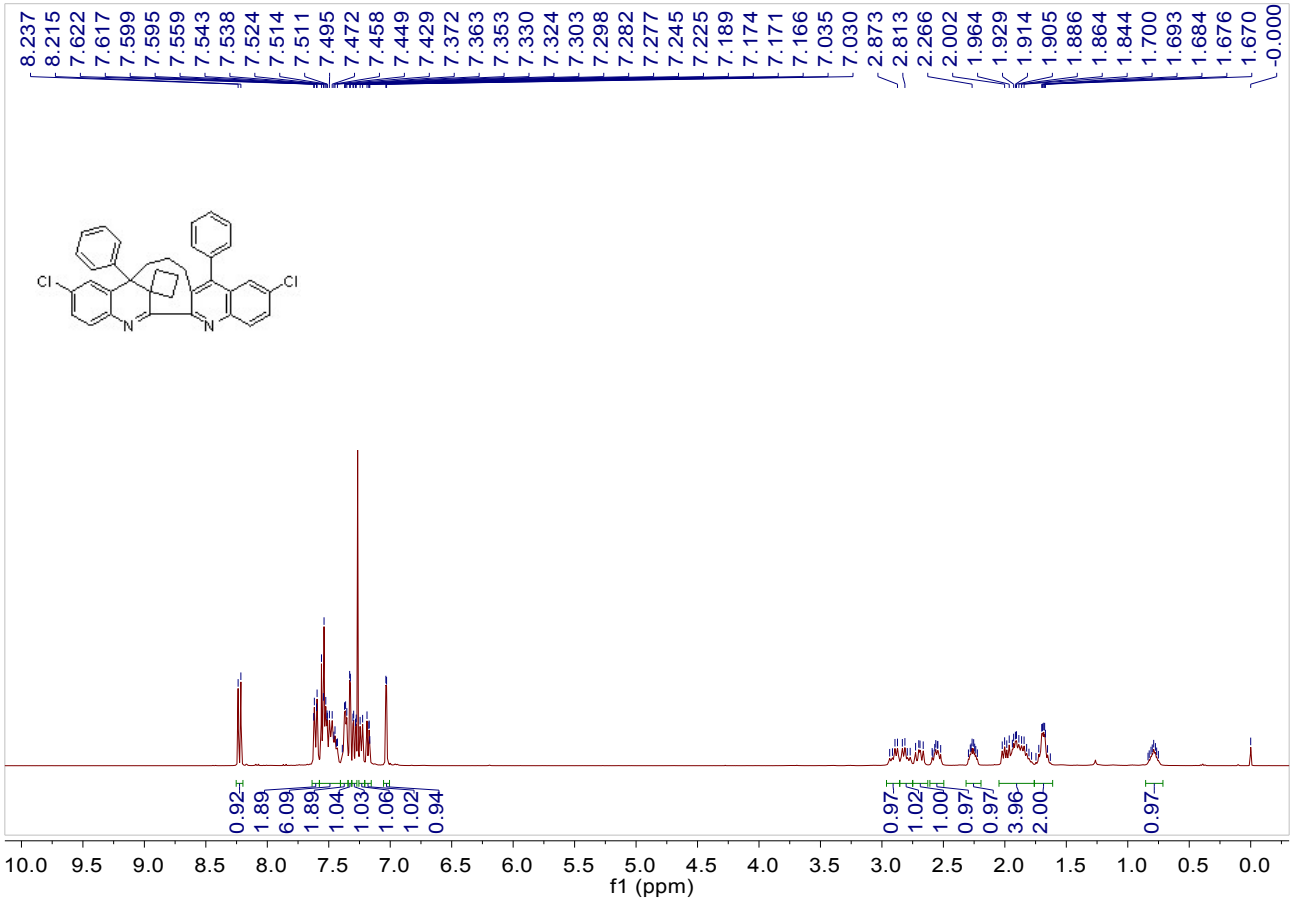


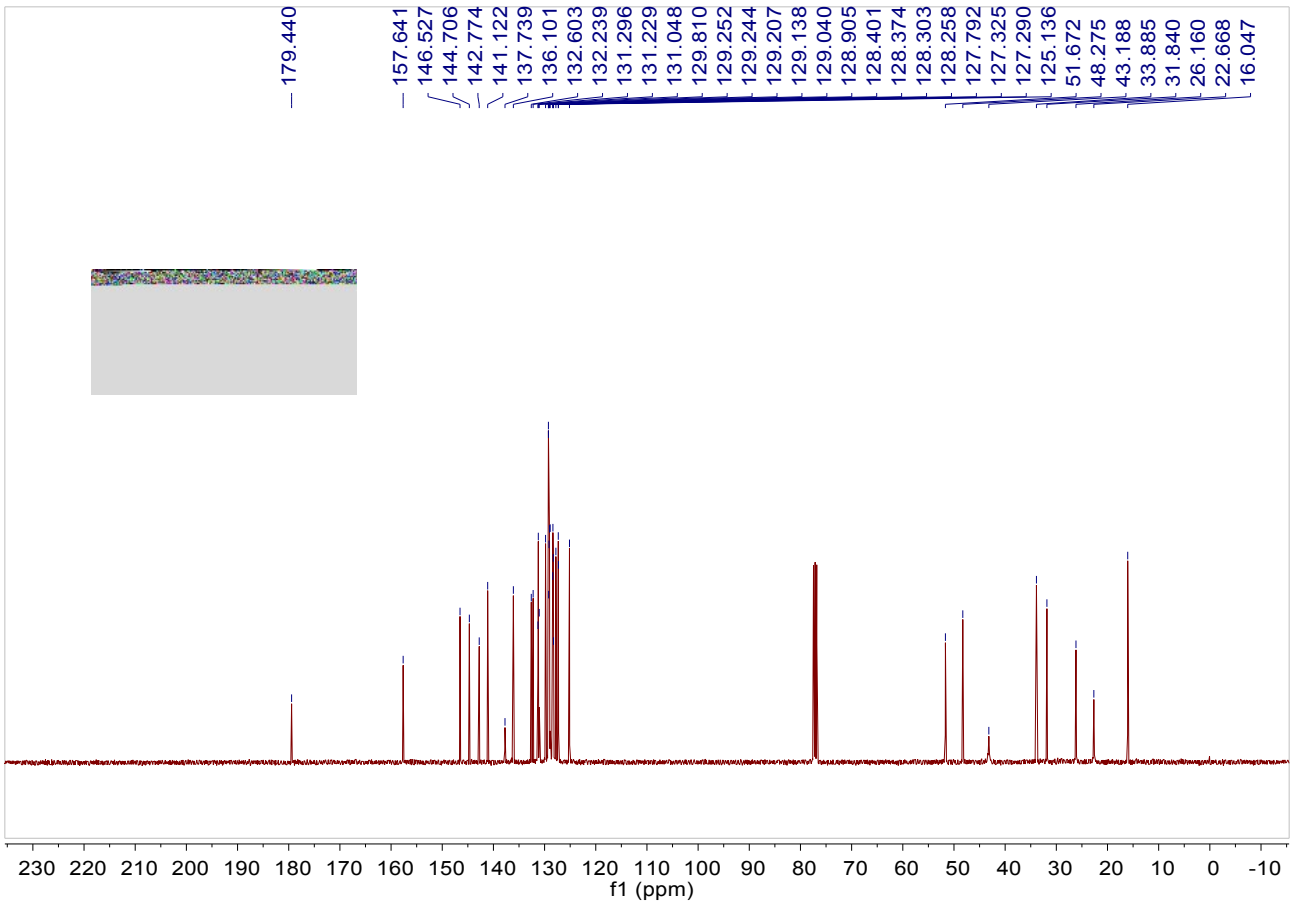


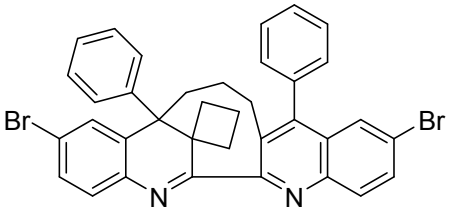


Compound **2r**: Yield: 298 mg, 53%; A brown solid; m.p. 318-320 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.75-0.84 (m, 1H), 1.63-1.75 (m, 2H), 1.78-2.02 (m, 4H), 2.22-2.30 (m, 1H), 2.52-2.59 (m, 1H), 2.70 (dd, *J* = 14.4 Hz, *J* = 10.4 Hz, 1H), 2.80 (dd, *J* = 16.6 Hz, *J* = 9.0 Hz, 1H), 2.90 (dd , *J* = 16.6 Hz, *J* = 8.8 Hz, 1H) 7.03 (d, *J* = 2.0 Hz, 1H), 7.17-7.19 (m, 1H), 7.23 (d, *J* = 8.0 Hz, 1H), 7.29 (dd, *J* = 8.4 Hz, *J* = 2.0 Hz, 1H), 7.33 (d, *J* = 2.4 Hz, 1H), 7.35-7.39 (m, 2H), 7.43-7.56 (m, 6H), 7.61 (dd, *J* = 9.0 Hz, *J* = 1.8 Hz, 2H), 8.23 (d, *J* = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.0, 22.7, 26.2, 31.8, 33.9, 43.2, 48.3, 51.7, 125.1, 127.29, 127.33, 127.8, 128.26, 128.30, 128.37, 128.40, 128.9, 129.0, 129.1, 129.21, 129.24, 129.3, 129.8, 131.0, 131.2, 131.3, 132.2, 132.6, 136.1, 137.7, 141.1, 142.8, 144.7, 146.5, 157.6, 179.4; IR (CH_3COCH_3): ν 3057, 3026, 2942, 2871, 1714, 1621, 1607, 1568, 1479, 1457, 1377, 1361, 1217, 1166, 1122, 1078, 1030, 993, 941,

831, 770, 703 cm^{-1}; MS (ESI) m/z 559.2 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{36}H_{29}N_2Cl_2$: 559.1702, Found: 559.1704.

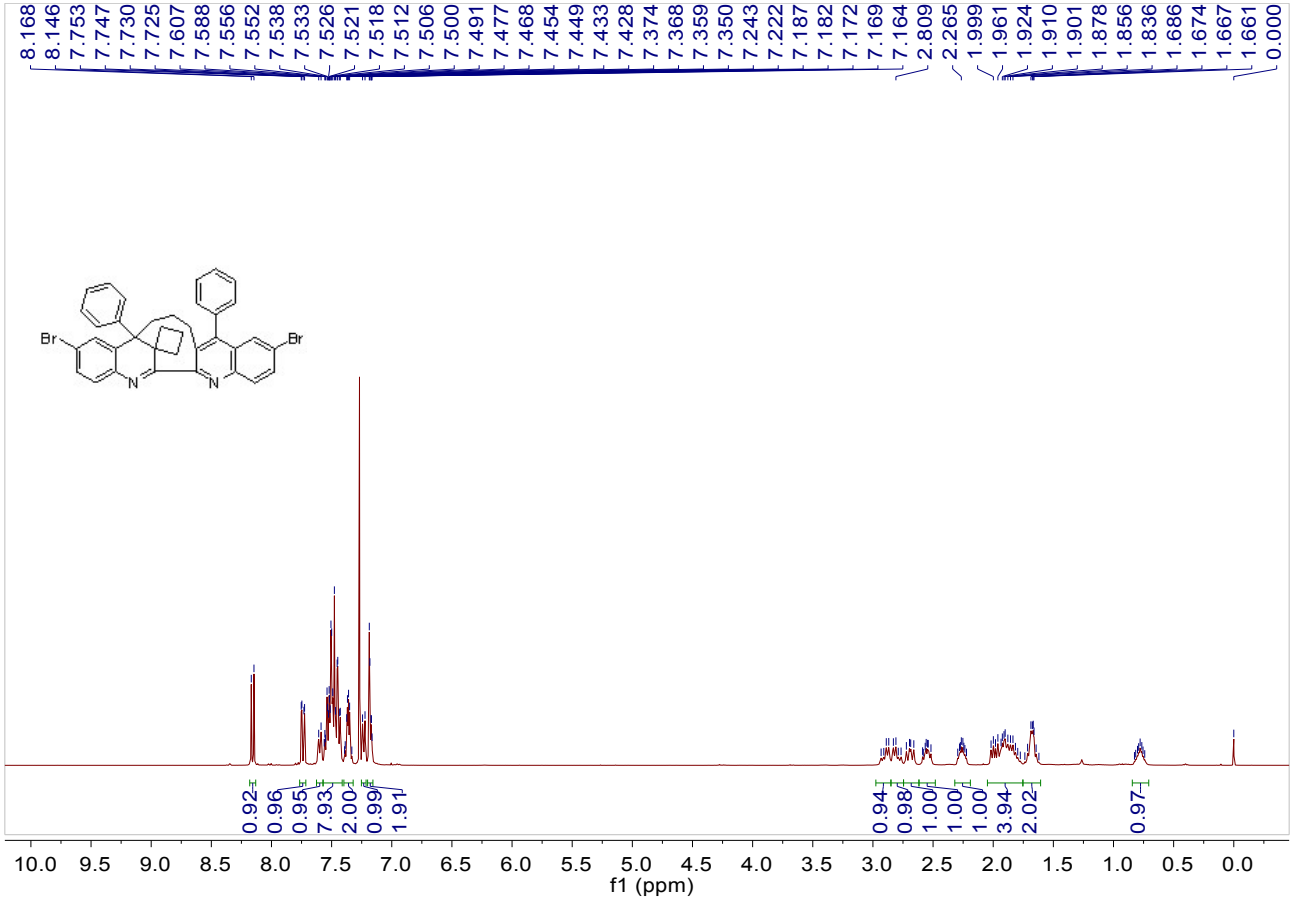


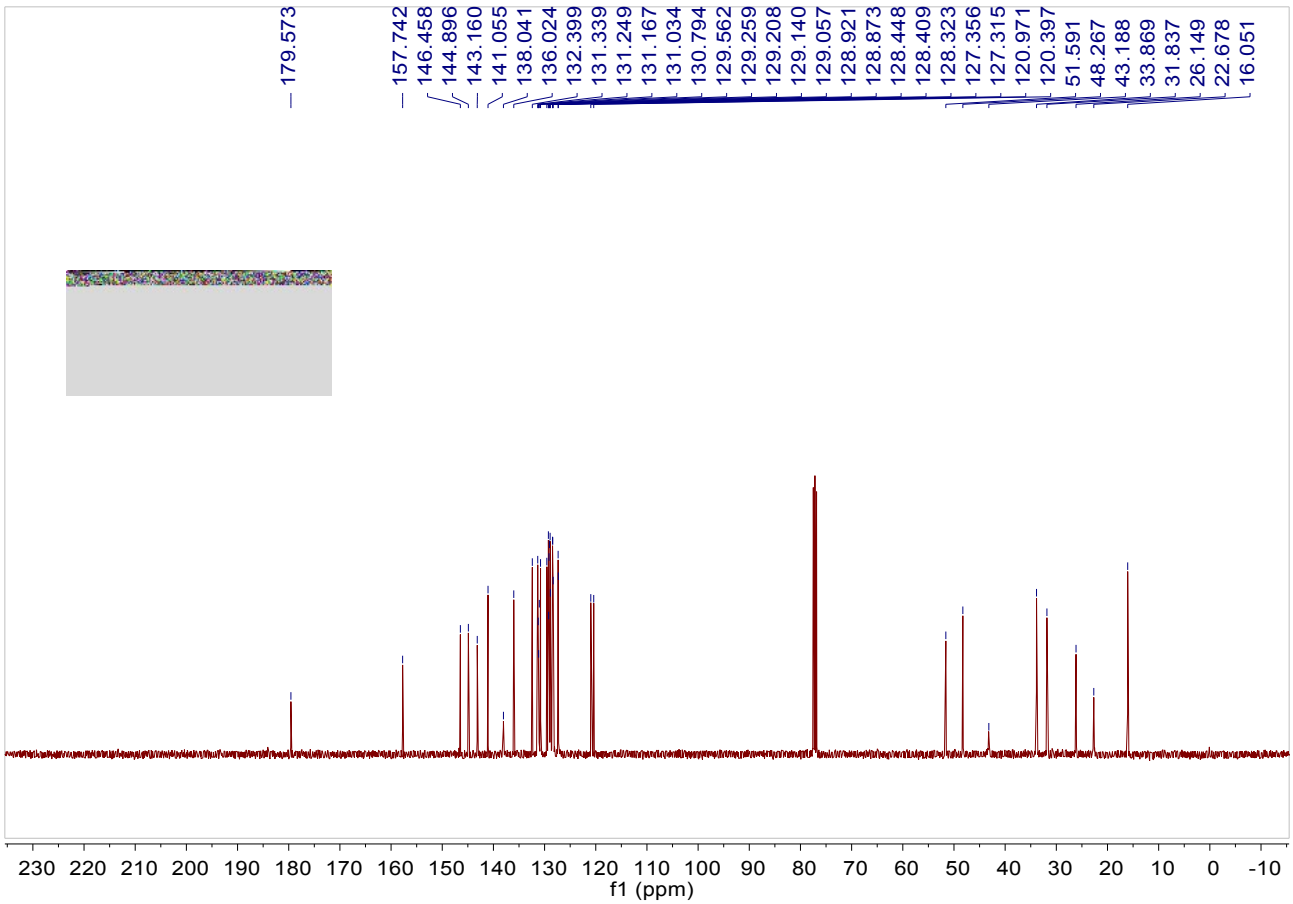


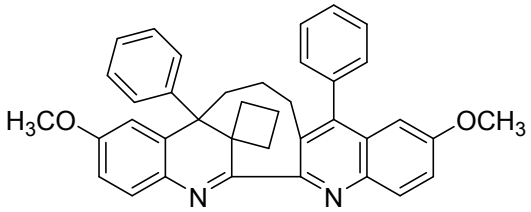


Compound **2s**: Yield: 342 mg, 53%; A brown solid; m.p. 317-319 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.74-0.83 (m, 1H), 1.62-1.74 (m, 2H), 1.78-2.02 (m, 4H), 2.22-2.30 (m, 1H), 2.52-2.59 (m, 1H), 2.69 (dd, *J* = 14.4 Hz, *J* = 10.4 Hz, 1H), 2.80 (dd, *J* = 17.2 Hz, *J* = 8.4 Hz, 1H), 2.90 (dd , *J* = 17.2 Hz, *J* = 8.8 Hz, 1H) 7.16-7.19 (m, 2H), 7.23 (d, *J* = 8.4 Hz, 1H), 7.33-7.39 (m, 2H), 7.43-7.56 (m, 8H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.74 (dd, *J* = 9.2 Hz, *J* = 2.4 Hz, 1H), 8.16 (d, *J* = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.1, 22.7, 26.1, 31.8, 33.9, 43.2, 48.3, 51.6, 120.4, 121.0, 127.3, 127.4, 128.3, 128.41, 128.45, 128.87, 128.92, 129.06, 129.14, 129.2, 129.3, 129.6, 130.8, 131.0, 131.17, 131.25, 131.3, 132.4, 136.0, 138.0, 141.1, 143.2, 144.9, 146.5, 157.7, 179.6; IR (CH_3COCH_3): ν 3003, 2945, 1711, 1621, 1597, 1477, 1442, 1414, 1359, 1220, 1091, 1032, 995, 914, 833, 770, 735, 713 cm^{-1}; MS (ESI) m/z 647.1 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{36}H_{29}N_2Br_2$:

647.0692, Found: 647.0696.

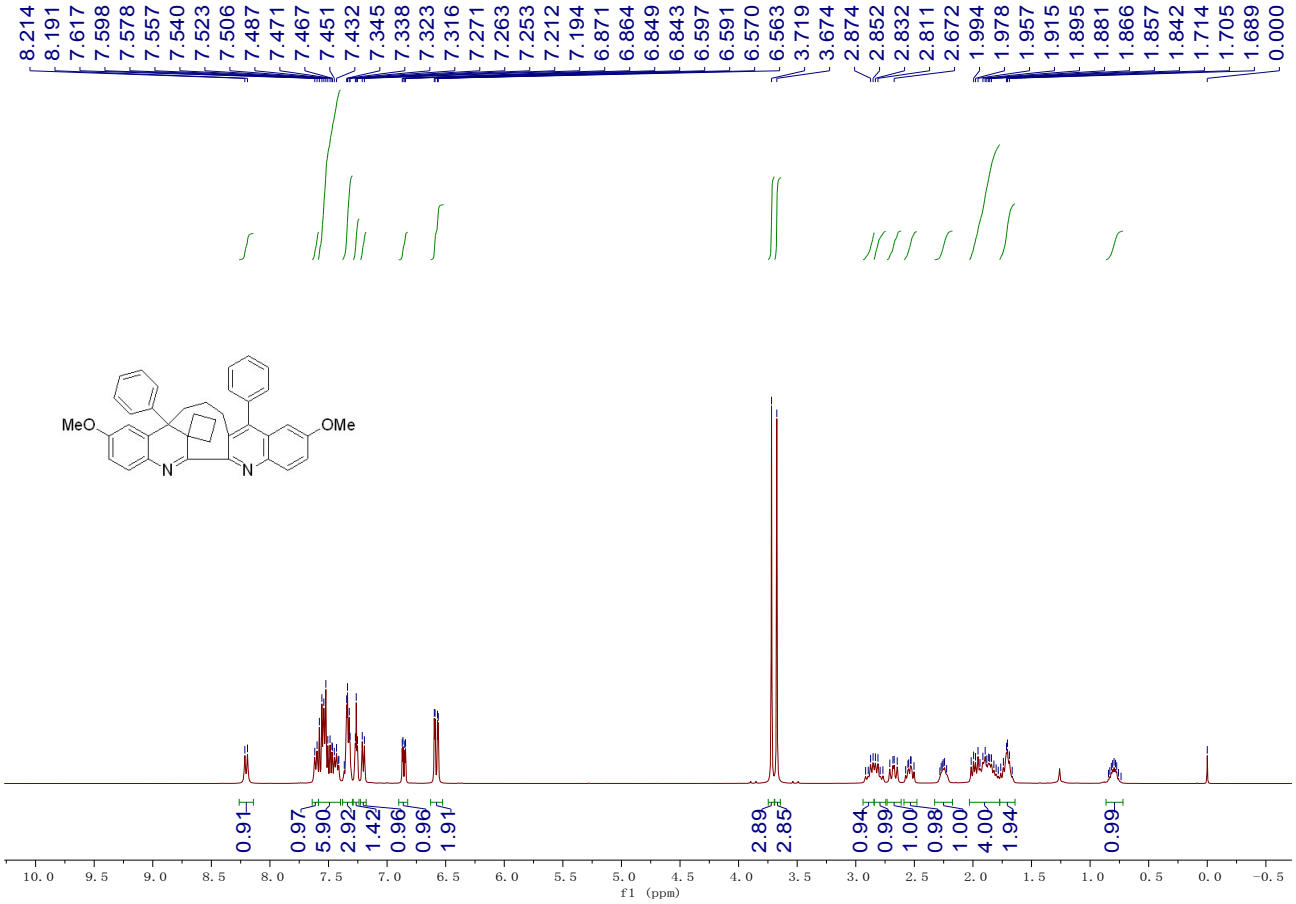


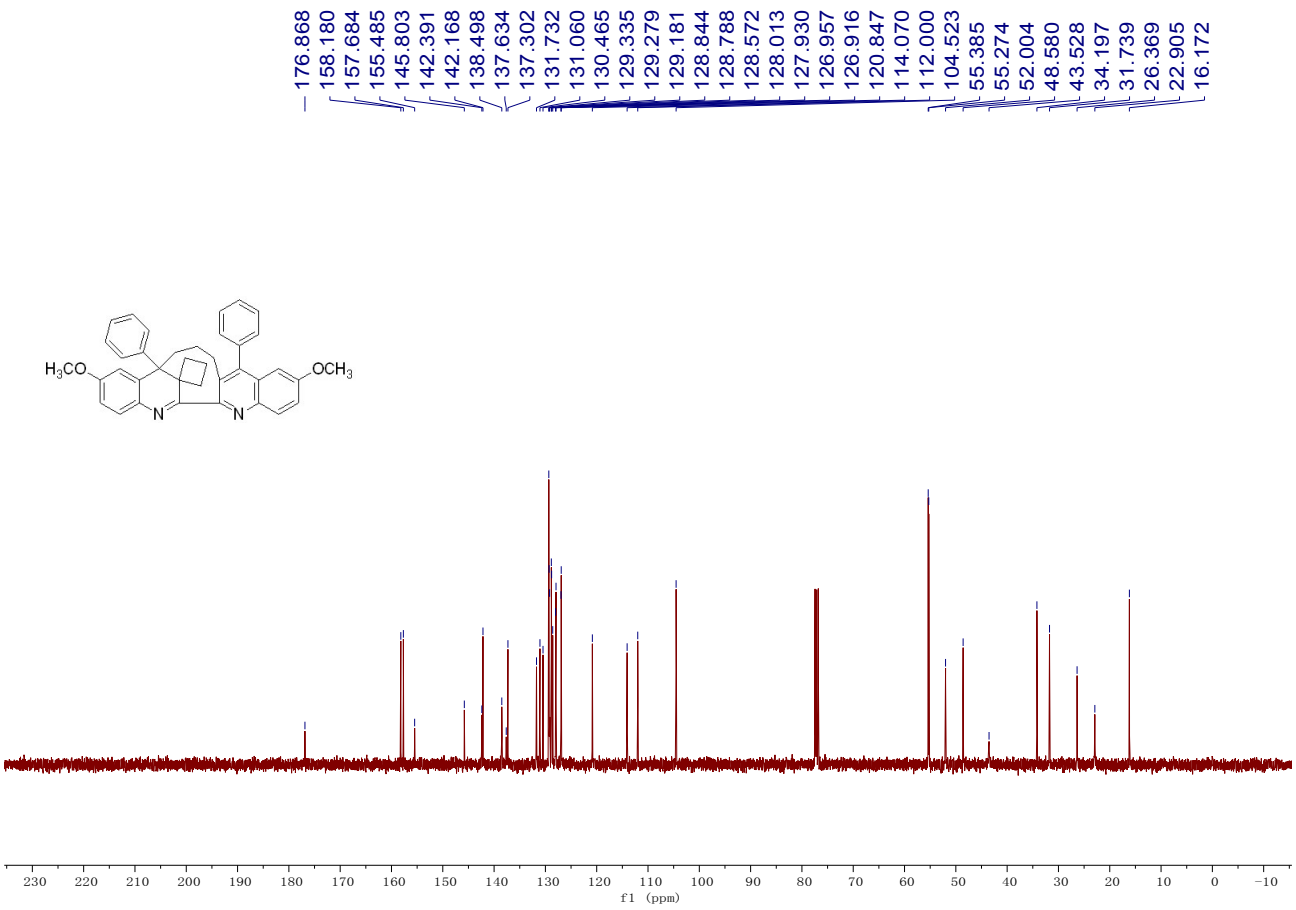


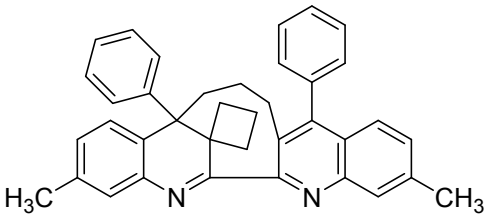


Compound **2t**: Yield: 209 mg, 38%; A brown solid; m.p. 243-245 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.74-0.84 (m, 1H), 1.67-1.74(m, 2H), 1.76-2.02 (m, 4H), 2.24-2.28 (m, 1H), 2.50-2.57 (m, 1H), 2.68 (dd, *J* = 14.8 Hz, *J* = 10.4 Hz, 1H), 2.80 (dd, *J* = 16.0 Hz, *J* = 8.4 Hz, 1H), 2.88 (dd, *J* = 16.0 Hz, *J* = 8.4 Hz, 1H), 3.67 (s, 3H), 3.72 (s, 3H), 6.58 (dd, *J* = 10.8 Hz, *J* = 2.6 Hz, 2H), 6.86 (dd, *J* = 8.8 Hz, *J* = 2.6 Hz, 1H), 7.20 (d, *J* = 7.2 Hz, 1H), 7.26 (t, *J* = 3.6 Hz, 1H), 7.32-7.37 (m, 3H), 7.41-7.58 (m, 6H), 7.61 (d, *J* = 7.6 Hz, 1H), 8.20 (d, *J* = 9.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.2, 22.9, 26.4, 31.7, 34.2, 43.5, 48.6, 52.0, 55.3, 55.4, 104.5, 112.0, 114.1, 120.8, 126.9, 127.0, 127.9, 128.0, 128.6, 128.79, 128.84, 129.2, 129.3, 129.3, 130.5, 131.1, 131.7, 137.3, 137.6, 138.5, 142.2, 142.4, 145.8, 155.5, 157.7, 158.2, 176.9; IR (CH_3COCH_3): ν 3055, 2936, 2854, 1713, 1618, 1571, 1490, 1442, 1361, 1274, 1227, 1183, 1153, 1119, 1034, 994, 832, 774, 732, 703

cm^{-1}; MS (ESI) m/z 551.3 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{38}H_{35}N_2O_2$: 551.26930, Found: 551.27093.

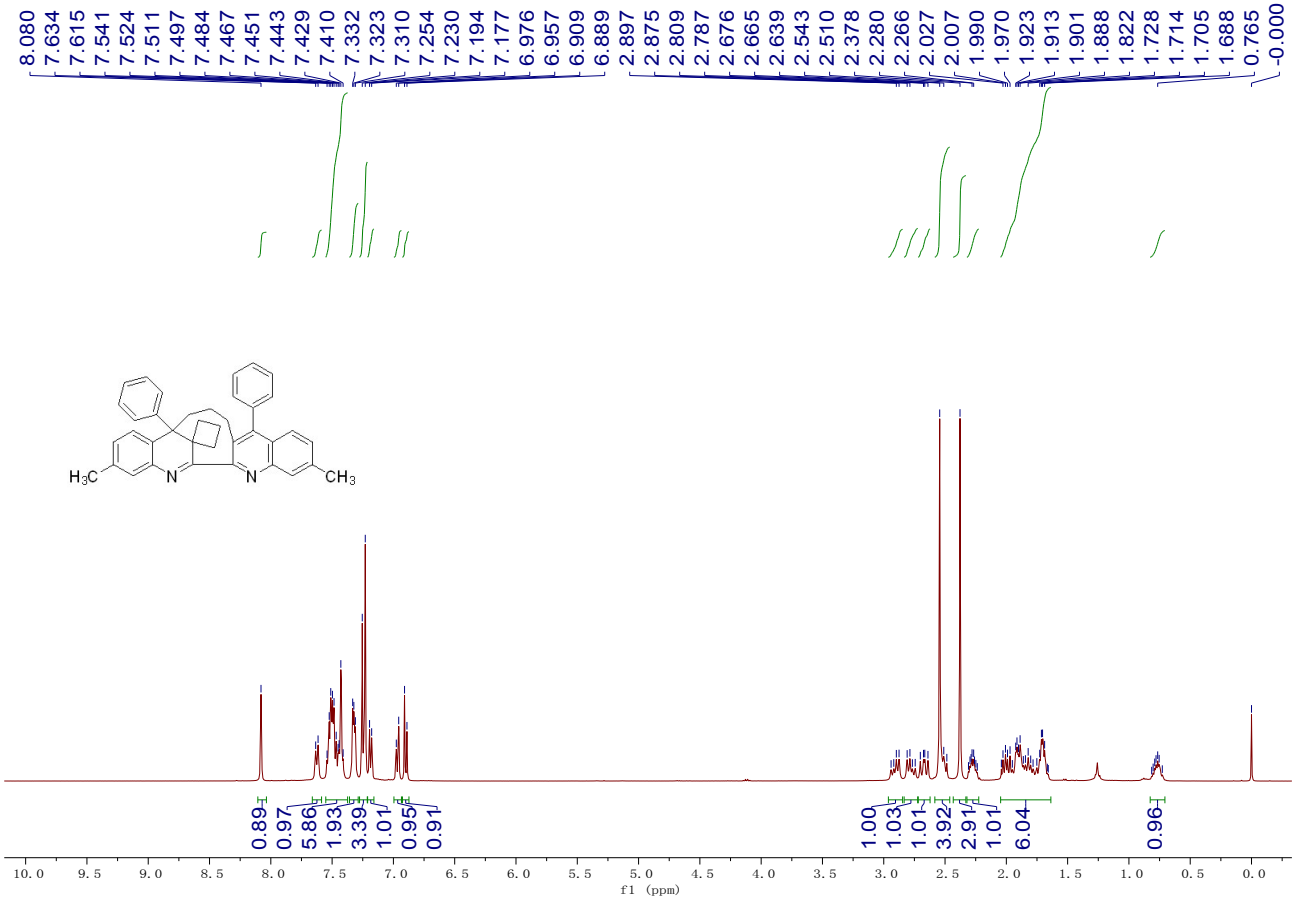


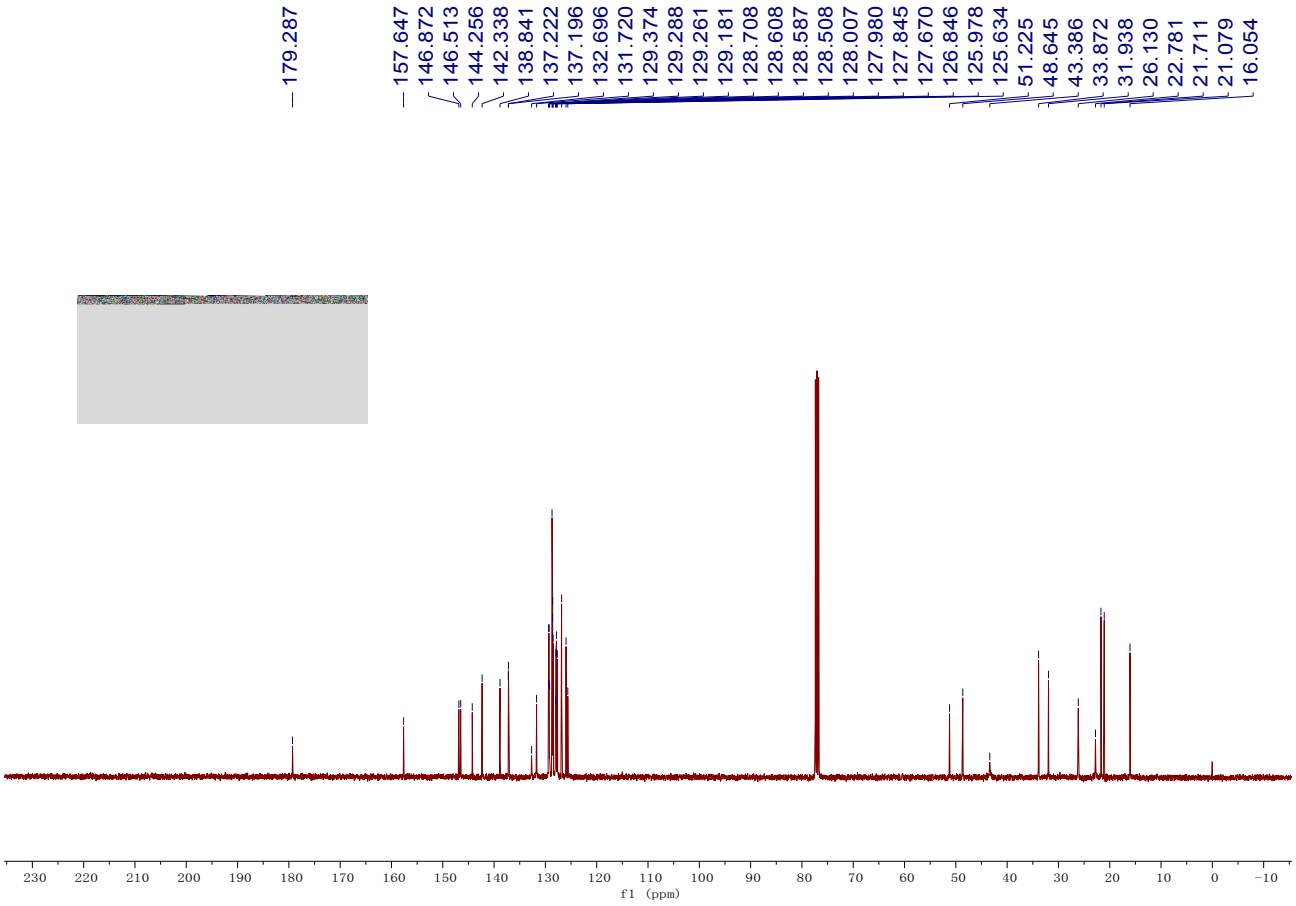


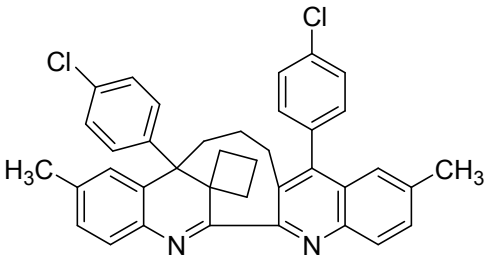


Compound **2u**: Yield: 262 mg, 51%; A brown solid; m.p. 310-312 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.73-0.81 (m, 1H), 1.66-2.04 (m, 6H), 2.24-2.31 (m, 1H), 2.38 (s, 3H), 2.49-2.54 (m, 4H), 2.67 (dd, *J* = 14.8 Hz, *J* = 10.4 Hz, 1H), 2.78 (dd, *J* = 17.2 Hz, *J* = 8.8 Hz, 1H), 2.91 (dd , *J* = 17.2 Hz, *J* = 8.8 Hz, 1H), 6.90 (d, *J* = 8.0 Hz, 1H), 6.97 (d, *J* = 7.6 Hz, 1H), 7.19 (d, *J* = 6.8 Hz, 1H), 7.23-7.25 (m, 3H), 7.31-7.33 (m, 2H), 7.41-7.54 (m, 6H), 7.62 (d, *J* = 7.6 Hz, 1H), 8.08 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.1, 21.1, 21.7, 22.8, 26.1, 31.9, 33.9, 43.4, 48.6, 51.2, 125.6, 126.0, 126.8, 127.7, 127.8, 127.98, 128.01, 128.5, 128.59, 128.61, 128.7, 129.2, 129.26, 129.29, 129.4, 131.7, 132.7, 137.20, 137.22, 138.8, 142.3, 144.3, 146.5, 146.9, 157.6, 179.3; IR (CH_3COCH_3): ν 3055, 3029, 2982, 2923, 2872, 1713, 1605, 1560, 1489, 1443, 1359, 1263, 1219, 1122, 1032, 994, 922, 883, 847, 799, 747, 703, 681 cm^{-1}; MS (ESI) m/z 519.3 $(M+H)^{+}$; HRMS

(ESI) Calcd. for $C_{38}H_{35}N_2$: 519.27948, Found:519.27968.

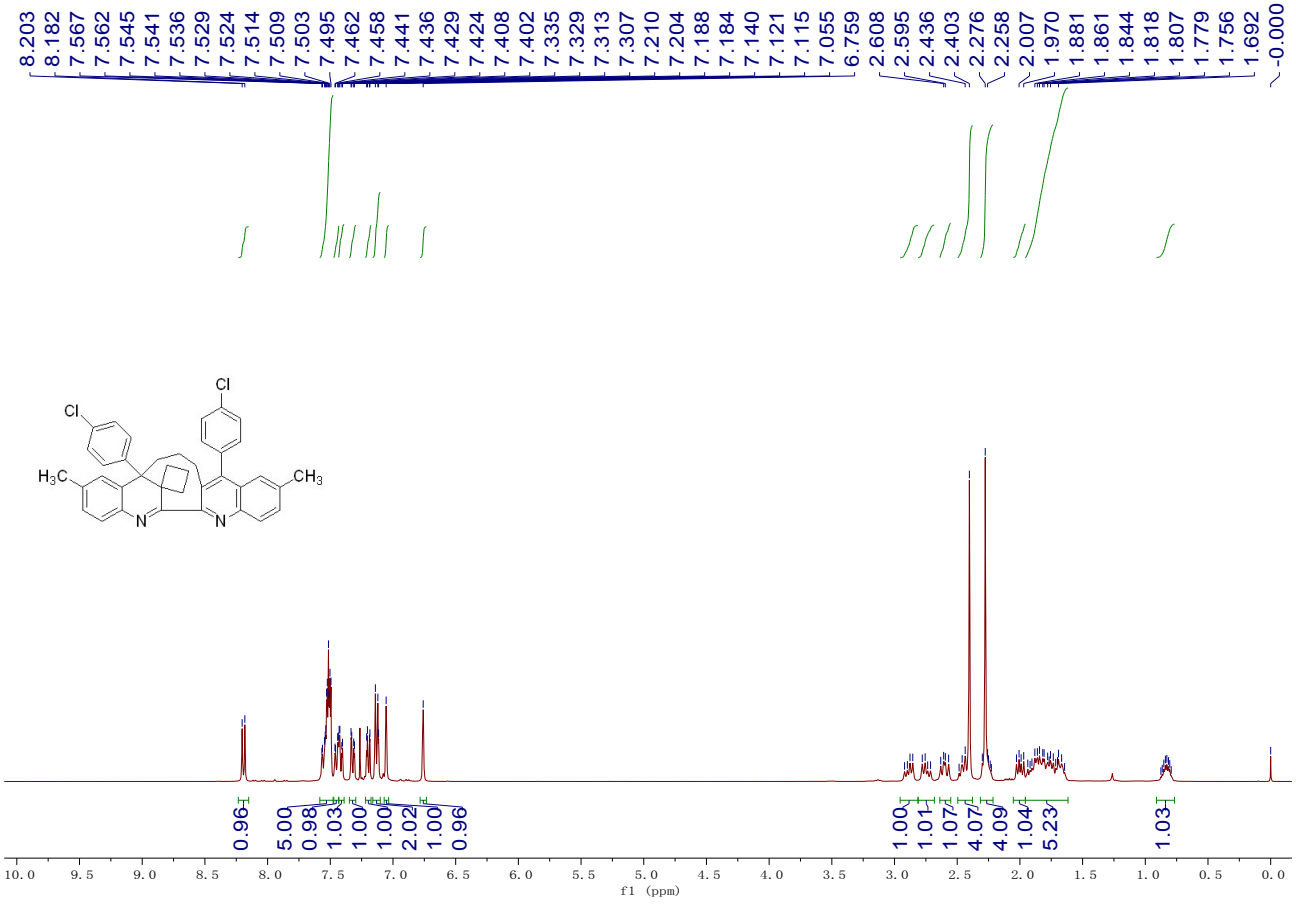


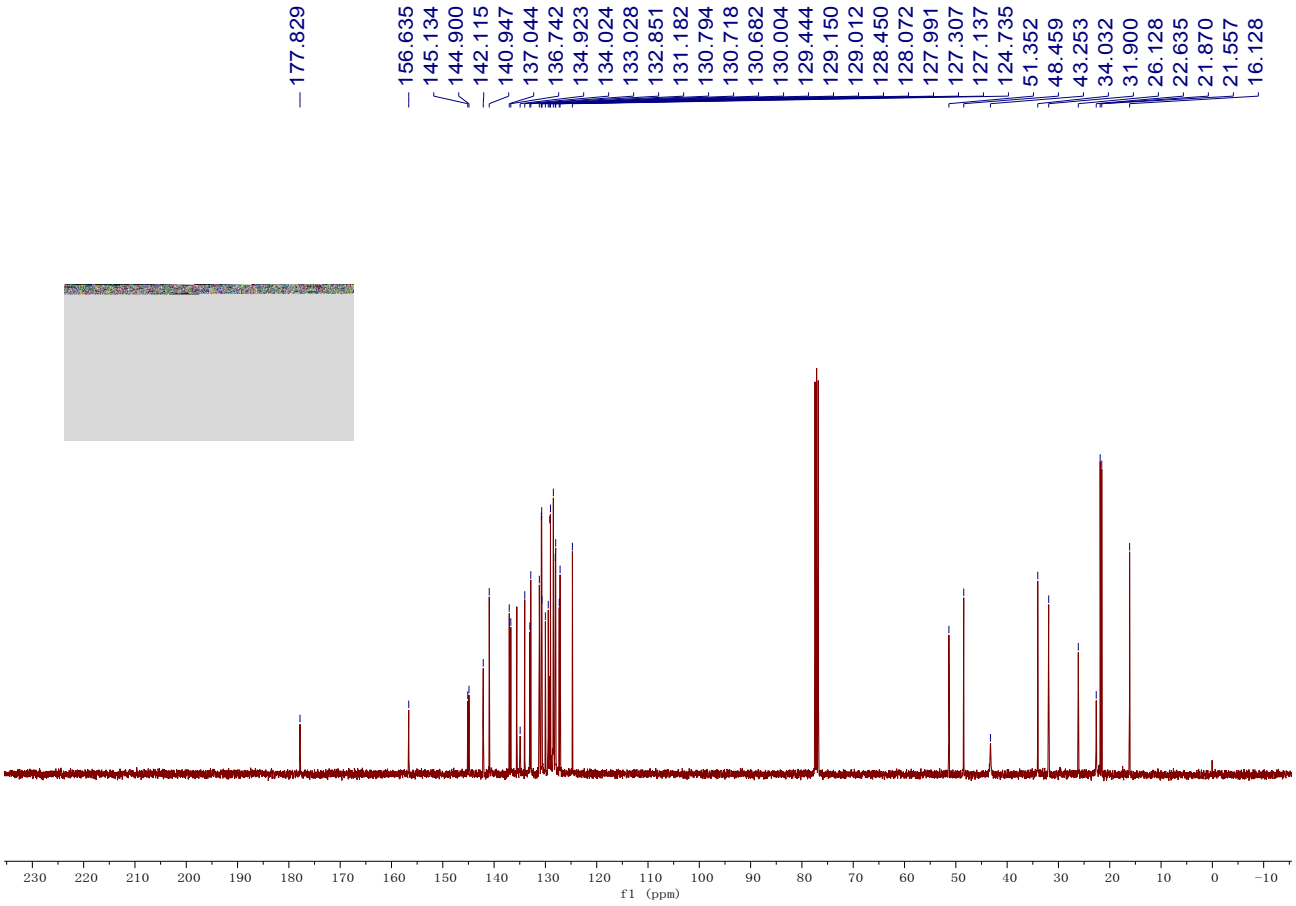


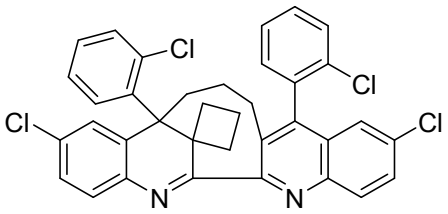


Compound **2v**: Yield: 287 mg, 49%; A brown solid; m.p. 297-299 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.79-0.88 (m, 1H), 1.64-1.94 (m, 5H), 2.00 (dd, *J* = 14.8 Hz, *J* = 8.0 Hz, 1H), 2.23-2.30 (m, 4H), 2.40-2.49 (m, 4H), 2.60 (dd, *J* = 14.4 Hz, *J* = 10.4 Hz, 1H), 2.75 (dd, *J* = 17.2 Hz, *J* = 9.2 Hz, 1H), 2.89 (dd, *J* = 17.2 Hz, *J* = 9.2 Hz, 1H), 6.76 (s, 1H), 7.06 (s, 1H), 7.12-7.14 (m, 2H), 7.20 (dd, *J* = 8.4 Hz, *J* = 2.0 Hz, 1H), 7.32 (dd, *J* = 8.8 Hz, *J* = 2.4 Hz, 1H), 7.42 (dd, *J* = 8.4 Hz, *J* = 2.2 Hz, 1H), 7.45 (dd, *J* = 8.4 Hz, *J* = 2.0 Hz, 1H), 7.50-7.57 (m, 5H), 8.19 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.1, 21.6, 21.9, 22.6, 26.1, 31.9, 34.0, 43.3, 48.5, 51.4, 124.7, 127.1, 127.3, 128.0, 128.1, 128.5, 129.0, 129.1, 129.4, 130.0, 130.68, 130.72, 130.8, 131.2, 132.9, 133.0, 134.0, 134.9, 136.7, 137.0, 140.9, 142.1, 144.9, 145.1, 156.6, 177.8; IR (CH_3COCH_3): ν

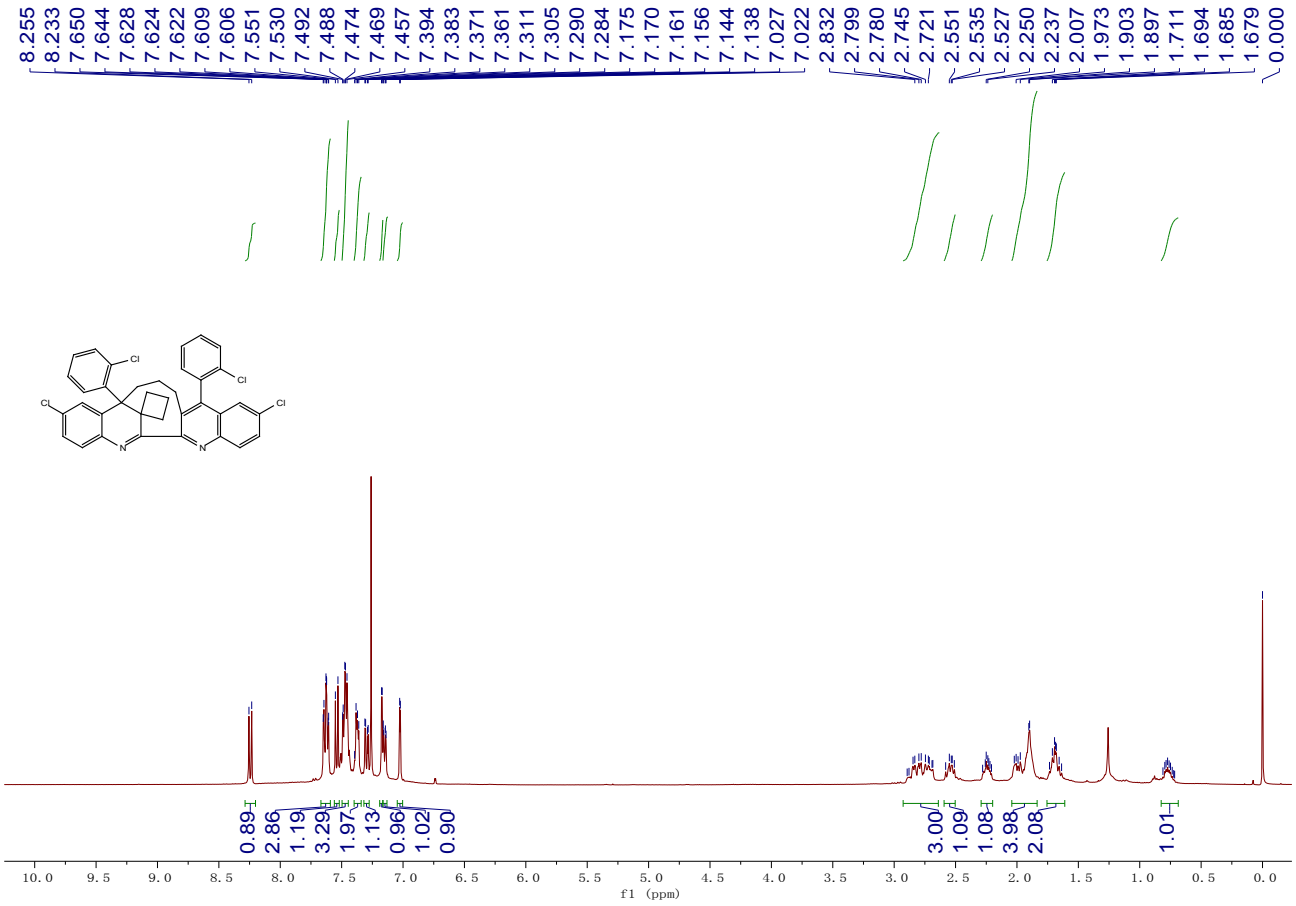
3006, 2923, 2862, 1711, 1621, 1592, 1488, 1421, 1360, 1220, 1090, 1013, 919, 828, 733 cm^{-1}; MS (ESI) m/z 587.2 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{38}H_{33}N_2Cl_2$: 587.20153, Found: 587.19984.

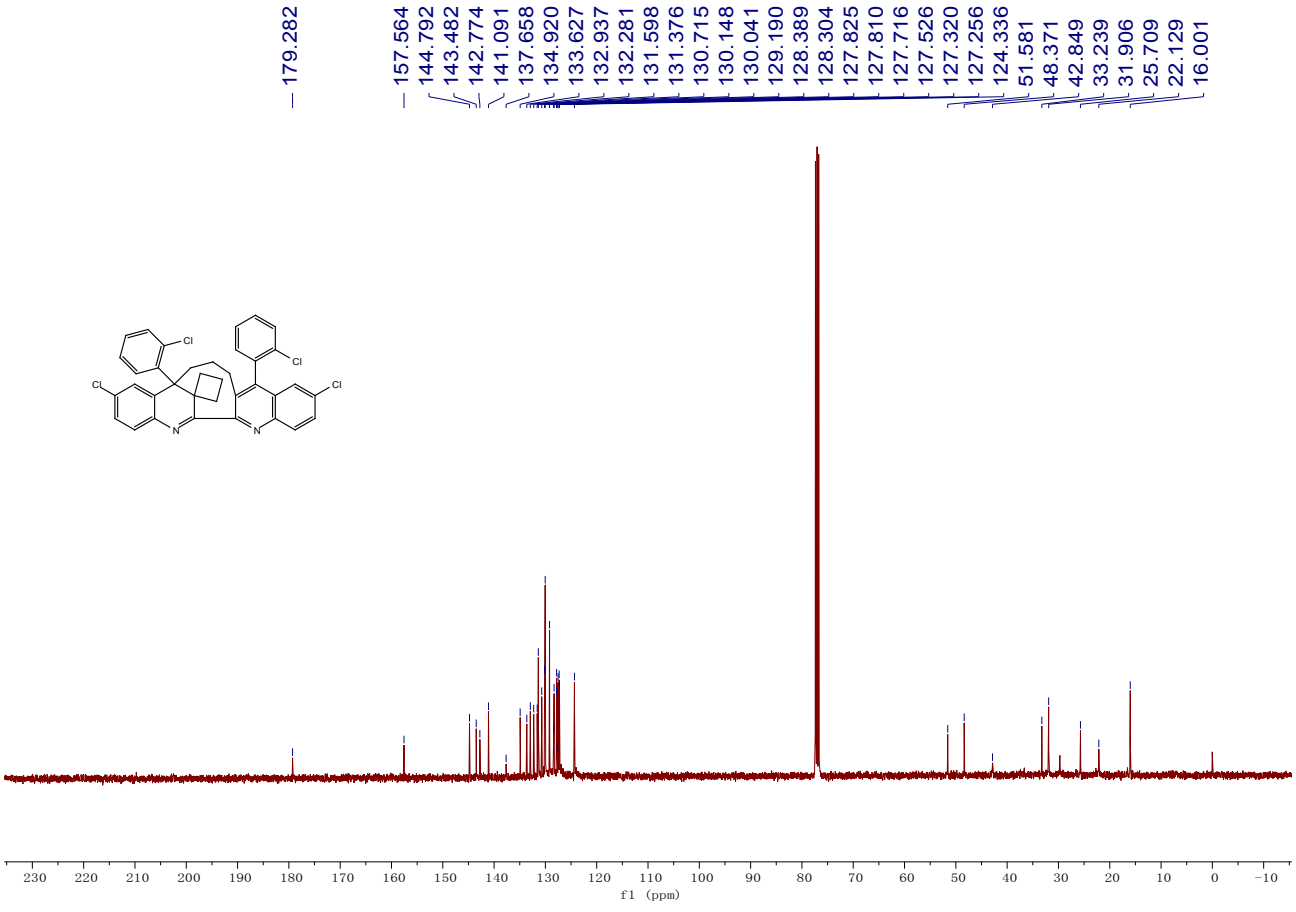




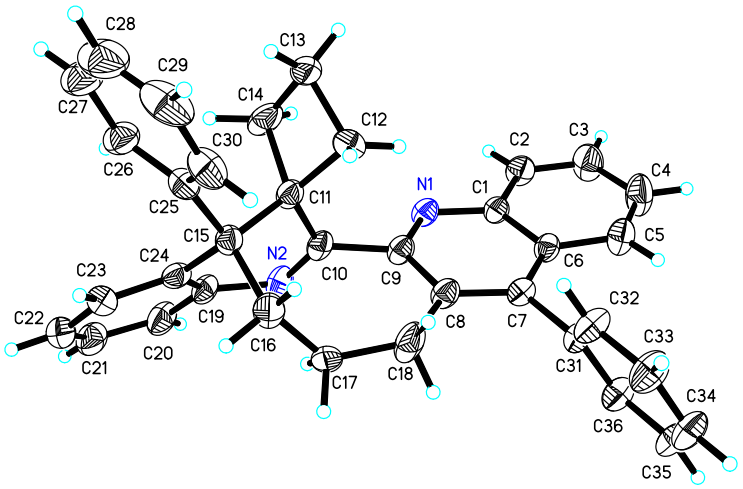


Compound **2w**: Yield: 87 mg, 14%; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.72-0.81 (m, 1H), 1.64-1.74 (m, 2H), 1.90-2.02 (m, 4H), 2.21-2.28 (m, 1H), 2.51-2.58 (m, 1H), 2.69-2.89 (m, 3H), 7.02 (d, *J* = 2.0 Hz, 1H), 7.15 (dd, *J* = 6.8 Hz, *J* = 2.0 Hz, 1H), 7.17 (d, *J* = 2.0 Hz, 1H), 7.30 (dd, *J* = 8.4 Hz, *J* = 2.4 Hz, 1H), 7.36-7.39 (m, 2H), 7.46-7.49 (m, 3H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.61-7.65 (m, 3H), 8.24 (d, *J* = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 16.0, 22.1, 25.7, 31.9, 33.2, 42.8, 48.4, 51.6, 124.3, 127.26, 127.32, 127.5, 127.7, 127.81, 127.83, 128.3, 128.4, 129.2, 130.0, 130.1, 130.7, 131.4, 131.6, 132.3, 132.9, 133.6, 134.9, 137.7, 141.1, 142.8, 143.5, 144.8, 157.6, 179.3; IR (CH_3COCH_3): ν 3058, 2942, 2864, 1713, 1063, 1567, 1470, 1401, 1360, 1219, 1168, 1125, 1079, 1054, 1035, 994, 938, 920, 830, 758, 736, 707 cm^{-1}; MS (ESI) m/z 627.1 $(M+H)^+$; HRMS (ESI) Calcd. for $C_{36}H_{27}N_2Cl_4$: 627.09229, Found: 627.09297.


8.255
8.233
7.650
7.644
7.628
7.624
7.622
7.609
7.606
7.551
7.530
7.492
7.488
7.474
7.469
7.457
7.394
7.383
7.371
7.361
7.311
7.305
7.290
7.284
7.175
7.170
7.161
7.156
7.144
7.138
7.027
7.022
2.832
2.799
2.780
2.745
2.721
2.551
2.535
2.527
2.250
2.237
2.007
1.973
1.903
1.897
1.711
1.694
1.685
1.679
0.000
Cl
Cl
Cl
Cl
N
N
0.89
2.86
1.19
3.29
1.97
1.13
0.96
1.02
0.90
3.00
1.09
1.08
3.98
2.08
1.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


179.282
157.564
144.792
143.482
142.774
141.091
137.658
134.920
133.627
132.937
132.281
131.598
131.376
130.715
130.148
130.041
129.190
128.389
128.304
127.825
127.810
127.716
127.526
127.320
127.256
124.336
51.581
48.371
42.849
33.239
31.906
25.709
22.129
16.001
Cl
Cl
Cl
Cl
N
N
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

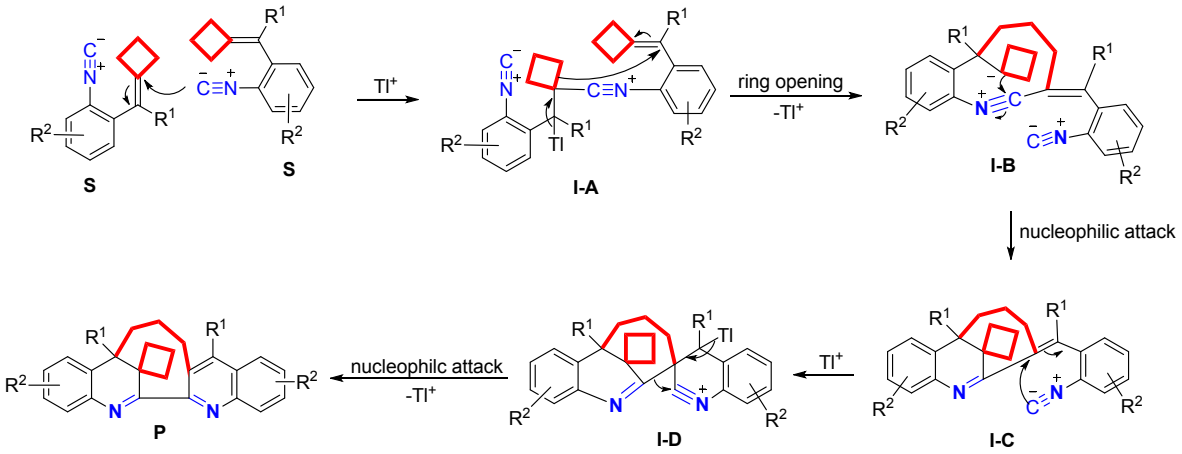
(F) X-ray Crystal Data of 2a



The crystal data of **2a** have been deposited in CCDC with number 1509688. Empirical Formula: $C_{36}H_{30}N_2$; Formula Weight: 490.62; Crystal Color, Habit: colorless, Crystal Dimensions: 0.200 x 0.160 x 0.130 mm^3; Crystal System: Monoclinic; Lattice Parameters: a = 13.796(2)Å, b = 13.582(2)Å, c = 14.676(2)Å, α = 90°, β = 110.931(4)°, γ = 90°, V = 2568.4(7)$Å^3$; Space group: P 21/c; Z = 4; D_{calc}= 1.269 g/cm^3; F_{000} = 1040; Final R indices [I>2sigma(I)] R1 = 0.0789, wR2 = 0.1731.

(G) Other Plausible Mechanisms of the Dimerization-Cyclization Reaction

Another plausible ionic reaction mechanism of dimerization-cyclization reaction

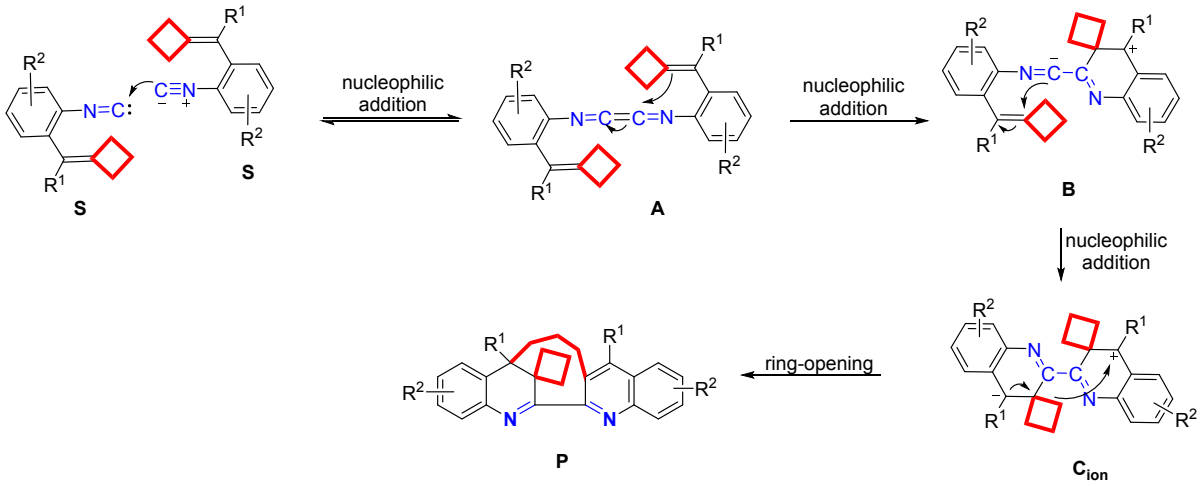


Scheme S6

For this ionic reaction mechanism, the C=C double bond of one substrate received the intermolecular nucleophilic attack of isocyanide group of another substrate at high temperature, affording the intermediate **I-A**. Then, the remaining C=C double bond of intermediate **I-A** could also receive the intramolecular nucleophilic attack of carbon anion along with the cyclobutane ring-opening process to give intermediate **I-B**. The subsequent intramolecular addition furnished the intermediate **I-C**, which underwent similar nucleophilic attacking process to give product **P** via intermediate **I-D**.

To simplify the calculation process, we investigated the reaction pathway starting from substrate **1a** without TlOAc additive. The proposed intermediate **I-A** and **I-D** can not be located by DFT calculation in gas phase at SMD/M06/6-311+G(d,p)//B3LYP/6-31G(d) level of theory with Gaussian 09 program.

Plausible ionic reaction mechanism of dimerization-cyclization reaction via 1,4-diazabutatriene intermediate

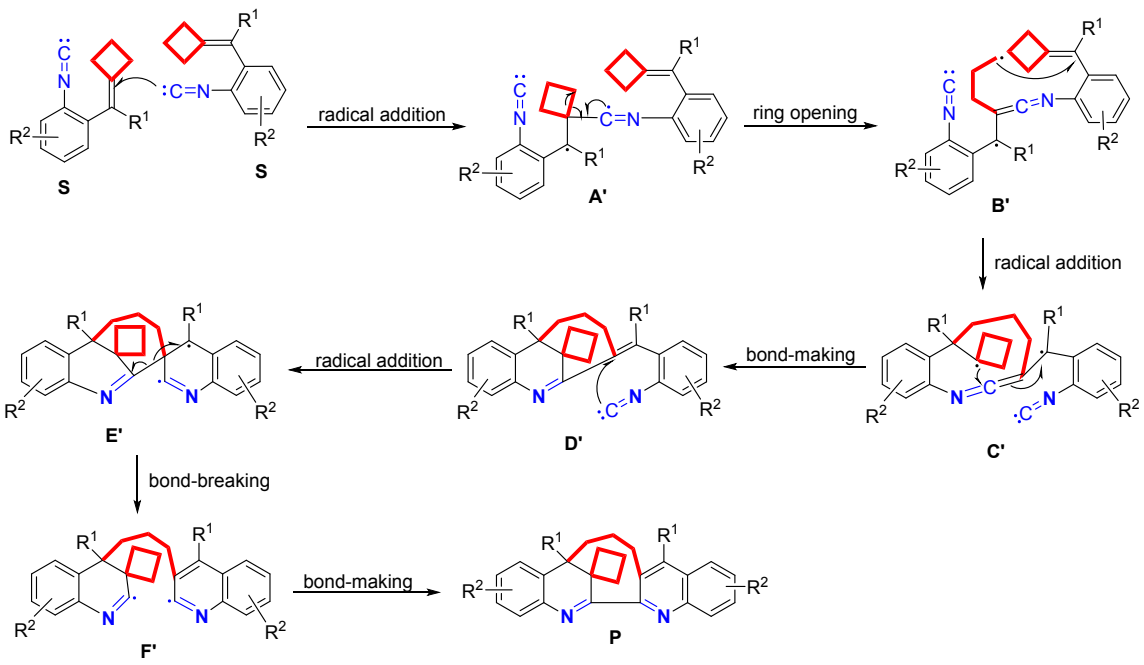


Scheme S7

For this ionic reaction mechanism, Firstly, the isocyanide carbon of one substrate underwent a nucleophilic attack on the isocyanide carbon of another substrate to give a 1,4-diazabutatriene intermediate **A**. Then, one C=C double bond of intermediate A underwent the intramolecular nucleophilic attack to 1,4-diazabutatriene unit, giving the intermediate **B**, which experienced another intramolecular nucleophilic attack to furnish intermediate $\mathbf{C_{ion}}$. Finally, intermediate $\mathbf{C_{ion}}$ underwent an intermolecular nucleophilic attack along with the cyclobutane ring-opening process to afford product. The Lewis acidic additive of TlOAc, which is quite stable at high temperature, could both activate the isocyano-group through σ-coordination and the C=C double bond by π-coordination, facilitating the reaction proceeding and improving the yield of this dimerization-cyclization reaction product. The key issue of this newly proposed reaction mechanism is the formation of 1,4-diazabutatriene unit.

To simplify the calculation process, we investigated the reaction pathway starting from substrate **1a** without TlOAc additive. The proposed intermediate from intermediate $\mathbf{C_{ion}}$ to product can not be located by DFT calculation in gas phase at SMD/M06/6-311+G(d,p)//B3LYP/6-31G(d) level of theory with Gaussian 09 program.

Another plausible biradical reaction mechanism of dimerization-cyclization reaction



Scheme S8

Firstly, the isocyano group of one substrate underwent a radical addition to the C=C double bond of another substrate at high temperature to give a biradical intermediate **A'**, which initiated the cyclobutane ring-opening to produce biradical intermediate **B'**. Then, the intramolecular radical addition took place to give biradical intermediate **C'**, which subsequently experienced a bond-making process to furnish intermediate **D'**. Finally, intermediate **D'** underwent a similar radical addition, bond-breaking and bond-making processes through biradical intermediates **E'** and **F'** to give the desired product. The Lewis acidic additive of TlOAc, which is quite stable at high temperature, could both activate the isocyano-group through σ-coordination and the C=C double bond by π-coordination, facilitating the reaction proceeding and improving the yield of this dimerization-cyclization reaction product. The key issue of this newly proposed reaction mechanism is the formation of the biradical intermediates as well as their reaction properties.

As a radical mediated process, a plausible biradical mechanism for this dimerization-cyclization reaction has been investigated by DFT calculations using the SMD/M06/6-311+G(d,p)//B3LYP/6-31G(d) level of theory with Gaussian 09 program.

The possible biradical reaction mechanisms along the singlet or triplet pathways were all

investigated theoretically. We first calculated the possible singlet pathway. The species reported in this paper are denoted as ^{m}ITEMx, where m = 1 for singlet and 3 for triplet spin state multiplicities; ITEMx = TSx for a transition state, A-F for a reaction intermediate, S for the substrate and P for the product. However, the suggested intermediates or transition states along the singlet pathway were not stable, and could not be located by calculations, indicating the infeasibility of possible biradical mechanism along the singlet pathway.

We subsequently calculated the possible triplet pathway, the solvation Gibbs free energy profile in 1,4-dioxane for the suggested triplet reaction pathway is shown in Figure 2 (the ΔG_{298} (kcal/mol), see Supporting Information for the details). First, substrate **S** is excited from the singlet state ^{1}S to the triplet state ^{3}S passing through an energy barrier of 45.5 kcal/mol, which is the rate determining step in the reaction, indicating the necessity of high temperature in this reaction. Second, the isocyano-group of one molecule of **1a** undergoes a radical addition to the C=C double bond of another molecule of **1a** via transition state **^{3}TS1'** with an energy barrier up to 6.9 kcal/mol to give an intermediate **^{3}A'**. Then, the intermediate **^{3}A'** undergoes a cyclobutane ring-opening to deliver an intermediate **^{3}B'** through the transition state **^{3}TS2'** peaked at 45.7 kcal/mol. Next, the intermediate **^{3}B'** passes through **^{3}TS3'** with an energy barrier of 22.9 kcal/mol to furnish an intermediate **^{3}C'**. A subsequent bond-making step generates an intermediate **^{3}D'** through **^{3}TS4'** with an energy barrier of 7.9 kcal/mol. The intermediate **^{3}D'** undergoes another radical addition to give an intermediate **^{3}E'** through transition state **^{3}TS5'** with an energy barrier of 23.7 kcal/mol. Subsequently, the intermediate **^{3}E'** passes through **^{3}TS6'** with an energy barrier of 21.2 kcal/mol to afford intermediate **^{3}F'**. Finally, another bond-making step generates the desired product **^{1}P** through **^{3}TS7'** with an energy barrier of 12.9 kcal/mol. Moreover, the total $\Delta G_{298,\ rxn}$ in 1,4-dioxane of this reaction is -76.0 kcal/mol overall, accounting for a thermodynamically favorable process. The calculation results support that this reaction proceeds through a biradical reaction mechanism in a triplet pathway.

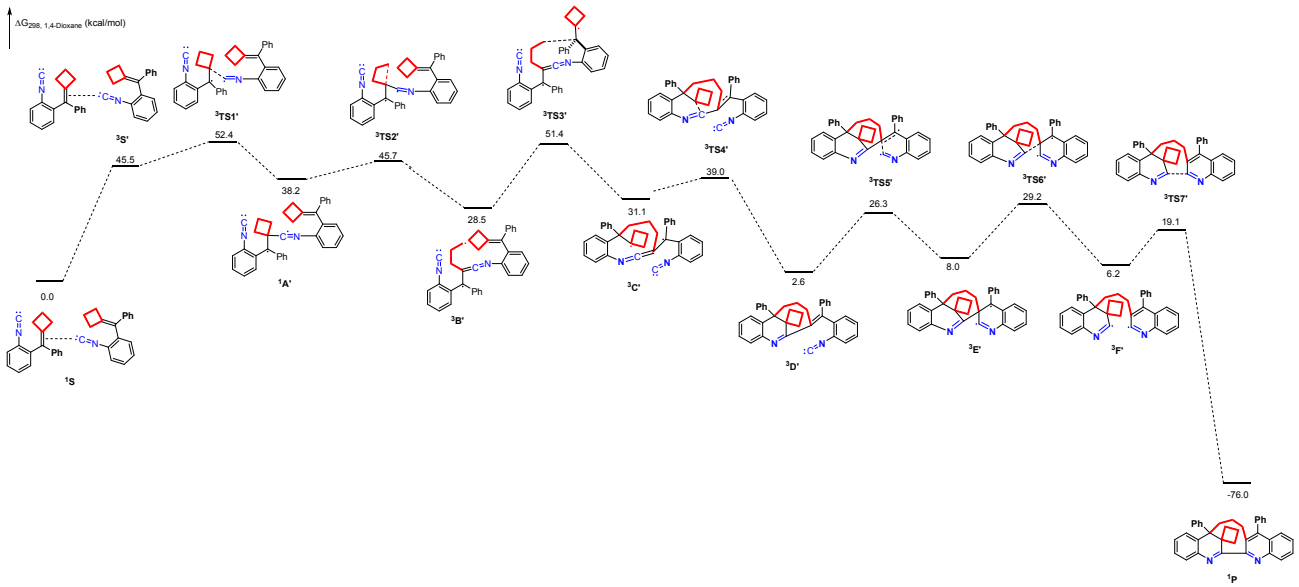

ΔG298, 1,4-Dioxane (kcal/mol)
0.0
45.5
52.4
38.2
45.7
28.5
51.4
31.1
39.0
2.6
26.3
8.0
29.2
6.2
19.1
-76.0
1S
3S'
3TS1'
1A'
3TS2'
3B'
3TS3'
3C'
3TS4'
3D'
3TS5'
3E'
3TS6'
3F'
3TS7'
1P

Figure S1

(H) Computational Details

The geometries of compounds not involving Ag atom have been optimized at B3LYP/6-31G(d) level; and the geometries of compounds involving Ag atom have been optimized at B3LYP/6-31G(d)/LANL2DZ level. The subsequent frequency calculations on the stationary points were carried out at the same level of theory to ascertain the nature of the stationary points as minima on the respective potential energy surfaces. The conformational space of flexible systems has first been searched manually. Thermochemical corrections to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at this same level. The thermochemical corrections have been combined with single-point energies calculated at the SMD/M06/6-311+G(d,p)/LANL2DZ//B3LYP/6-31G(d)/LANL2DZ or SMD/M06/6-311+G(d,p)//B3LYP/6-31G(d) level to yield free energy G_{298} at 298.15 K. All quantum mechanical calculations have been performed with Gaussian 09.

Table S4. The total energies, enthalpies and free energies of all species in gas phase shown in Scheme 2

	E_{tot}	H_{298}	G_{298}
S' + Ag^+	-855.812220	-855.546588	-855.612770
TS1'	-855.776548	-855.512562	-855.575846
IntA'	-855.793667	-855.528595	-855.590760
TS2'	-855.737515	-855.474538	-855.535718
P' + Ag^+	-855.930296	-855.661684	-855.722682

Table S5. The total energies, enthalpies and free energies of all species in 1,4-dioxane shown in Scheme 2, $\varepsilon = 2.2099$

	E_{tot}	H_{298}	G_{298}
S' + Ag^+	-855.521950	-855.256318	-855.322500
TS1'	-855.487614	-855.223628	-855.286912
IntA'	-855.499613	-855.234540	-855.296705
TS2'	-855.442583	-855.179606	-855.240786

P' + Ag^+	-855.624175	-855.355563	-855.416561

Table S6. The total energies, enthalpies and free energies of all species in gas phase shown in Scheme 3

	E_{tot}	H_{298}	G_{298}
S	-1499.235195	-1498.646729	-1498.757543
TS1	-1499.203255	-1498.616714	-1498.722890
IntA	-1499.232753	-1498.644096	-1498.748129
TS2	-1499.216203	-1498.628918	-1498.727954
IntB	-1499.256610	-1498.666629	-1498.766492
^{3}IntB	-1499.231609	-1498.643212	-1498.744239
^{3}TS3	-1499.219658	-1498.632238	-1498.728868
^{3}IntC	-1499.272033	-1498.681984	-1498.777578
^{3}TS4	-1499.258337	-1498.670428	-1498.766488
^{3}IntD	-1499.293752	-1498.704856	-1498.805814
^{3}TS5	-1499.232367	-1498.644590	-1498.736456
P	-1499.365122	-1498.770233	-1498.859905

Table S7. The total energies, enthalpies and free energies of all species in 1,4-dioxane shown in Scheme 3, $\varepsilon = 2.2099$

	E_{tot}	H_{298}	G_{298}
S	-1498.450016	-1497.861550	-1497.972364
TS1	-1498.423991	-1497.837450	-1497.943626
IntA	-1498.454387	-1497.865731	-1497.969764
TS2	-1498.435140	-1497.847856	-1497.946892
IntB	-1498.483202	-1497.893221	-1497.993084
^{3}IntB	-1498.458141	-1497.869744	-1497.970771

^{3}TS3	-1498.443723	-1497.856303	-1497.952933
^{3}IntC	-1498.500639	-1497.910590	-1498.006184
^{3}TS4	-1498.483977	-1497.896068	-1497.992128
^{3}IntD	-1498.513001	-1497.924105	-1498.025063
^{3}TS5	-1498.465054	-1497.877277	-1497.969143
P	-1498.600831	-1498.005942	-1498.095614

Table S8. The total energies, enthalpies and free energies of all species in gas phase shown in Scheme S8

	E_{tot}	H_{298}	G_{298}
^{1}S	-1499.232735	-1498.644456	-1498.756637
^{3}S'	-1499.152954	-1498.567783	-1498.682619
^{3}TS1'	-1499.140010	-1498.555358	-1498.659671
^{3}Int A'	-1499.164393	-1498.577160	-1498.681200
^{3}TS2'	-1499.156548	-1498.571745	-1498.676243
^{3}IntB'	-1499.182998	-1498.597675	-1498.705254
^{3}TS3'	-1499.145513	-1498.560591	-1498.660431
^{3}IntC'	-1499.176481	-1498.588287	-1498.686953
^{3}TS4'	-1499.163990	-1498.576465	-1498.670599
^{3}IntD'	-1499.225424	-1498.635225	-1498.728987
^{3}TS5'	-1499.186887	-1498.597915	-1498.687471
^{3}IntE'	-1499.220677	-1498.628777	-1498.717118
^{3}TS6'	-1499.188650	-1498.598689	-1498.688399
^{3}IntF'	-1499.230969	-1498.638890	-1498.735656
^{3}TS7'	-1499.211656	-1498.621724	-1498.713776
^{1}P	-1499.365122	-1498.770233	-1498.859905

Table S9. The total energies, enthalpies and free energies of all species in 1,4-dioxane shown in Scheme S8, ε = 2.2099

	E_{tot}	H_{298}	G_{298}
^{1}S'	-1498.450638	-1497.862358	-1497.974539
^{3}S'	-1498.372396	-1497.787224	-1497.902060
^{3}TS1'	-1498.371428	-1497.786777	-1497.891090
^{3}IntA'	-1498.396858	-1497.809625	-1497.913665
^{3}TS2'	-1498.382020	-1497.797217	-1497.901715
^{3}IntB'	-1498.406800	-1497.821477	-1497.929056
^{3}TS3'	-1498.377697	-1497.792775	-1497.892615
^{3}IntC'	-1498.414507	-1497.826312	-1497.924978
^{3}TS4'	-1498.405771	-1497.818245	-1497.912379
^{3}IntD'	-1498.466804	-1497.876605	-1497.970367
^{3}TS5'	-1498.432070	-1497.843097	-1497.932653
^{3}IntE'	-1498.465402	-1497.873502	-1497.961843
^{3}TS6'	-1498.428290	-1497.838329	-1497.928039
^{3}IntF'	-1498.459915	-1497.867836	-1497.964602
^{3}TS7'	-1498.441947	-1497.852014	-1497.944066
^{1}P	-1498.600831	-1498.005942	-1498.095614

(I) Archive Entries

S' + Ag^+

1\1\GINC-OM112\SP\RM06\GenECP\C17H13Ag1N1(1+)\WEIY\01-Apr-2020\0\\#p M
06/genecp geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Title Card
Required\\1,1\C,0,3.195615547,-1.7141944019,-0.1011900954\C,0,1.14715
88098,-1.648761532,-1.3713799279\C,0,1.4891971751,-2.8508707243,-1.992
9229139\C,0,2.6898198974,-3.4852736796,-1.6664680366\C,0,3.5480921493,
-2.9156820797,-0.7293202572\H,0,0.2330455909,-1.1335875921,-1.66478320
58\H,0,0.8251091309,-3.2837662564,-2.7343219875\H,0,2.964110619,-4.418
1349044,-2.1484140712\H,0,4.4930222958,-3.3833612717,-0.4743165287\C,0
,1.975489786,-1.0718243319,-0.3996446773\C,0,1.6128021777,0.2041622484
,0.3093219149\C,0,1.8197014958,1.480784638,-0.3812666217\C,0,2.4183545
042,1.5029882733,-1.6619201771\C,0,1.4659582777,2.7151520305,0.2166135
177\C,0,2.6649657654,2.7091917418,-2.3110167416\H,0,2.7042874389,0.573
9167467,-2.1412299085\C,0,1.7048969943,3.9130158624,-0.4395042899\H,0,
0.996380169,2.72889689,1.1933375634\C,0,2.30829843,3.9154856107,-1.705
464897\H,0,3.1357311005,2.7071669871,-3.2890170285\H,0,1.4264980754,4.
8508297787,0.0311631736\H,0,2.4975329457,4.8563562622,-2.2134965107\C,
0,1.1577230804,0.1017058233,1.6284470272\C,0,1.460901784,-0.71645449,2
.8374213927\C,0,1.3428106529,0.8082902539,2.9207515439\H,0,2.448792135
6,-1.162702628,2.909236736\H,0,0.6775589261,-1.2943046236,3.3207892069
\H,0,0.4919683761,1.2129271563,3.4635301882\H,0,2.2581524456,1.3879577
706,3.0316648815\N,0,4.0662675204,-1.1358568502,0.8053960233\C,0,4.805
1331364,-0.6248940449,1.5750821838\Ag,0,-0.9328364331,-0.2635716631,0.
8178125232\\Version=ES64L-G16RevA.03\State=1-A\HF=-855.52195\RMSD=4.36
5e-09\Dipole=-3.2945188,-0.4670415,-0.3556658\Quadrupole=-3.255343,7.0
167005,-3.7613574,-1.1732751,-12.1006265,2.6628728\PG=C01 [X(C17H13Ag1
N1)]\\@

TS1'

1\1\GINC-OM112\SP\RM06\GenECP\C17H13Ag1N1(1+)\WEIY\01-Apr-2020\0\\#p M
06/genecp geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Title Card
Required\\1,1\C,0,-0.1182368517,0.1238404119,-0.0107894321\C,0,-0.067
5592442,0.1070896124,1.4939747893\C,0,1.2091659341,-0.075609507,2.1042
502055\C,0,2.4145309786,0.2519238683,0.0785194703\H,0,-2.1673541112,0.
3175146323,1.9464852167\C,0,-1.1676541732,0.1791074964,2.3539397245\C,
0,1.3666098883,-0.197602759,3.4802413752\C,0,0.2413098675,-0.123806575
8,4.3032573777\C,0,-1.01946115,0.0701968153,3.7414114902\H,0,2.3601763
18,-0.3409199396,3.8908160288\H,0,0.3532576163,-0.2143125623,5.3787531
111\H,0,-1.8958567437,0.1340216058,4.3785976279\C,0,-0.4272161088,-1.1
905637385,-0.6950437944\C,0,-1.0664662301,-2.2341687937,0.0085787037\C
,0,-0.0858604568,-1.4122536869,-2.0492598933\C,0,-1.3591121391,-3.4436
507132,-0.6196073423\H,0,-1.3208959354,-2.1069881946,1.0548394407\C,0,
-0.3779297319,-2.6247309645,-2.6671468779\H,0,0.432121399,-0.645255885
7,-2.6128846161\C,0,-1.0195504683,-3.6452063087,-1.9585109626\H,0,-1.8
451487729,-4.2336695124,-0.0550224238\H,0,-0.0924808411,-2.777683042,-
3.7036719974\H,0,-1.2431956714,-4.5901956654,-2.4438397779\N,0,2.29953
29479,-0.0714888135,1.2224932699\C,0,0.7668336001,1.0510493753,-0.6235
785162\C,0,1.0771655724,2.5134279629,-0.5866714664\C,0,1.0330030658,1.
7524051854,-1.9061691874\H,0,2.0510211204,2.8301200395,-0.2272815179\H
,0,0.2685260947,3.195397415,-0.3361315819\H,0,0.2126420565,1.928255203
2,-2.5980311611\H,0,1.9854315858,1.5527934859,-2.388949978\Ag,0,-2.109
5601155,0.991374563,-0.7612239748\\Version=ES64L-G16RevA.03\State=1-A\
HF=-855.4876136\RMSD=5.173e-09\Dipole=-2.3028015,1.4524239,-0.5551789\
Quadrupole=-5.181786,-2.2966651,7.4784512,-1.1410582,3.7399219,-2.1308
36\PG=C01 [X(C17H13Ag1N1)]\\@

IntA'

1\1\GINC-OM112\SP\RM06\GenECP\C17H13Ag1N1(1+)\WEIY\01-Apr-2020\0\\#p M
06/genecp geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Title Card

Required\\1,1\C,0,-5.2150992126,0.4628819064,-2.6145458658\C,0,-4.655
5246018,1.839388443,-2.3094124924\C,0,-5.1973995315,2.6582091732,-1.27
89392168\C,0,-6.8662649885,1.1622573766,-1.1423156302\H,0,-2.992910377
,1.7469587786,-3.6838120469\C,0,-3.4911308927,2.3378724619,-2.91918864
69\C,0,-4.6835364735,3.8972117784,-0.9189326453\C,0,-3.5481211357,4.36
35410682,-1.5808179524\C,0,-2.9516798426,3.5767566972,-2.5690323695\H,
0,-5.1571048965,4.4650908457,-0.1255928875\H,0,-3.1206434047,5.3232570
867,-1.309698885\H,0,-2.0557503291,3.9265393202,-3.0723390245\C,0,-4.3
509692058,-0.6616286843,-2.0924586595\C,0,-3.5604096755,-0.4875064784,
-0.9397544185\C,0,-4.3292458064,-1.925817943,-2.7164671306\C,0,-2.7881
900457,-1.5329368574,-0.4343960519\H,0,-3.5472581053,0.4714659613,-0.4
321390014\C,0,-3.5538228451,-2.9692285428,-2.2173752853\H,0,-4.9149706
299,-2.0906238919,-3.620610794\C,0,-2.7807370522,-2.7761683616,-1.0693
0807\H,0,-2.1881053547,-1.3726728517,0.456401279\H,0,-3.5462464393,-3.
9279468807,-2.727221573\H,0,-2.1728561291,-3.5865073263,-0.6786127724\
N,0,-6.3386400549,2.0929805083,-0.606483112\C,0,-6.7339827915,0.300795
1407,-2.2793656799\C,0,-7.9700732692,0.2841329124,-3.2111189071\C,0,-7
.5772970037,-0.9485287375,-2.4807899801\H,0,-7.7530944398,0.3596762439
,-4.2739403193\H,0,-8.8388196453,0.8461690729,-2.8809771561\H,0,-8.174
790617,-1.2785170696,-1.6377163287\H,0,-7.0927684822,-1.7488709255,-3.
0275187216\Ag,0,-5.113664341,0.3291073649,-4.8696498046\\Version=ES64L
-G16RevA.03\State=1-A\HF=-855.4996125\RMSD=5.560e-09\Dipole=-0.9141787
,-0.0925289,-1.7520722\Quadrupole=-2.2103265,1.0719126,1.1384139,3.245
4512,2.6076823,3.6503768\PG=C01 [X(C17H13Ag1N1)]\\@

TS2'

1\1\GINC-OM112\SP\RM06\GenECP\C17H13Ag1N1(1+)\WEIY\01-Apr-2020\0\\#p M
06/genecp geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Title Card
Required\\1,1\C,0,0.3275705046,0.2249771831,0.3614433637\C,0,-1.15459
54091,0.4028165621,0.0695204307\C,0,-1.9998821312,0.9656849728,1.09839

51247\C,0,-0.45717373,0.432513364,2.5463131123\H,0,-1.1323908694,-0.13
37139954,-2.020069892\C,0,-1.7358066929,0.2385979299,-1.1959972017\C,0
,-3.3442646375,1.2792146241,0.8578337709\C,0,-3.8823668947,1.054158545
6,-0.4023448469\C,0,-3.0761937694,0.5455213401,-1.429626229\H,0,-3.940
7502553,1.6873052951,1.6667831405\H,0,-4.9248611963,1.2875782689,-0.59
40780757\H,0,-3.4927316316,0.395067035,-2.420639353\C,0,1.1867605914,1
.4184704989,0.0558857647\C,0,0.6527729798,2.6341886199,-0.4182621967\C
,0,2.5820660235,1.3457493737,0.2882997582\C,0,1.4868092593,3.719408308
,-0.6795150977\H,0,-0.4140432407,2.7302253811,-0.5837071818\C,0,3.4075
897912,2.4351074898,0.0422763481\H,0,3.0145477324,0.4194215427,0.66181
88957\C,0,2.8618039893,3.6270076949,-0.4499585803\H,0,1.0593256203,4.6
454054742,-1.052032698\H,0,4.4749389791,2.3582947202,0.2259268172\H,0,
3.5058170472,4.4781221741,-0.6493557905\N,0,-1.3180786142,1.3212214016
,2.2726695347\C,0,0.5624994218,-0.1986783596,1.8182299618\C,0,-0.63826
84267,-1.3288052451,2.7865345778\C,0,0.8038641656,-1.5485593101,2.4263
820726\H,0,-1.378321811,-1.7320002957,2.1004611587\H,0,-0.9358301542,-
1.3206464432,3.8364292994\H,0,1.5061469733,-1.5869502737,3.2586368527\
H,0,1.002414857,-2.3307092213,1.6929970904\Ag,0,1.1285416582,-1.385774
4156,-0.9615686013\\Version=ES64L-G16RevA.03\State=1-A\HF=-855.4425834
\RMSD=4.774e-09\Dipole=0.567986,-2.6478489,-0.2361707\Quadrupole=3.015
3156,0.2447742,-3.2600898,-2.2515675,-1.233992,-5.0566222\PG=C01 [X(C1
7H13Ag1N1)]\\@

P' + Ag^+

1\1\GINC-OM112\SP\RM06\GenECP\C17H13Ag1N1(1+)\WEIY\01-Apr-2020\0\\#p M
06/genecp geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Title Card
Required\\1,1\C,0,-1.6169721246,1.9729282838,0.1386126646\C,0,-2.3532
80355,-0.1979483633,0.0660643399\C,0,-0.9913163757,-0.6649982591,-0.04
24456475\C,0,0.1143226908,0.2720696066,-0.0133804856\C,0,-0.272678504,
1.5961514455,0.0289577902\H,0,-4.4332400826,-0.7679381135,0.1417074698

\C,0,-3.40975717,-1.1325971271,0.0482428597\C,0,-0.7909072926,-2.05995
37968,-0.2191148332\C,0,-1.8456540797,-2.9475807387,-0.2462683566\C,0,
-3.1683546641,-2.4822078794,-0.0988491587\H,0,0.2208443006,-2.42303495
81,-0.3543930011\H,0,-1.6586269785,-4.0068975288,-0.3903036578\H,0,-3.
9970699482,-3.1831816837,-0.1151111418\C,0,-1.3172646676,3.4518120349,
0.2543065862\C,0,0.2085200324,3.0372149834,0.1354342506\C,0,1.53852741
06,-0.1249750963,-0.010023703\C,0,2.0304915847,-1.0861285486,0.8924944
917\C,0,2.4390747222,0.516557207,-0.8793623522\C,0,3.3884906423,-1.399
0041301,0.9168647133\H,0,1.3554370969,-1.5625204266,1.5971788934\C,0,3
.7926267847,0.1869815987,-0.8637605728\H,0,2.0701246494,1.2527509655,-
1.5877104602\C,0,4.2706083494,-0.7694711955,0.0354802559\H,0,3.7582441
989,-2.1319659211,1.6276765814\H,0,4.4742746491,0.6767419887,-1.552718
5506\H,0,5.3270098661,-1.0204202302,0.0518961124\N,0,-2.6499132903,1.1
554331254,0.1825356444\H,0,-1.5935605421,3.9110439813,1.2097863439\H,0
,0.8098199917,3.2633250184,1.0207295799\H,0,0.7121887206,3.4373527493,
-0.7485569971\H,0,-1.6918257784,4.0724436505,-0.5670507077\Ag,0,-4.680
2526672,1.8792916479,0.4290248588\\Version=ES64L-G16RevA.03\State=1-A\
HF=-855.6241753\RMSD=9.371e-09\Dipole=-2.8905468,1.5830869,0.299554\Qu
adrupole=26.1379953,-1.7693003,-24.368695,-12.2791848,-3.988936,-0.764
2741\PG=C01 [X(C17H13Ag1N1)]\\@

S

1\1\GINC-OM103\SP\RM06\6-311+G(d,p)\C36H30N2\WEIY\14-Jul-2020\0\\#p M0
6/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Title
Card Required\\0,1\C,0,3.5305680828,-2.4920571313,-0.4740354424\C,0,2
.5151559021,-1.5645698677,-0.6928849108\C,0,2.8334381713,-0.313205777,
-1.2362457011\C,0,4.1586368843,0.0368085255,-1.570964643\C,0,5.1535210
458,-0.9218658812,-1.3380937335\C,0,4.8502172954,-2.1722705956,-0.7973
730534\H,0,3.2868838411,-3.4627577506,-0.0521501601\H,0,1.479003544,-1
.790665668,-0.4564695313\H,0,6.1815200447,-0.6685248099,-1.5812512223\

H,0,5.645149484,-2.8929683227,-0.626184003\C,0,4.4939081203,1.37842538
8,-2.1456933193\C,0,4.8715293462,1.4585506246,-3.4338320104\C,0,5.0913
501874,0.4148858768,-4.5203535023\C,0,5.4308333514,2.5650575054,-4.318
9330056\C,0,5.9768011364,1.4573135918,-5.2683677963\H,0,4.1675146803,0
.1833865841,-5.067376639\H,0,5.5550367287,-0.5326135694,-4.2290302118\
H,0,4.6500997559,3.1687853394,-4.7993850121\H,0,6.1505634712,3.2505157
08,-3.8573068271\H,0,5.7867131495,1.5880881469,-6.3372713485\H,0,7.045
0349256,1.2745489985,-5.1193566205\C,0,4.4281539067,2.5569137858,-1.23
96415913\C,0,4.7319309639,2.4209818302,0.1270741437\C,0,4.0707288795,3
.8326238443,-1.7112414443\C,0,4.7042865435,3.5209061424,0.982526501\H,
0,4.9992119343,1.4441248503,0.5194133008\C,0,4.0418622733,4.9321346884
,-0.8551943226\H,0,3.7827735192,3.9569874221,-2.7494788863\C,0,4.36254
93977,4.783577001,0.4953151082\H,0,4.9493438817,3.389797723,2.03341700
66\H,0,3.7543427222,5.9060147928,-1.2431659813\H,0,4.3362726918,5.6407
274409,1.1627920745\C,0,0.9113002906,1.3334840884,-1.6567643124\C,0,-1
.0664102288,-1.6514617683,-0.1369233599\C,0,-2.9939619502,0.0035975947
,-0.4939452619\C,0,-2.6593347535,1.2366177071,-1.0756343259\C,0,-4.326
6638471,-0.3252484724,-0.1621850783\C,0,-3.6614545761,2.1607851677,-1.
3469463203\H,0,-1.6193094996,1.442473858,-1.3136957216\C,0,-5.31229182
79,0.6251565985,-0.4767957038\C,0,-4.992224784,1.8519354509,-1.0513925
295\H,0,-3.4031482865,3.1151527147,-1.7963806795\H,0,-6.347593648,0.38
58630939,-0.2520072275\H,0,-5.7805576187,2.5676709165,-1.2678958768\C,
0,-4.7238587371,-1.615861442,0.4754252499\C,0,-4.1981558577,-2.0036661
412,1.6505641015\C,0,-3.2593730943,-1.3425743565,2.6499541525\C,0,-4.3
939322033,-3.209526091,2.5628170204\C,0,-3.7162861152,-2.3938041098,3.
7044061883\H,0,-3.4432957393,-0.2853990315,2.8729492676\H,0,-2.2035956
96,-1.4539920509,2.3763424954\H,0,-5.4106266856,-3.5713491205,2.737090
4208\H,0,-3.7850215434,-4.0637412412,2.2381287667\H,0,-4.4451299644,-1
.9869619449,4.4116683608\H,0,-2.9255938239,-2.899574735,4.2652460785\C
,0,-5.7573442733,-2.4218474135,-0.2421203445\C,0,-6.9202872407,-2.8710

630331,0.4039485277\C,0,-5.5921386935,-2.7325611081,-1.6029173447\C,0,
-7.8746237881,-3.6257706821,-0.2792620662\H,0,-7.0852739141,-2.6073459
436,1.4443604351\C,0,-6.5428124026,-3.4894146616,-2.2855432766\H,0,-4.
7049923449,-2.3826424068,-2.1238435293\C,0,-7.6877217039,-3.9418236962
,-1.6256163808\H,0,-8.7696635824,-3.9588664107,0.2400699024\H,0,-6.389
5375856,-3.7260186333,-3.3353231334\H,0,-8.4309301618,-4.5288260506,-2
.1586145957\N,0,1.8040675027,0.588858467,-1.4638309322\N,0,-1.96794840
37,-0.9078854794,-0.2864893618\\Version=ES64L-G16RevA.03\State=1-A\HF=
-1498.450016\RMSD=6.469e-09\Dipole=0.2135999,-0.0935968,-0.0437441\Qua
drupole=12.2190627,-8.2610758,-3.9579869,-2.1008291,-7.9039305,-3.8730
975\PG=C01 [X(C36H30N2)]\\@

TS1

1\1\GINC-OM103\SP\RM06\6-311+G(d,p)\C36H30N2\WEIY\14-Jul-2020\0\\#p M0
6/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Title
Card Required\\0,1\C,0,-0.0171669223,-0.0003789299,0.0380292802\C,0,-
0.0076477408,-0.037738454,1.4290038871\C,0,1.2115908761,-0.0296085688,
2.1214077837\C,0,2.4447499968,-0.0153542234,1.4302630674\C,0,2.3975199
165,0.0161536205,0.0304346409\C,0,1.187900724,0.0276066858,-0.66577078
65\H,0,-0.9648639145,0.0045860614,-0.492902847\H,0,-0.9326493062,-0.05
96180765,1.9961674382\H,0,3.3377979581,0.0324790625,-0.5139917037\H,0,
1.1880346977,0.0534698843,-1.751779655\C,0,3.7570796947,-0.0347436776,
2.1572356356\C,0,4.3970928761,1.1352217952,2.3334815853\C,0,4.06057239
54,2.5570799582,1.9143391048\C,0,5.7571377294,1.5640234387,2.869217435
\C,0,5.5555798826,2.9302776226,2.14870406\H,0,3.3847528469,3.036249635
6,2.6349635283\H,0,3.6495491291,2.7031724006,0.9096212705\H,0,5.774422
4892,1.6715652331,3.9611993704\H,0,6.6182712044,0.9521065035,2.5763556
931\H,0,5.7495123888,3.8277989234,2.7425420118\H,0,6.1209211341,2.9962
636303,1.2142421056\C,0,4.2797404517,-1.3511357513,2.6094672096\C,0,3.
8888758806,-2.5372607866,1.9600614358\C,0,5.1734246722,-1.4633413907,3

.692114687\C,0,4.3871301011,-3.7769284044,2.3572400241\H,0,3.190555868
4,-2.48615599,1.1305392541\C,0,5.6703571142,-2.7034172524,4.0880024852
\H,0,5.4619533164,-0.5778234761,4.2466340366\C,0,5.2844753599,-3.86808
55051,3.4218311723\H,0,4.0704641311,-4.6746159836,1.8321483643\H,0,6.3
554289937,-2.7608000734,4.9305226968\H,0,5.6711090093,-4.8343411715,3.
7346046044\C,0,1.424960868,0.3917529861,4.5952399223\C,0,2.1155135822,
1.9352751785,5.0185873808\C,0,2.5340499887,1.7629064318,7.4445370688\C
,0,1.470092761,0.9751260149,7.9084089768\C,0,3.6136809651,2.0994606435
,8.2877041947\C,0,1.4765093914,0.5014666746,9.2166075537\H,0,0.6612675
941,0.7338788041,7.2264107768\C,0,3.6016819073,1.5893494566,9.59330216
29\C,0,2.5462213442,0.8075001704,10.0613268303\H,0,0.6498826066,-0.106
0441224,9.5746227801\H,0,4.4366700096,1.8211667398,10.2487248993\H,0,2
.5567158139,0.4416876125,11.0844039088\C,0,4.7654435639,2.9364543684,7
.8181156678\C,0,4.57899433,4.2490819781,7.5922827956\C,0,3.3451071151,
5.1375142988,7.6307634153\C,0,5.4237314824,5.3641526907,6.989467627\C,
0,4.1023889823,6.138467819,6.7063383067\H,0,3.1546835197,5.5508344181,
8.6305095643\H,0,2.4130413231,4.7108894742,7.2501335795\H,0,6.05280139
6,5.8801351768,7.7270366567\H,0,6.0568671046,5.0959015405,6.1358232073
\H,0,4.0795274,7.1928576445,6.9961286481\H,0,3.7877186258,6.049890478,
5.6628674289\C,0,6.0710637649,2.2519408729,7.6239512097\C,0,7.29610050
04,2.9184658004,7.8126602668\C,0,6.1154274255,0.8965702612,7.242862687
3\C,0,8.5109564069,2.2665620764,7.6055853847\H,0,7.2973533162,3.948652
5627,8.1515402068\C,0,7.3307794917,0.2459549248,7.0350177772\H,0,5.186
9775097,0.3498224807,7.1082359742\C,0,8.5363455289,0.9278942409,7.2112
821197\H,0,9.4416885567,2.8052437221,7.7650739841\H,0,7.3348645695,-0.
8004702046,6.7399387033\H,0,9.4836377809,0.4194416362,7.0534255583\N,0
,1.1888362257,-0.0483629857,3.5062707209\N,0,2.5172835771,2.227066937,
6.1254766199\\Version=ES64L-G16RevA.03\State=1-A\HF=-1498.4239912\RMSD
=2.920e-09\Dipole=0.0843074,0.2983901,-0.1741969\Quadrupole=-0.6308266
,-4.778809,5.4096356,3.7130008,5.4246721,2.5030174\PG=C01 [X(C36H30N2)

]\\@

IntA

1\1\GINC-OM103\SP\RM06\6-311+G(d,p)\C36H30N2\WEIY\14-Jul-2020\0\\#p M0
6/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Title
Card Required\\0,1\C,0,4.2203382984,-3.1694073924,0.0201977969\C,0,2.
9297699747,-2.730855277,0.2928669294\C,0,2.4304708516,-1.5394463679,-0
.2624587625\C,0,3.2632462828,-0.7498168301,-1.1004365533\C,0,4.5588002
628,-1.2154938485,-1.3598084385\C,0,5.0392068542,-2.4087144,-0.8156958
423\H,0,4.5843131036,-4.0959565507,0.4550708553\H,0,2.2631539333,-3.30
15364431,0.9318532636\H,0,5.2028218224,-0.6148823459,-1.9966848048\H,0
,6.0513290828,-2.7351684474,-1.0391414802\C,0,2.8271674443,0.558571591
7,-1.6845371136\C,0,2.5626379438,0.6335269413,-3.0009283784\C,0,2.6145
670097,-0.3857368568,-4.1297412774\C,0,2.2722571794,1.7682042714,-3.97
38347404\C,0,2.6726279295,0.8065836505,-5.1326523503\H,0,1.682285005,-
0.9599945922,-4.2163101369\H,0,3.4479241051,-1.0957020762,-4.132983015
5\H,0,1.2092488249,2.0378242693,-4.0116861451\H,0,2.8504543122,2.69048
34688,-3.8458765141\H,0,1.9951936798,0.7616587853,-5.990018037\H,0,3.6
880037088,0.9935605986,-5.4946225331\C,0,2.798661904,1.743860792,-0.78
20431731\C,0,3.7243769931,1.8579247948,0.2710736475\C,0,1.8675287895,2
.7835683483,-0.9577476565\C,0,3.7380452091,2.9799658648,1.0982038697\H
,0,4.4453482643,1.0628389545,0.4363121016\C,0,1.8820916515,3.904681024
9,-0.1294310914\H,0,1.1002959642,2.6915646407,-1.7181928789\C,0,2.8198
970954,4.0123062467,0.8992378427\H,0,4.4688382611,3.0467233785,1.90027
53485\H,0,1.1466375313,4.6909271744,-0.2802951482\H,0,2.8278823612,4.8
86050015,1.5455454877\C,0,0.4048099628,-0.3363393969,-0.4284088802\C,0
,-0.6898088698,0.3430562862,-0.5759108508\C,0,-2.7372585131,1.52506510
74,-0.7533698627\C,0,-3.1661342528,2.8281434474,-1.0696796011\C,0,-3.6
700213781,0.5828008949,-0.2447397207\C,0,-4.480544842,3.2254654328,-0.
8622873594\H,0,-2.4281561507,3.5132344778,-1.4753410325\C,0,-4.9972500

383,1.0013976774,-0.0783861457\C,0,-5.4050928133,2.3036890301,-0.36583
6243\H,0,-4.7860028844,4.2409403603,-1.098513423\H,0,-5.720202355,0.27
97203082,0.2924530935\H,0,-6.4408431499,2.5930487789,-0.2102687659\C,0
,-3.3292716526,-0.8422944834,0.0831213421\C,0,-2.7859215192,-1.1215194
122,1.2814635803\C,0,-2.2855186223,-0.2322675389,2.4078246313\C,0,-2.1
93179538,-2.3643196333,1.9311632562\C,0,-1.3884267843,-1.4199409406,2.
8725602523\H,0,-3.0729496401,0.0090656123,3.1347660122\H,0,-1.78683820
94,0.7003025993,2.1243126301\H,0,-2.9333273747,-2.9646527322,2.4772423
416\H,0,-1.6247525064,-3.0320874123,1.2749816972\H,0,-1.4039968729,-1.
6588647461,3.9399195907\H,0,-0.3539471974,-1.3087862813,2.5390307404\C
,0,-3.6624129487,-1.8759165526,-0.9323804589\C,0,-3.9892166658,-3.1959
600139,-0.5686915852\C,0,-3.6671009839,-1.555423156,-2.303001271\C,0,-
4.2832970865,-4.1572875065,-1.5340061696\H,0,-4.0400011694,-3.46540399
07,0.4803700468\C,0,-3.9582960886,-2.5177104492,-3.2679560404\H,0,-3.4
329194244,-0.5422356913,-2.6148800734\C,0,-4.2655350942,-3.8258185171,
-2.8899296746\H,0,-4.5380876816,-5.1674524581,-1.2231724746\H,0,-3.946
5085514,-2.2425068376,-4.3195867088\H,0,-4.4969775397,-4.5755065795,-3
.6418474932\N,0,1.0953482866,-1.2611957892,0.0750583487\N,0,-1.3865724
042,1.2734727928,-1.05348398\\Version=ES64L-G16RevA.03\State=1-A\HF=-1
498.4543874\RMSD=5.002e-09\Dipole=0.1611063,-0.1268379,-0.0738932\Quad
rupole=2.866963,0.2836503,-3.1506133,-7.0960964,-3.3323424,-2.1577828\
PG=C01 [X(C36H30N2)]\\@

TS2

1\1\GINC-OM103\SP\RM06\6-311+G(d,p)\C36H30N2\WEIY\14-Jul-2020\0\\#p M0
6/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Title
Card Required\\0,1\C,0,0.0141613823,0.2243954949,-0.0809633288\C,0,0.
0642699169,0.3695636786,1.3016472438\C,0,1.2899750938,0.3445470359,1.9
845484026\C,0,2.4976540898,0.1312528019,1.2716571529\C,0,2.4172018451,
-0.0165215625,-0.1188994429\C,0,1.1970548232,0.0346201391,-0.796568408

9\H,0,-0.9420299746,0.257067202,-0.5955072406\H,0,-0.8394084926,0.5213
223925,1.8837918499\H,0,3.3372854853,-0.1822421725,-0.6730811206\H,0,1
.1729110502,-0.0835205557,-1.8764280102\C,0,3.8227445059,0.0237676904,
1.9606170067\C,0,4.6911351795,1.0474303085,1.8861622937\C,0,4.64359440
93,2.3994636115,1.1902963739\C,0,6.1411246152,1.2551587603,2.299575810
5\C,0,6.1978240615,2.4533985533,1.3047274155\H,0,4.1516943806,3.166416
7581,1.8037035666\H,0,4.2041620734,2.4369832905,0.1881033774\H,0,6.242
6052184,1.5794596626,3.3425940315\H,0,6.8276132765,0.4164524104,2.1369
408486\H,0,6.6309698242,3.3842795355,1.681302063\H,0,6.6911813115,2.18
9639703,0.364515382\C,0,4.1425315008,-1.2635075511,2.641748072\C,0,3.6
928739577,-2.4835485541,2.1051482498\C,0,4.903527286,-1.3001905812,3.8
239702894\C,0,4.0178089002,-3.6968873005,2.7093634348\H,0,3.0898259501
,-2.4800242501,1.2019509505\C,0,5.2251033073,-2.5151628981,4.428144579
5\H,0,5.2005435316,-0.3713035539,4.2980682718\C,0,4.7903645553,-3.7193
943023,3.872011199\H,0,3.6651808849,-4.6268831872,2.2704529511\H,0,5.8
060395001,-2.518023333,5.3470497707\H,0,5.0405883026,-4.6649141428,4.3
460002769\C,0,2.1491422492,0.8365469515,4.1421467779\N,0,1.2143088282,
0.5362556119,3.3753756993\C,0,2.6012361163,1.2192888526,5.3309043747\N
,0,3.6954110217,1.2186095872,5.9974743484\C,0,3.8454293462,1.803843319
6,7.2287372248\C,0,5.0080858474,1.4693221761,7.9699162423\C,0,3.025229
5179,2.9037988282,7.6625936849\C,0,5.3638773132,2.1820820735,9.0946902
752\H,0,5.6090311157,0.6369838712,7.6159767157\C,0,3.482539259,3.66875
46836,8.7656772229\C,0,4.6029339878,3.3053631269,9.4867867821\H,0,6.24
34466235,1.8957819032,9.6649397459\H,0,2.8947653285,4.5298598422,9.070
7506422\H,0,4.8971771742,3.8828196453,10.358953908\C,0,1.8315485664,3.
254894686,6.9270120768\C,0,1.0575009589,2.2037673229,6.423920008\C,0,-
0.290681918,2.259116295,5.7170221936\C,0,0.6070215265,0.9626014466,7.2
302835114\C,0,-0.8516181759,1.3334779927,6.8369112951\H,0,-0.253937015
4,1.7277438715,4.7586797746\H,0,-0.7516879435,3.2357824018,5.557703535
1\H,0,0.9199123148,0.0116509005,6.7900554669\H,0,0.86891269,0.97114207

09,8.2923021119\H,0,-1.497816713,0.5115898491,6.5149361873\H,0,-1.3565
76135,1.8983260852,7.626914239\C,0,1.5421962249,4.6877572587,6.6581584
554\C,0,0.2792915519,5.2493797391,6.9231068846\C,0,2.5496163759,5.5380
995795,6.1646375275\C,0,0.0275352724,6.5998780325,6.684643928\H,0,-0.5
016320148,4.6260208429,7.3486628197\C,0,2.298138037,6.8872935515,5.922
1854019\H,0,3.5339151233,5.1256371733,5.9622684959\C,0,1.0343685276,7.
4238930602,6.1777553208\H,0,-0.9540524247,7.0113777809,6.9054868881\H,
0,3.090208534,7.520720409,5.5310259265\H,0,0.8379101186,8.4762263088,5
.9906706441\\Version=ES64L-G16RevA.03\State=1-A\HF=-1498.4351404\RMSD=
4.509e-09\Dipole=-0.4154728,0.5768655,-0.4029098\Quadrupole=0.2328813,
-3.0247781,2.7918968,-1.1362994,1.9774935,2.387458\PG=C01 [X(C36H30N2)
]\\@

IntB

1\1\GINC-OM103\SP\RM06\6-311+G(d,p)\C36H30N2\WEIY\14-Jul-2020\0\\#p M0
6/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Title
Card Required\\0,1\C,0,-3.7112636299,-3.733352471,0.6043491322\C,0,-2
.5470013821,-3.1519779156,0.1081376862\C,0,-2.4346806147,-1.7595520178
,0.0298561194\C,0,-3.5106213048,-0.9216148128,0.3963260121\C,0,-4.6728
857566,-1.5365094392,0.8820164737\C,0,-4.7776884868,-2.9237474731,0.99
67629617\H,0,-3.7847248491,-4.814761498,0.6776405253\H,0,-1.7071534291
,-3.762280828,-0.2094882597\H,0,-5.5061652745,-0.9031577394,1.17459698
08\H,0,-5.6916927508,-3.3680672121,1.3808338038\C,0,-3.4335547165,0.56
53563208,0.2331970074\C,0,-3.1419736893,1.3378234753,1.2913937181\C,0,
-2.8862374546,1.0331725436,2.7594238979\C,0,-3.1167274294,2.8380323323
,1.5458015551\C,0,-3.2096154855,2.5267039157,3.0705610225\H,0,-1.83305
71506,0.7852727647,2.9502880517\H,0,-3.5076952818,0.2650871386,3.23219
61258\H,0,-2.1580986741,3.2954442462,1.2754239248\H,0,-3.9195519408,3.
4294110944,1.0914247781\H,0,-2.5087259841,3.055303866,3.7225967897\H,0
,-4.223322909,2.6571391862,3.4611306053\C,0,-3.7123571602,1.1238060612

,-1.121379879\C,0,-4.7546204961,0.607683445,-1.9113446154\C,0,-2.93998
77754,2.1764126986,-1.6423685275\C,0,-5.03990342,1.1498518929,-3.16336
6808\H,0,-5.3491253733,-0.2215448853,-1.538493744\C,0,-3.2250772971,2.
7145810868,-2.8972654428\H,0,-2.080931577,2.5297330931,-1.0811648029\C
,0,-4.2795462113,2.2104229847,-3.6602996548\H,0,-5.8565511137,0.740833
8524,-3.7531048646\H,0,-2.6089531567,3.5214807212,-3.2863986281\H,0,-4
.4985052959,2.6300312706,-4.6387871296\C,0,-0.4824497207,-0.3677660739
,-0.0466217202\N,0,-1.2184743888,-1.2383693497,-0.4727819279\C,0,0.474
8948881,0.4981121999,0.3336873298\N,0,0.2929155121,1.8300649441,0.0179
000532\C,0,1.0470667559,2.7084363929,0.6392874833\C,0,0.877423504,4.10
74063953,0.3113265217\C,0,1.9584386553,2.3508485173,1.7476047107\C,0,1
.476433854,5.0798284377,1.0465290389\H,0,0.2373257073,4.338017479,-0.5
349673505\C,0,2.5092119599,3.4436969733,2.5315423882\C,0,2.2926763698,
4.7392393936,2.1877738722\H,0,1.3333936398,6.1266682195,0.7921520707\H
,0,3.1329253015,3.2003035511,3.3850979332\H,0,2.7387231091,5.538345696
5,2.7738815137\C,0,2.2136683373,1.028199411,2.0090237055\C,0,1.7454886
985,-0.0154317364,1.0047006878\C,0,1.7535865048,-1.5053743626,1.489166
7377\C,0,2.9085116393,-0.4204291425,-0.0020047298\C,0,3.1063892909,-1.
7439858491,0.7731125265\H,0,0.9412192061,-2.0776728141,1.0326766186\H,
0,1.7230292453,-1.6678110887,2.5688974503\H,0,2.5020822041,-0.57201676
39,-1.0075889671\H,0,3.7577261346,0.267859232,-0.0633198747\H,0,3.1874
041044,-2.6560463701,0.1742302263\H,0,3.9538190922,-1.7033739806,1.462
981707\C,0,3.029607712,0.6150493736,3.1890141051\C,0,4.43260468,0.6808
031726,3.1605150676\C,0,2.4078302983,0.1571695243,4.3627387845\C,0,5.1
897156068,0.292655714,4.2674476814\H,0,4.9292500365,1.0449963453,2.265
2229086\C,0,3.1645125386,-0.2315473489,5.4686776583\H,0,1.3225996675,0
.1187595823,4.4075961517\C,0,4.5583990819,-0.1674004977,5.4238734422\H
,0,6.2740843123,0.3532126251,4.2248661066\H,0,2.6630036532,-0.57920129
38,6.3680652228\H,0,5.1476492488,-0.4690393263,6.2855768909\\Version=E
S64L-G16RevA.03\State=1-A\HF=-1498.483202\RMSD=2.828e-09\Dipole=0.5267

532,-0.4591037,1.3054294\Quadrupole=4.878254,1.4957778,-6.3740318,4.18
54559,3.2950114,-2.6999537\PG=C01 [X(C36H30N2)]\\@

^{3}IntB

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\14-Jul-2020\0\\#p
uM06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\T
itle Card Required\\0,3\C,0,-3.2784964008,-3.9706955711,-0.3132382903\
C,0,-2.1306597075,-3.1858087472,-0.3960429566\C,0,-2.2188535799,-1.798
1982527,-0.2428047877\C,0,-3.4664334468,-1.1620858952,-0.0553768814\C,
0,-4.6034045655,-1.9780392271,0.0143790376\C,0,-4.5187660956,-3.366703
5904,-0.1039564663\H,0,-3.2021241749,-5.0493335988,-0.417227809\H,0,-1
.1561065883,-3.6334427536,-0.5649412217\H,0,-5.5696515374,-1.504037662
8,0.1650662888\H,0,-5.4194691239,-3.9710624368,-0.0428383766\C,0,-3.56
70351588,0.3293204862,0.0274951471\C,0,-3.6651188916,0.9258588008,1.22
5896115\C,0,-3.7763187117,0.3924558555,2.6468447544\C,0,-3.8934442317,
2.3559468454,1.6907204598\C,0,-4.3543376212,1.7797643451,3.0637831798\
H,0,-2.7943860405,0.1963496623,3.0986298278\H,0,-4.4036490672,-0.49113
48749,2.8055543796\H,0,-2.9557487816,2.9183912748,1.77249494\H,0,-4.60
69847503,2.9576473028,1.1169390159\H,0,-3.9277146173,2.2410274551,3.95
8878663\H,0,-5.4438280021,1.7597871143,3.1618714353\C,0,-3.5641171774,
1.0899979277,-1.2558408013\C,0,-4.3013350873,0.630005146,-2.3610298061
\C,0,-2.8290623258,2.2800978644,-1.3923018735\C,0,-4.3332910266,1.3544
513625,-3.5514133736\H,0,-4.858223648,-0.2996498351,-2.2841770691\C,0,
-2.8592523854,3.0006999162,-2.5863967116\H,0,-2.188486718,2.6029297818
,-0.5777418579\C,0,-3.6161995137,2.5470211701,-3.667822336\H,0,-4.9174
819663,0.9849173005,-4.3905420887\H,0,-2.2743658346,3.9127842553,-2.67
57825649\H,0,-3.636402555,3.1094483207,-4.5977254922\C,0,-0.5318072905
,-0.1989526672,0.3854244961\N,0,-1.0204797813,-1.0519417886,-0.3307481
81\C,0,0.280421678,0.7178313124,1.0087143705\N,0,-0.0334542236,2.00944
6514,0.8642702982\C,0,0.8436235317,2.95884393,1.3599937797\C,0,0.47372

07892,4.3025105717,1.2402880811\C,0,2.1289642107,2.6218454905,1.911516
0276\C,0,1.3395191294,5.3316750562,1.626538288\H,0,-0.5020845189,4.522
736473,0.8175465232\C,0,2.9988047243,3.6841854459,2.2462323001\C,0,2.6
075873208,5.0178488933,2.1164579092\H,0,1.0289343514,6.3678291136,1.52
48721748\H,0,3.9906053004,3.4545283308,2.6208391379\H,0,3.2986783375,5
.8084505686,2.3959449687\C,0,2.476449183,1.2405125449,2.0635340703\C,0
,1.4044267694,0.1951709934,1.9097768566\C,0,0.7977314014,-0.3333673374
,3.2955931005\C,0,1.7950360165,-1.2997379103,1.6275661489\C,0,0.836846
4253,-1.7779700768,2.7473501493\H,0,-0.1675716159,0.0917761162,3.58614
82463\H,0,1.5158895692,-0.1818694257,4.1065570117\H,0,1.617061008,-1.6
635289218,0.6109863816\H,0,2.8380678011,-1.4877941765,1.8856785404\H,0
,-0.1327389618,-2.1106509128,2.3650785514\H,0,1.2210952763,-2.54636573
25,3.4246820477\C,0,3.8104830795,0.8480506173,2.5901890926\C,0,4.75555
41532,0.2124556523,1.7646701169\C,0,4.1690698596,1.1057131857,3.926249
7891\C,0,6.0070081574,-0.158371873,2.2571880511\H,0,4.5064011548,0.022
6348645,0.7240114097\C,0,5.4196759023,0.7323234456,4.4204995644\H,0,3.
4576276525,1.6057066661,4.578093812\C,0,6.3427700728,0.0975358004,3.58
80258567\H,0,6.7223574048,-0.6432027984,1.5979124843\H,0,5.6718395293,
0.9386328516,5.4575321666\H,0,7.3173253045,-0.1919756786,3.9718107385\
\Version=ES64L-G16RevA.03\State=3-A\HF=-1498.4581414\S2=2.022808\S2-1=
0.\S2A=2.000298\RMSD=2.676e-09\Dipole=0.1052991,-1.0869554,0.9845099\Q
uadrupole=5.4690183,1.3348917,-6.80391,1.8047217,4.5798087,1.3572501\P
G=C01 [X(C36H30N2)]\\@

^{3}TS3

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\14-Jul-2020\0\\#p
uM06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\T
itle Card Required\\0,3\C,0,-4.0395264305,-3.9773925078,-0.9315797056\
C,0,-2.7577483952,-3.4561814666,-1.0564868944\C,0,-2.4460472156,-2.192
0283934,-0.5322960699\C,0,-3.4481762315,-1.4223494819,0.1220174209\C,0

,-4.7502582754,-1.9501834196,0.1747235002\C,0,-5.0450947775,-3.2149925
19,-0.324319108\H,0,-4.2631743391,-4.9648054402,-1.3258780935\H,0,-1.9
761266462,-4.007693895,-1.5706057581\H,0,-5.5298758301,-1.3558291576,0
.6435923113\H,0,-6.0555073522,-3.6063872044,-0.2447044981\C,0,-3.12764
32374,-0.0946041804,0.6804328382\C,0,-2.0290403167,0.0027808045,1.5034
336388\C,0,-1.531834818,-1.0104690153,2.5518593314\C,0,-1.4500576352,1
.1637357652,2.3025152061\C,0,-1.333316595,0.1957716137,3.5170951896\H,
0,-0.5841047029,-1.4963690566,2.3016368479\H,0,-2.2535010676,-1.780605
4665,2.8425338591\H,0,-0.4699682524,1.4520647723,1.9104599649\H,0,-2.0
481928816,2.0699136818,2.4141835111\H,0,-0.3958608847,0.2242455944,4.0
803076914\H,0,-2.1698189603,0.303606909,4.2144619525\C,0,-3.9397567349
,1.0644290808,0.2327430075\C,0,-4.4436430519,2.0090437381,1.1455298029
\C,0,-4.2682190907,1.220534265,-1.1269760104\C,0,-5.2237393242,3.08067
65769,0.7135322265\H,0,-4.2480986227,1.8821372981,2.2057918448\C,0,-5.
0423477131,2.2949369315,-1.559952028\H,0,-3.898300647,0.4961916264,-1.
8467621836\C,0,-5.5215758237,3.2322469711,-0.6420614725\H,0,-5.6084221
153,3.7926973417,1.4392891104\H,0,-5.2716692369,2.400945536,-2.6171548
514\H,0,-6.1287303978,4.068221845,-0.9790215648\C,0,-0.6059361769,-0.7
377557768,-0.2064654849\N,0,-1.1836673148,-1.6573309972,-0.8201059747\
C,0,0.6083236847,0.0196518641,-0.4185183223\N,0,0.4704479316,1.3103735
542,-0.4617047201\C,0,1.5961302104,2.1066880516,-0.6548712002\C,0,1.38
47017127,3.4696286976,-0.8789808643\C,0,2.925388703,1.5800636861,-0.58
22296838\C,0,2.4593690475,4.3417054619,-1.0554658875\H,0,0.3579941119,
3.8214687638,-0.9098182284\C,0,3.9964130436,2.4933940682,-0.764404907\
C,0,3.7669384513,3.8439357746,-0.9990967708\H,0,2.2803884299,5.3978906
442,-1.2359362963\H,0,5.0147915975,2.1207950399,-0.747579783\H,0,4.611
3391591,4.5118330761,-1.1475252429\C,0,3.1056110252,0.1758745084,-0.35
77851127\C,0,1.9232652613,-0.745019795,-0.572701758\C,0,1.954963471,-2
.1392822796,0.1587132775\C,0,1.9078469247,-1.5569196155,-1.9615259181\
C,0,1.8913288076,-2.8984617379,-1.1899078278\H,0,1.1071935327,-2.31250

49032,0.8263058078\H,0,2.8735612305,-2.2977913362,0.7255638248\H,0,1.0
175506659,-1.3606218892,-2.5639978261\H,0,2.7917867122,-1.3652565239,-
2.5748787036\H,0,0.9712201459,-3.4690550609,-1.3356557206\H,0,2.743408
624,-3.557274466,-1.3837991762\C,0,4.4269036606,-0.3494583069,0.040928
5492\C,0,5.0370419237,-1.4641831376,-0.5730785425\C,0,5.1266706774,0.2
624928826,1.1052905699\C,0,6.278923944,-1.9351621946,-0.1500633702\H,0
,4.548313398,-1.9558333452,-1.4067889791\C,0,6.3646290643,-0.212208187
2,1.5306239913\H,0,4.6738508895,1.1092456116,1.612073557\C,0,6.9509032
544,-1.3143358105,0.9040382808\H,0,6.7253295038,-2.7893010909,-0.65288
54317\H,0,6.8696308437,0.2766543718,2.3598457412\H,0,7.9176914519,-1.6
847367496,1.2336881164\\Version=ES64L-G16RevA.03\State=3-A\HF=-1498.44
37233\S2=2.048958\S2-1=0.\S2A=2.001463\RMSD=9.968e-09\Dipole=0.3563574
,-0.5352451,0.5109384\Quadrupole=6.3393407,0.4241602,-6.7635009,-3.778
8281,0.0992113,3.9406697\PG=C01 [X(C36H30N2)]\\@

^{3}IntC

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\14-Jul-2020\0\\#p
uM06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\T
itle Card Required\\0,3\C,0,0.2586954853,-0.4140699247,-0.3859436159\C
,0,0.2469844046,-0.6997037286,0.9752383748\C,0,1.3933051727,-0.5114070
347,1.7583813185\C,0,2.5950699143,0.0130979207,1.1658929775\C,0,2.5994
344976,0.2015990299,-0.2460282685\C,0,1.4516351527,0.0140989696,-0.996
6419046\H,0,-0.6386027762,-0.5577970632,-0.9811666717\H,0,-0.637482717
2,-1.1042149869,1.4587039801\H,0,3.5134680494,0.5232514181,-0.73301831
68\H,0,1.4762227839,0.1942232472,-2.0681393036\C,0,3.6996032449,0.2718
4647,2.0191582888\C,0,3.3938633309,0.320419803,3.5049848716\C,0,2.8161
420618,1.7821498127,3.8595015841\C,0,4.5761015288,0.6840497654,4.45881
26693\C,0,4.2261158403,2.1849937907,4.3366545564\H,0,2.1019466531,1.71
72333266,4.6880127742\H,0,2.356991515,2.3314907406,3.0331891116\H,0,4.
3809736386,0.3148019342,5.4644226696\H,0,5.5759989196,0.3611988988,4.1

657488318\H,0,4.2870064594,2.7853514823,5.2497040845\H,0,4.7981342106,
2.6840035821,3.5490685145\C,0,5.0456903033,0.5931979221,1.4917684476\C
,0,5.287247385,1.7472344995,0.7228639882\C,0,6.1277260968,-0.271292539
7,1.7459827837\C,0,6.5617416541,2.0261732338,0.2279769837\H,0,4.469382
8028,2.4346624345,0.5249743156\C,0,7.3994085201,0.0064881632,1.2469724
764\H,0,5.9567181617,-1.1741858821,2.3257598459\C,0,7.6223979502,1.156
8085165,0.4869344404\H,0,6.7249582337,2.926661065,-0.3585196552\H,0,8.
2172809298,-0.6802742629,1.4489375729\H,0,8.6143745024,1.3731895746,0.
0997416716\C,0,2.3779739918,-0.7621289222,3.8479235534\N,0,1.383922502
2,-1.0120519167,3.0563380771\C,0,2.4751815123,-1.5719569508,5.10288113
17\N,0,3.6758836359,-1.9722028603,5.3775493632\C,0,3.9231171715,-2.737
7071095,6.5084212188\C,0,5.2216806201,-3.2230164519,6.6966772535\C,0,2
.9114624613,-2.9639888165,7.5009331444\C,0,5.560019189,-3.9243410494,7
.8509235478\H,0,5.9532546919,-3.0239586583,5.9192420556\C,0,3.30120594
56,-3.648111179,8.6907059125\C,0,4.5907576453,-4.1239346452,8.85121703
23\H,0,6.5699278711,-4.3010123847,7.9852207527\H,0,2.5639398425,-3.809
2129174,9.4699925833\H,0,4.8558175791,-4.6557325685,9.7613712733\C,0,1
.6051607316,-2.4827177387,7.2629087353\C,0,1.2316911049,-1.9512290977,
5.8967563065\C,0,0.0405372782,-0.9173784781,5.8805803046\C,0,0.2428077
586,-2.9662764055,5.1310057308\C,0,-0.9387628762,-1.9991756718,5.36690
92478\H,0,0.2059280308,-0.1185770405,5.1571902918\H,0,-0.1963290078,-0
.472379213,6.8493740773\H,0,0.5190752589,-3.0686120729,4.0830070216\H,
0,0.1725736938,-3.9540685601,5.5945232239\H,0,-1.5077038113,-1.7306766
615,4.4725215147\H,0,-1.6343513208,-2.3482580504,6.1353842851\C,0,0.55
85209006,-2.6274968917,8.3183194322\C,0,-0.1427113634,-3.8326767047,8.
494787876\C,0,0.2733092421,-1.5627525625,9.1903456018\C,0,-1.110156211
8,-3.9610497925,9.4931182575\H,0,0.0804196055,-4.677959982,7.849854258
5\C,0,-0.6926714476,-1.6901180061,10.1892142589\H,0,0.8247745482,-0.63
18868214,9.0879731706\C,0,-1.391261126,-2.8889665577,10.3410662845\H,0
,-1.6407964267,-4.9025032549,9.6094602487\H,0,-0.8950735735,-0.8527834

422,10.8520008901\H,0,-2.143843687,-2.9890394317,11.1185609928\\Versio
n=ES64L-G16RevA.03\State=3-A\HF=-1498.500639\S2=2.074534\S2-1=0.\S2A=2
.003604\RMSD=6.150e-09\Dipole=-0.1211061,0.4863299,0.3762203\Quadrupol
e=1.7482274,-4.3699744,2.621747,3.0250658,-7.3644127,-7.8158365\PG=C01
[X(C36H30N2)]\\@

^{3}TS4

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\13-Jul-2020\0\\#p
uM06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\T
itle Card Required\\0,3\C,0,-0.0010255907,-0.069442112,0.0026450957\C,
0,-0.0029032808,-0.0997030137,1.3848509318\C,0,1.2093633484,-0.0786644
615,2.1064587134\C,0,2.4574016132,-0.0066822327,1.4107562064\C,0,2.425
6285277,-0.0175933737,-0.013086333\C,0,1.2258731945,-0.0390292693,-0.6
955087342\H,0,-0.9382481992,-0.0846661684,-0.5466537847\H,0,-0.9271102
289,-0.1534740283,1.9524934709\H,0,3.3600412976,0.0033684847,-0.563257
1305\H,0,1.2265935423,-0.03531529,-1.7824077905\C,0,3.6522594786,0.048
4608359,2.1827656252\C,0,3.5626949339,0.1767173531,3.6141879031\C,0,3.
7863123485,2.142382358,4.0618648341\C,0,4.8701598767,0.1735140663,4.44
90168357\C,0,5.1951121451,1.6768338481,4.3792541454\H,0,3.1227880958,2
.3322658402,4.9042868877\H,0,3.5877204064,2.7738900807,3.1979500554\H,
0,4.6622722874,-0.1465435215,5.4666063533\H,0,5.6391344997,-0.49081681
69,4.0462103799\H,0,5.6185147142,2.0949499871,5.3008100657\H,0,5.88023
93675,1.9064966652,3.5582593289\C,0,4.9737812958,0.0689161369,1.485450
5216\C,0,5.4099703632,1.2071944772,0.7866853422\C,0,5.8003066141,-1.06
66988191,1.4877922387\C,0,6.6392968554,1.2153740601,0.1254865382\H,0,4
.777105627,2.0905766196,0.7619418294\C,0,7.0285032712,-1.0602862798,0.
8255872915\H,0,5.4679822149,-1.9625379775,2.0054842764\C,0,7.453635027
1,0.0818558585,0.1446897119\H,0,6.9589048965,2.1080818393,-0.405907818
9\H,0,7.6511654851,-1.9510232613,0.8383206903\H,0,8.4101882057,0.08701
30349,-0.3709136979\C,0,2.2432750107,-0.1665637793,4.1861403265\N,0,1.

148463493,-0.2019544705,3.4720563516\C,0,2.0540486272,-0.4783727557,5.
647368873\N,0,2.8847658761,-1.3414269355,6.1349093883\C,0,2.8278812773
,-1.6971284513,7.4768867587\C,0,3.6815495651,-2.7136625504,7.918749044
3\C,0,1.9973649259,-0.9894665621,8.4086207922\C,0,3.7508678951,-3.0486
730967,9.268305986\H,0,4.2924712999,-3.2193593076,7.1768856548\C,0,2.1
291119405,-1.3221009041,9.7897473769\C,0,2.9761106191,-2.3356060399,10
.2020236542\H,0,4.4127981663,-3.8432207376,9.6006375767\H,0,1.53680318
18,-0.7807946925,10.5198463853\H,0,3.0434728465,-2.5807611557,11.25882
7731\C,0,1.1223567059,0.0044316731,7.9166682452\C,0,0.8860606207,0.118
0652577,6.4262137286\C,0,0.3187805096,1.5031474434,5.9382164713\C,0,-0
.5476627549,-0.5059631805,6.0321065264\C,0,-1.1096964208,0.9186152643,
5.8285216892\H,0,0.7266228043,1.7900934644,4.9692148086\H,0,0.45068941
8,2.3319671156,6.6374022614\H,0,-0.4803751877,-1.0813812916,5.11028171
67\H,0,-1.0032697551,-1.1137871864,6.8190364703\H,0,-1.6177601085,1.09
1234184,4.8756133986\H,0,-1.7668584263,1.2408839497,6.6411539572\C,0,0
.3161783969,0.8237053299,8.8689543774\C,0,-0.8612159759,0.3228959053,9
.4508463974\C,0,0.7366680171,2.1143748121,9.2332753335\C,0,-1.60189350
95,1.0929075921,10.3494429486\H,0,-1.1926823442,-0.6811548512,9.201022
2546\C,0,-0.0021198594,2.8845316047,10.1321873662\H,0,1.6583026933,2.5
092451369,8.8138926846\C,0,-1.1767536158,2.3776267121,10.6904810517\H,
0,-2.5102864135,0.6850819875,10.7852972688\H,0,0.3440538499,3.87954301
41,10.3996150584\H,0,-1.7528042897,2.9767782173,11.3905306392\\Version
=ES64L-G16RevA.03\State=3-A\HF=-1498.4839772\S2=2.089781\S2-1=0.\S2A=2
.005097\RMSD=6.531e-09\Dipole=0.2874146,0.8732315,0.1408032\Quadrupole
=1.8683462,-6.4187094,4.5503631,-1.702252,-9.6934006,-0.8805666\PG=C01
[X(C36H30N2)]\\@

^{3}IntD

1\1\GINC-OM112\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\14-Jul-2020\0\\#p
uM06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\T

itle Card Required\\0,3\C,0,0.617876787,2.1255766821,0.7164000101\C,0,
0.7935700906,1.8354393409,2.04987913\C,0,1.9077447478,1.0664415939,2.4
781061271\C,0,2.848439264,0.5896356064,1.5165310435\C,0,2.6415431504,0
.9124677465,0.1471668793\C,0,1.5518403344,1.6605213327,-0.2410029869\H
,0,-0.2368999865,2.7135784307,0.393233659\H,0,0.0969770975,2.177956649
6,2.8088813691\H,0,3.3531250879,0.5614340341,-0.5925014466\H,0,1.40668
18385,1.897312976,-1.2915937154\C,0,3.9605528818,-0.1730169646,1.99562
15869\C,0,4.0786615653,-0.4406356403,3.3561447029\C,0,6.1437879126,-3.
5555845399,4.4463366534\C,0,5.2432148431,-1.2417969088,3.9041999394\C,
0,5.0152912739,-2.7882631608,3.8488797501\H,0,6.1941957101,-3.72012585
65,5.5189008893\H,0,7.0217118852,-3.8115166749,3.8597856737\H,0,6.1499
154577,-1.0052156242,3.3392037607\H,0,5.4315746386,-0.9607826762,4.943
9103469\H,0,4.0813128651,-2.9949071763,4.3813644985\H,0,4.8753651386,-
3.0733298893,2.7988286325\C,0,4.986411573,-0.6471784467,1.0111143998\C
,0,6.1626944332,0.0867281465,0.79762773\C,0,4.7764515414,-1.8147632835
,0.262604229\C,0,7.111372442,-0.343131134,-0.1313348063\H,0,6.33074310
59,0.9995286645,1.3633204726\C,0,5.7250733504,-2.2445238658,-0.6671685
978\H,0,3.863378506,-2.3851571625,0.4106559586\C,0,6.8958005351,-1.510
8806733,-0.8653841187\H,0,8.0178890181,0.2369440592,-0.2827827756\H,0,
5.5472600354,-3.1530240569,-1.2364533333\H,0,7.6344036974,-1.845504378
9,-1.5887706\C,0,3.0605692799,0.0862556343,4.2269014355\N,0,2.04329050
47,0.8161349364,3.8086959004\C,0,3.0908428057,-0.1764738971,5.71497371
65\N,0,3.002006955,-1.4176617854,6.0555385143\C,0,3.0599720612,-1.7808
236232,7.3983952185\C,0,2.8558250121,-3.1264789284,7.7191259064\C,0,3.
3951496741,-0.8324927871,8.4221872908\C,0,2.9845795857,-3.5738807189,9
.0315404151\H,0,2.6028363017,-3.807508669,6.9119735386\C,0,3.560508717
7,-1.3304879361,9.7496752374\C,0,3.3489318233,-2.6656625422,10.0428967
913\H,0,2.8194867519,-4.6205959426,9.2702459508\H,0,3.8395736806,-0.64
03636294,10.5388796446\H,0,3.4668850833,-3.0149289874,11.0654400072\C,
0,3.5652400928,0.5236147872,8.0673534542\C,0,3.1758069162,0.9927872399

,6.6846618181\C,0,3.9339561028,2.2727236044,6.1594088958\C,0,1.8530885
256,1.9107409566,6.7246114348\C,0,2.7149951383,3.1696044582,6.47938235
58\H,0,4.1418587239,2.2061768701,5.089479835\H,0,4.8649927609,2.510107
426,6.6789734698\H,0,1.1922914188,1.6684843556,5.8931821203\H,0,1.3008
522439,1.8601408073,7.6669477518\H,0,2.3785594491,3.8224762921,5.66867
96622\H,0,2.8573983122,3.7738452439,7.3796951668\C,0,4.0017941895,1.51
56648428,9.0941052275\C,0,3.0868360126,2.0888298303,9.9940597365\C,0,5
.3544281618,1.881320588,9.2031992293\C,0,3.506234509,3.012139207,10.95
34564407\H,0,2.0404568388,1.8007242032,9.9449164568\C,0,5.7750246441,2
.8034825526,10.1623755946\H,0,6.0812937678,1.4271795389,8.5349838546\C
,0,4.8509153898,3.3760015605,11.0378426639\H,0,2.7802714451,3.44384936
,11.6376225294\H,0,6.8266882109,3.0701538907,10.2278590731\H,0,5.17727
0556,4.0946438552,11.7848094791\\Version=ES64L-G16RevA.03\State=3-A\HF
=-1498.5130011\S2=2.04904\S2-1=0.\S2A=2.001347\RMSD=2.939e-09\Dipole=0
.7339078,0.7527142,-0.4018633\Quadrupole=-5.2606672,-7.0512029,12.3118
701,-1.2694245,-2.6532694,5.4447178\PG=C01 [X(C36H30N2)]\\@

^{3}TS5

1\1\GINC-OM112\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\14-Jul-2020\0\\#p
uM06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\T
itle Card Required\\0,3\C,0,-1.5422329698,-0.2623768523,-0.8716030684\
C,0,-1.5414850798,1.3276152323,1.7765535279\C,0,-0.1514793229,0.802395
3983,1.9387289265\C,0,0.8350320593,1.2759621176,0.8340984132\C,0,0.938
3696144,-1.0126049449,-0.335888764\C,0,-0.5306936321,-1.1536002583,-0.
2081023641\C,0,-2.179265781,-1.0671476491,-2.1090177934\C,0,-1.1748961
027,-0.3640286118,-3.04108948\C,0,-0.9658137691,0.7142170352,-1.952019
8754\C,0,-2.6364221212,0.1387865038,0.157742669\N,0,-0.9730074749,-2.2
165004762,0.4990866424\C,0,-4.1959352026,-0.9266922727,1.8265554028\C,
0,-4.5829216696,-2.0258785145,2.543278922\C,0,-3.8206930871,-3.2456089
596,2.4848253512\C,0,-2.6676013643,-3.3024990858,1.7609526751\C,0,-3.0

359655256,-0.9450019906,0.9835198344\C,0,-2.1869826837,-2.1578767346,1
.0325839815\C,0,-5.6207328982,2.913936704,-1.3463718033\C,0,-4.3360718
106,3.3688857737,-1.0474587818\C,0,-3.3751587964,2.4934890692,-0.54343
68406\C,0,-3.6641224313,1.1355276827,-0.3064942881\C,0,-4.9620646756,0
.6947346697,-0.6415407902\C,0,-5.9253506927,1.5676921329,-1.1458464592
\H,0,-6.369456295,3.5966846905,-1.7385474128\H,0,-4.0755766154,4.41199
00811,-1.2069224133\H,0,-2.3847907754,2.8788656324,-0.3335004808\H,0,-
5.2132429583,-0.3528582162,-0.5148922099\H,0,-6.9142630798,1.188090851
8,-1.3894139995\C,0,1.6166012361,0.1699736571,0.1431498973\N,0,1.57110
3175,-2.0628862385,-0.84041038\C,0,2.9236653362,-2.0174876987,-0.96218
61083\C,0,2.9972291283,0.2270924956,0.013540146\C,0,3.6967050729,-0.88
15659136,-0.5686307385\C,0,3.5799765957,-3.1477230578,-1.51985636\C,0,
4.945700517,-3.1503873193,-1.6920884964\C,0,5.7119999449,-2.0222711102
,-1.3145212371\C,0,5.10244879,-0.913437807,-0.765394409\C,0,3.84815986
83,2.5838976471,-0.2711466453\C,0,4.5906669647,3.6804329536,0.16957903
4\C,0,5.2806027075,3.6187226503,1.3815650844\C,0,5.2267285855,2.453113
8465,2.1481319345\C,0,4.4880067659,1.3551464046,1.704685866\H,0,3.3141
441619,2.6335193267,-1.2165465038\H,0,4.6304481961,4.5825107088,-0.435
4209222\H,0,5.8576955756,4.4727697998,1.7258010037\H,0,5.7614387331,2.
3963882744,3.0926843041\H,0,4.4503832296,0.4476895176,2.3014590162\C,0
,3.7846219738,1.4083729971,0.4916234531\H,0,2.9614688722,-3.9937963829
,-1.8026952677\H,0,5.440080054,-4.0176385342,-2.1218907488\H,0,6.78890
27747,-2.0295579637,-1.4602494098\H,0,5.6972275096,-0.0520358917,-0.47
991363\H,0,-0.2749319928,-0.9653386156,-3.1982657963\H,0,-1.5511995811
,-0.0229659559,-4.0101910976\H,0,0.0523631532,1.0816184076,-1.81237040
06\H,0,-1.630245714,1.5649602674,-2.1121275509\H,0,-2.1515670345,-2.15
60372702,-2.0297481182\H,0,-3.2065555814,-0.7358958678,-2.2865104889\H
,0,-0.1685326419,-0.2911582804,2.008402804\H,0,0.2258202038,1.13022593
12,2.9232122694\H,0,0.2675742352,1.8440075371,0.0871309773\H,0,1.54122
79937,1.9905753317,1.2613610119\H,0,-1.635629428,2.3476903464,1.415622

0958\H,0,-2.2552977875,1.0790795739,2.5579352724\H,0,-4.780986271,-0.0
143699335,1.8865769046\H,0,-5.4715040266,-1.9824713093,3.1668251448\H,
0,-4.1582788381,-4.1112025243,3.0484716978\H,0,-2.044371316,-4.1911290
083,1.7378378708\\Version=ES64L-G16RevA.03\State=3-A\HF=-1498.4650536\
S2=2.034908\S2-1=0.\S2A=2.000606\RMSD=6.903e-09\Dipole=-0.5553397,2.20
13713,0.3034659\Quadrupole=11.0262168,-4.4699054,-6.5563114,2.3913603,
2.6193522,-1.6622429\PG=C01 [X(C36H30N2)]\\@

P

1\1\GINC-OM103\SP\RM06\6-311+G(d,p)\C36H30N2\WEIY\01-Apr-2020\0\\#p M0
6/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Title
Card Required\\0,1\C,0,-3.5949359942,-1.8826259889,-2.8524252133\C,0,
-3.3645964891,-3.8174471174,-1.1159747792\C,0,-2.6278364558,-2.8712663
948,-0.1267629963\C,0,-1.1068529487,-2.6457100554,-0.4053197564\C,0,-1
.1143926138,-1.1881070534,-2.5071044408\C,0,-2.1145282241,-2.142772005
8,-3.0841534386\C,0,-4.2497990711,-1.2471827649,-4.1439485015\C,0,-4.8
695420159,-0.1221335882,-3.2838222578\C,0,-4.0219604364,-0.5894440263,
-2.0752120376\C,0,-4.1845814536,-3.2564169852,-2.3576826583\N,0,-1.694
7273373,-3.1574792908,-3.7474296645\C,0,-4.6969956861,-5.3506914218,-3
.8193897984\C,0,-4.3266196886,-6.2409022639,-4.8333757334\C,0,-3.12627
36086,-6.0616022278,-5.5202497862\C,0,-2.2825205483,-5.0108046553,-5.1
651804831\C,0,-3.8950576092,-4.2555243585,-3.4929440738\C,0,-2.6513031
694,-4.1138614314,-4.1569894371\C,0,-8.4217595442,-2.7143991195,-1.391
1551222\C,0,-7.4549610237,-2.694581502,-0.3874589327\C,0,-6.1086525848
,-2.8910884335,-0.7002572815\C,0,-5.6799723857,-3.111131112,-2.0205839
446\C,0,-6.6737756916,-3.1247636284,-3.0165742665\C,0,-8.0211824925,-2
.9314570021,-2.7093479371\H,0,-9.4710025638,-2.5668057208,-1.150230071
5\H,0,-7.7437067278,-2.5277959799,0.6471565751\H,0,-5.3861356811,-2.86
70769332,0.1085380223\H,0,-6.3985795574,-3.3086349484,-4.0485596595\H,
0,-8.7585219343,-2.9562880794,-3.5076825468\C,0,-0.6811420108,-1.39491

47208,-1.156443374\N,0,-0.7535039127,-0.1814298026,-3.2736649987\C,0,0
.1110687481,0.7388426508,-2.7554008618\C,0,0.182063934,-0.4526917643,-
0.6110182393\C,0,0.6028142685,0.6569453661,-1.4164546162\C,0,0.5118622
806,1.8170447593,-3.5857302744\C,0,1.3653957763,2.7861342991,-3.108938
6391\C,0,1.8474102688,2.7160136096,-1.7802446711\C,0,1.4753665485,1.67
88704644,-0.9525733277\C,0,-0.1096421506,-0.1759925647,1.8769919118\C,
0,0.3666713194,-0.2747861182,3.1851333949\C,0,1.6502446784,-0.76630414
54,3.4289746094\C,0,2.4555742245,-1.1565554695,2.3574444199\C,0,1.9803
657191,-1.0555013913,1.0491136399\H,0,-1.108265559,0.2098043419,1.6894
50894\H,0,-0.2657159272,0.0340593556,4.0133373804\H,0,2.0209396332,-0.
844148522,4.4474699487\H,0,3.4558936393,-1.5408739661,2.5385229734\H,0
,2.6093260306,-1.3598256736,0.216788555\C,0,0.6900600093,-0.5677089863
,0.7931787079\H,0,0.1192654991,1.8423109312,-4.5974799769\H,0,1.669207
714,3.6097378869,-3.7494375585\H,0,2.5158425086,3.4884818082,-1.409553
4199\H,0,1.8482141149,1.6342247128,0.0651878595\H,0,-4.6850728894,0.89
88628176,-3.630685698\H,0,-5.9433525207,-0.2497410851,-3.1234246135\H,
0,-3.1808192742,0.0738482664,-1.8624225733\H,0,-4.5786934083,-0.750344
6142,-1.1497851281\H,0,-3.4806804034,-0.8822093785,-4.8302859425\H,0,-
4.9364965366,-1.8814462042,-4.7073564257\H,0,-2.6860994665,-3.35037696
,0.8585685615\H,0,-3.1349636354,-1.9093245154,-0.0134002442\H,0,-0.587
8520251,-2.6472545495,0.5553842129\H,0,-0.7272978221,-3.5173844957,-0.
9550459258\H,0,-2.6119638719,-4.5086119886,-1.5047396477\H,0,-4.057633
9263,-4.4510925635,-0.5539689402\H,0,-5.6292478664,-5.5117174498,-3.28
7671916\H,0,-4.9780801384,-7.0758769944,-5.0775061467\H,0,-2.836581206
3,-6.7497110476,-6.3097971127\H,0,-1.3187000169,-4.87009247,-5.6452758
459\\Version=ES64L-G16RevA.03\State=1-A\HF=-1498.6008307\RMSD=5.363e-0
9\Dipole=-0.3762731,0.2924243,1.6259911\Quadrupole=4.5447152,-5.417802
1,0.8730869,5.7450268,7.1844476,1.9425058\PG=C01 [X(C36H30N2)]\\@

^{1}S'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2\WEIY\08-Apr-2020\0\\#p uM
06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Titl
e Card Required\\0,1\C,0,5.408018,-1.277929,-0.099785\C,0,4.380988,-0.
573164,0.564484\C,0,4.281902,-0.750203,1.953738\C,0,5.133106,-1.604739
,2.649803\C,0,6.130143,-2.306627,1.967077\C,0,6.270564,-2.140393,0.594
375\H,0,3.510298,-0.201313,2.485765\H,0,5.019129,-1.72403,3.7237\H,0,6
.799368,-2.974806,2.501283\H,0,7.045247,-2.661232,0.040999\N,0,5.60640
9,-1.119835,-1.4632\C,0,5.791493,-0.998928,-2.623184\C,0,3.435244,0.35
0403,-0.135511\C,0,3.494288,1.789885,0.242685\C,0,4.73254,2.406751,0.4
99905\C,0,2.328629,2.568844,0.357986\C,0,4.807179,3.757203,0.835129\H,
0,5.645413,1.822356,0.425158\C,0,2.4063,3.920156,0.695604\H,0,1.354088
,2.113985,0.211552\C,0,3.643008,4.522387,0.932298\H,0,5.776964,4.21264
4,1.019632\H,0,1.490885,4.499846,0.784647\H,0,3.699619,5.574994,1.1975
16\C,0,2.561917,-0.126224,-1.040574\C,0,1.580314,0.521948,-2.006048\C,
0,2.301521,-1.505225,-1.628697\C,0,1.598829,-0.80124,-2.828012\H,0,1.9
18032,1.439924,-2.500273\H,0,0.600589,0.718021,-1.554563\H,0,3.162929,
-2.141281,-1.850546\H,0,1.591788,-2.079803,-1.018298\H,0,2.252923,-0.7
37083,-3.702168\H,0,0.6282,-1.204025,-3.130349\C,0,-1.428521,1.711258,
-0.048534\N,0,-2.584504,1.689794,-0.279836\C,0,-3.945151,1.678753,-0.5
43707\C,0,-4.727265,0.568155,-0.161416\C,0,-4.513764,2.792237,-1.17528
9\C,0,-6.099635,0.624331,-0.439491\C,0,-5.880544,2.815491,-1.437196\H,
0,-3.874423,3.625579,-1.447618\C,0,-6.675531,1.729459,-1.067353\H,0,-6
.7166,-0.225309,-0.161665\H,0,-6.320372,3.678595,-1.927999\H,0,-7.7425
22,1.73935,-1.271133\C,0,-4.120681,-0.626164,0.50802\C,0,-4.405121,-0.
857605,1.80223\C,0,-5.297389,-0.15213,2.814442\C,0,-4.135672,-2.003061
,2.769335\C,0,-5.310023,-1.471877,3.643908\H,0,-6.257393,0.238147,2.46
27\H,0,-4.773172,0.661391,3.333707\H,0,-4.211261,-3.01857,2.36453\H,0,
-3.169481,-1.91513,3.282605\H,0,-6.229534,-2.045163,3.494355\H,0,-5.12
1421,-1.38018,4.716966\C,0,-3.262055,-1.520453,-0.314698\C,0,-2.18681,
-2.233312,0.245553\C,0,-3.514673,-1.682227,-1.689165\C,0,-1.412892,-3.

093091,-0.532129\H,0,-1.93707,-2.090836,1.291137\C,0,-2.739423,-2.5402
59,-2.467292\H,0,-4.332894,-1.136256,-2.149691\C,0,-1.686395,-3.25425,
-1.892254\H,0,-0.587218,-3.632328,-0.074919\H,0,-2.960329,-2.652246,-3
.525594\H,0,-1.081737,-3.923911,-2.497598\\Version=ES64L-G16RevA.03\St
ate=1-A\HF=-1498.4506375\S2=0.\S2-1=0.\S2A=0.\RMSD=3.554e-09\Dipole=-2
.6545711,-0.3932091,1.5020186\Quadrupole=9.8601533,-0.8956106,-8.96454
27,-11.9155814,18.5299748,-6.1651149\PG=C01 [X(C36H30N2)]\\@

^{3}S'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\08-Apr-2020\0\\#p
M06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti
tle Card Required\\0,3\C,0,4.8907401388,-1.2831119427,0.7642519872\C,0
,3.8178901795,-0.390148656,0.9752563358\C,0,3.369622572,-0.2337615661,
2.2965677153\C,0,3.9299658419,-0.946143216,3.3538335018\C,0,4.97848277
01,-1.8390798137,3.1169378014\C,0,5.461417317,-2.0045375301,1.82424451
82\H,0,2.557964824,0.4637407431,2.4821180009\H,0,3.5495165969,-0.80576
71143,4.3618462771\H,0,5.4226920578,-2.3986490756,3.9350328806\H,0,6.2
843579139,-2.6797761034,1.6133792355\N,0,5.4269526454,-1.4571722051,-0
.5027707811\C,0,5.8972794775,-1.6192684207,-1.573729829\C,0,3.17596985
84,0.394277539,-0.1246326593\C,0,3.301070137,1.8769252361,-0.057748191
8\C,0,4.4993594637,2.4710747319,0.3792126848\C,0,2.2368754764,2.721710
549,-0.422269446\C,0,4.639413541,3.8566773983,0.4266997187\H,0,5.33207
5432,1.8383660278,0.6736136118\C,0,2.3793955224,4.1084829813,-0.372652
1713\H,0,1.2840981266,2.2940353421,-0.718390263\C,0,3.5797636758,4.683
52021,0.0477768489\H,0,5.579072559,4.2910487016,0.7588268732\H,0,1.541
2671665,4.7409840677,-0.6546746665\H,0,3.6867500982,5.7644814346,0.087
3122202\C,0,2.4989155061,-0.2314228919,-1.1041037831\C,0,1.8615700053,
0.2268808613,-2.4077387173\C,0,2.2403308126,-1.692938597,-1.4389145648
\C,0,1.9523698136,-1.2469904157,-2.9037537932\H,0,2.4023651515,0.99530
34087,-2.9716066375\H,0,0.8244623701,0.5587226869,-2.2813230268\H,0,3.

0495870704,-2.4105168963,-1.277751836\H,0,1.335811533,-2.0686878402,-0
.9417926527\H,0,2.8151526106,-1.4123787561,-3.5552314481\H,0,1.0570216
103,-1.6621742073,-3.3747520293\C,0,-1.4241571276,1.7056606856,-1.2133
354877\N,0,-2.5704598726,1.6787522997,-0.9373547334\C,0,-3.9140311971,
1.7003335361,-0.6005543274\C,0,-4.5311854112,0.5714016252,0.0000796205
\C,0,-4.6195180966,2.8925131613,-0.817873433\C,0,-5.872294222,0.734047
5917,0.4078661969\C,0,-5.9502534043,2.9993289729,-0.4314395988\H,0,-4.
0992741239,3.7272139675,-1.2764006141\C,0,-6.5747518561,1.913766004,0.
1911222669\H,0,-6.3696353289,-0.1057828667,0.8822849757\H,0,-6.4914505
14,3.9246195979,-0.604118748\H,0,-7.6128445412,1.98676351,0.5029208511
\C,0,-3.8278637434,-0.6980315527,0.2755813216\C,0,-3.9281084731,-1.207
2229683,1.6476774755\C,0,-3.188494206,-0.8581981082,2.9230691583\C,0,-
4.8230056485,-2.2196957066,2.334918724\C,0,-4.0406473486,-1.9408216892
,3.6564468184\H,0,-3.34754609,0.1715943725,3.2789139809\H,0,-2.1016104
054,-1.0279473057,2.9116278221\H,0,-5.8938274185,-1.9641686085,2.37251
05518\H,0,-4.7557804263,-3.2467578327,1.9453361389\H,0,-4.6518978576,-
1.563620677,4.4808615411\H,0,-3.4606396024,-2.7948272027,4.0168727074\
C,0,-3.1125467242,-1.4378629384,-0.732128679\C,0,-2.3008709232,-2.5473
902227,-0.3679102305\C,0,-3.232541823,-1.1507413719,-2.1193283508\C,0,
-1.6393506295,-3.303298202,-1.3253985766\H,0,-2.1949563963,-2.79636475
09,0.6837319137\C,0,-2.573114655,-1.9156530668,-3.0710967959\H,0,-3.87
17737893,-0.3350755471,-2.4409020663\C,0,-1.7684524465,-2.9949460417,-
2.6857100754\H,0,-1.0220995951,-4.142376358,-1.0151645272\H,0,-2.69072
41745,-1.6761501131,-4.1246042574\H,0,-1.2574838035,-3.5933198647,-3.4
345362777\\Version=ES64L-G16RevA.03\State=3-A\HF=-1498.3723957\S2=2.03
602\S2-1=0.\S2A=2.000759\RMSD=4.969e-09\Dipole=-2.8265929,-0.1169752,1
.7786741\Quadrupole=-0.6356827,2.5734486,-1.9377659,-7.1200911,13.6923
834,-6.2056366\PG=C01 [X(C36H30N2)]\\@

^{3}TS1'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\31-Mar-2020\0\\#p
M06/6-311+G(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti
tle Card Required\\0,3\C,0,0.1834523497,-0.0036566351,0.0136723873\C,0
,0.0945970265,0.0638275229,1.4254807217\C,0,1.3110156947,0.1413639293,
2.1330285051\C,0,2.542058768,0.1358803018,1.4819622031\C,0,2.600436321
5,0.0544333958,0.0872286217\C,0,1.4201986492,-0.0110619619,-0.64529378
23\H,0,1.2722754149,0.1866145539,3.2171645877\H,0,3.4574607967,0.18900
92145,2.0647102378\H,0,3.5570402351,0.0468180413,-0.4265497923\H,0,1.4
331200465,-0.056624444,-1.7294937546\N,0,-0.9688229768,-0.0195350249,-
0.7563539632\C,0,-1.9357624748,-0.0161857284,-1.434592173\C,0,-1.18982
91693,0.0049286609,2.1624334365\C,0,-1.59655383,1.0951521897,2.9893989
873\C,0,-0.8840946745,2.3359788195,3.0047053369\C,0,-2.7723292118,1.02
4818344,3.8009803927\C,0,-1.2996383587,3.3998289015,3.7881502636\H,0,-
0.0100638287,2.4525294467,2.3738383928\C,0,-3.1763325369,2.0982859773,
4.5799687207\H,0,-3.347854218,0.108124306,3.8199721441\C,0,-2.44646818
98,3.2947855056,4.5883330777\H,0,-0.7342640007,4.3281403688,3.77054122
56\H,0,-4.0727864415,2.0065129772,5.1879486452\H,0,-2.7707818855,4.133
2334033,5.1980961796\C,0,-2.0087847777,-1.2371048932,2.0126585745\C,0,
-3.425156941,-1.3876248937,1.4666724101\C,0,-1.5871983204,-2.562457280
8,1.3933383771\C,0,-3.0937217403,-2.8745918392,1.1607818756\H,0,-3.590
812529,-0.7866629148,0.5626252366\H,0,-4.2473719092,-1.1932346269,2.16
48783654\H,0,-1.0410411656,-2.4307739347,0.4489296015\H,0,-1.009235457
2,-3.2522844587,2.0198803643\H,0,-3.3661848232,-3.2412648635,0.1674638
626\H,0,-3.4958834558,-3.5479424396,1.9218292846\C,0,-2.2117591224,-2.
0658636008,4.1230173462\N,0,-1.2197128631,-1.9774316853,4.7749645883\C
,0,-0.0897207427,-1.8255457866,5.5393194744\C,0,0.8752546865,-2.860569
8915,5.6013278563\C,0,0.0913851499,-0.62395834,6.2480271438\C,0,2.0108
498696,-2.6390257032,6.389982778\C,0,1.2333328548,-0.4398321267,7.0203
160363\H,0,-0.6682232519,0.1472576212,6.1717207292\C,0,2.198115859,-1.
4477686776,7.0935152627\H,0,2.7526445032,-3.4300335293,6.4561698329\H,

0,1.3674327513,0.4901707312,7.565521805\H,0,3.0885425229,-1.3113030778
,7.7005767634\C,0,0.6858326368,-4.1478296699,4.8611293016\C,0,1.504558
2043,-4.4376984137,3.832928636\C,0,2.6991673136,-3.7200871757,3.218012
2853\C,0,1.7390171345,-5.668918682,2.9660285987\C,0,3.1359800617,-5.08
40848899,2.6024114802\H,0,3.3982714496,-3.2257459397,3.8996764021\H,0,
2.4010268752,-2.9892176467,2.4547435387\H,0,1.7025770332,-6.6410542318
,3.4706905947\H,0,1.0744401043,-5.7167523406,2.0938875406\H,0,3.943397
8742,-5.5554942417,3.1704501188\H,0,3.4054656645,-5.0809606689,1.54260
24226\C,0,-0.3801769284,-5.071313819,5.3375295835\C,0,-1.0817372777,-5
.9123390908,4.4553792995\C,0,-0.7079437283,-5.1309576898,6.7040735027\
C,0,-2.0556984913,-6.79244174,4.9239919118\H,0,-0.8834968912,-5.855738
571,3.390478311\C,0,-1.6807936861,-6.0120056538,7.1727418655\H,0,-0.18
82916039,-4.4843794053,7.4051399113\C,0,-2.358046934,-6.8502569417,6.2
855651813\H,0,-2.5889043602,-7.4261037155,4.2198778702\H,0,-1.91069713
49,-6.0421928934,8.234749446\H,0,-3.1199687007,-7.5341969734,6.6496737
608\\Version=ES64L-G16RevA.03\State=3-A\HF=-1498.3714281\S2=2.04378\S2
-1=0.\S2A=2.001155\RMSD=6.122e-09\Dipole=2.3632915,0.0920788,1.0093064
\Quadrupole=2.9861686,3.7261546,-6.7123232,5.1042493,-10.8810725,10.17
1005\PG=C01 [X(C36H30N2)]\\@

^{3}IntA'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\31-Mar-2020\0\\#p
M06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti
tle Card Required\\0,3\C,0,-2.0403060327,-1.3123663715,1.1473447691\C,
0,-1.0404200824,-0.5520962822,0.4961463218\C,0,-1.3880314163,0.7481291
177,0.0942115819\C,0,-2.6577448053,1.2736075738,0.3325477627\C,0,-3.62
49503927,0.5051247502,0.9830249949\C,0,-3.3176517349,-0.7894696173,1.3
894541859\H,0,-0.6394127639,1.3546840932,-0.4059918756\H,0,-2.88722862
25,2.2864592621,0.0139853709\H,0,-4.6151181993,0.9089483407,1.17255667
64\H,0,-4.0515958743,-1.4113564145,1.8915263427\N,0,-1.7743813913,-2.6

128314113,1.5478326945\C,0,-1.5595240251,-3.7261507419,1.8792299346\C,
0,0.3248443523,-1.0887336642,0.2469150475\C,0,1.2370936161,-1.2515813,
1.3424081445\C,0,0.9036333778,-0.8015641167,2.6541590573\C,0,2.5149111
595,-1.8635004974,1.1836599796\C,0,1.7767455014,-0.9632712466,3.720089
357\H,0,-0.0525636875,-0.3177314209,2.8220951693\C,0,3.3788913656,-2.0
211053825,2.2576172767\H,0,2.8278848429,-2.209585751,0.2041030768\C,0,
3.0215165476,-1.5760856505,3.5355146284\H,0,1.4862055604,-0.6096845186
,4.7060420532\H,0,4.3439238607,-2.4950341491,2.0986568478\H,0,3.703661
8724,-1.6993744728,4.3716348775\C,0,0.6964354589,-1.5720468902,-1.1597
587276\C,0,0.6451319712,-3.1556876706,-1.2614266681\C,0,-0.4488486015,
-1.5588831674,-2.2462502993\C,0,-0.7159245389,-3.0591722755,-1.9888441
231\H,0,0.6696380758,-3.6991874952,-0.3143553402\H,0,1.4482022099,-3.5
179729209,-1.9102898815\H,0,-1.2652598848,-0.8508122624,-2.0891413591\
H,0,-0.0223950382,-1.388750169,-3.2396457614\H,0,-1.5592284206,-3.2239
391515,-1.3124376118\H,0,-0.8503025192,-3.6913662871,-2.8713971592\C,0
,1.9668189278,-0.9507368178,-1.6823483187\N,0,2.4043631423,0.176114766
3,-1.8960030431\C,0,1.9933593038,1.5139651574,-1.9108891784\C,0,2.7549
163004,2.5050598079,-1.2425954406\C,0,0.8621785837,1.880577479,-2.6651
080309\C,0,2.2794142388,3.8262729713,-1.2866734302\C,0,0.4470191221,3.
2074150815,-2.724654\H,0,0.3186137693,1.1087582931,-3.2010006404\C,0,1
.1504080534,4.1861396148,-2.0188540591\H,0,2.8316213617,4.5872601191,-
0.742506487\H,0,-0.4277603502,3.4720222925,-3.3130175494\H,0,0.8300171
877,5.2237709597,-2.0484611783\C,0,4.0159251228,2.2187013875,-0.493552
7868\C,0,5.0516129569,1.5799902848,-1.0641418453\C,0,5.332795951,1.062
4726646,-2.465697983\C,0,6.4476437679,1.1929351838,-0.5885201606\C,0,6
.8383975801,0.9608120197,-2.079458244\H,0,5.0666632199,1.7276905051,-3
.2955290995\H,0,4.8660009115,0.0891021631,-2.6534207908\H,0,7.02539868
76,1.9319998708,-0.0262393512\H,0,6.436365825,0.263063383,-0.004134855
4\H,0,7.4337489762,1.7840713135,-2.4858686048\H,0,7.3405919466,0.01737
32847,-2.3120581236\C,0,4.1054917342,2.7459682074,0.9037257321\C,0,5.1

184215518,3.6418907675,1.2817325104\C,0,3.1604490675,2.3650062667,1.87
04081643\C,0,5.1955883294,4.1291068756,2.5874911119\H,0,5.8403200703,3
.9689950297,0.5386116052\C,0,3.2395907558,2.8464531749,3.17615174\H,0,
2.3687987816,1.6731398915,1.59812741\C,0,4.2576899569,3.730560854,3.54
08948264\H,0,5.9856585696,4.825703219,2.85689396\H,0,2.5058591927,2.52
51198253,3.9108522344\H,0,4.3166842728,4.1086549944,4.5582435023\\Vers
ion=ES64L-G16RevA.03\State=3-A\HF=-1498.3968575\S2=2.04048\S2-1=0.\S2A
=2.000908\RMSD=4.886e-09\Dipole=-0.8174041,1.2936267,-0.4087277\Quadru
pole=13.8972592,-14.2485869,0.3513278,-8.0768566,5.1285572,7.1725377\P
G=C01 [X(C36H30N2)]\\@

^{3}TS2'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\31-Mar-2020\0\\#p
M06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti
tle Card Required\\0,3\C,0,-0.9461478659,0.1596327456,-0.5286346536\C,
0,-0.217697978,-0.1042867351,0.6557608921\C,0,1.0768899125,-0.63041688
05,0.5024671064\C,0,1.6295686214,-0.8729171052,-0.7537547572\C,0,0.892
4213595,-0.5942572126,-1.9068953418\C,0,-0.3958085455,-0.0802665014,-1
.7946422097\H,0,1.6595461151,-0.8270213666,1.3980253586\H,0,2.63771517
62,-1.2699167418,-0.8323241068\H,0,1.3160845919,-0.7776440278,-2.88984
87471\H,0,-0.9942447407,0.133848942,-2.6741300662\N,0,-2.246223099,0.6
321947737,-0.4546077759\C,0,-3.3643415536,1.0090767054,-0.3982370082\C
,0,-0.7624709431,0.1811657558,2.0077829444\C,0,-1.0415039583,1.5643913
164,2.3719423145\C,0,-0.4092804103,2.6328759995,1.6894339061\C,0,-1.94
18481141,1.9000049362,3.4124106191\C,0,-0.6549029758,3.9565294804,2.03
48586603\H,0,0.2952305616,2.4134533471,0.8932105972\C,0,-2.182680058,3
.2270943915,3.7533690987\H,0,-2.4707206683,1.1159744185,3.9402935055\C
,0,-1.5418523163,4.2645777559,3.0705596561\H,0,-0.1482293215,4.7531444
877,1.4960404505\H,0,-2.8825502943,3.4497584163,4.5542962331\H,0,-1.73
51540879,5.2999736841,3.3376816323\C,0,-1.0216140544,-0.920212097,2.92

27380828\C,0,-3.0134378401,-1.4640660849,2.6472945927\C,0,-0.910073781
7,-2.3985152915,2.4449582679\C,0,-2.3224619509,-2.5549944015,1.8543905
671\H,0,-3.6021511772,-0.7042564466,2.1401526709\H,0,-3.3309877119,-1.
6939051469,3.6625806063\H,0,-0.0808935628,-2.5995264597,1.7606705415\H
,0,-0.7807026181,-3.0416769604,3.3213021504\H,0,-2.3292828992,-2.31765
5714,0.7856686038\H,0,-2.7492051536,-3.559641795,1.9732549816\C,0,-0.7
111504003,-0.7590676126,4.2925838261\N,0,-1.2075870296,-0.679165551,5.
425894971\C,0,-0.5089704873,-0.6225249234,6.6579620129\C,0,-1.25360990
15,-0.3724076805,7.8283079406\C,0,0.8820907138,-0.8044127453,6.7302395
968\C,0,-0.5610496215,-0.2860217607,9.0467190337\C,0,1.5424506118,-0.7
310823983,7.9501012159\H,0,1.4263425755,-0.9962632983,5.8096792235\C,0
,0.817552645,-0.4672648048,9.1165753448\H,0,-1.1269032622,-0.077587634
2,9.9506029667\H,0,2.6190128451,-0.8739204281,7.9929644289\H,0,1.32570
04557,-0.4048808345,10.0750131884\C,0,-2.7416442092,-0.1811232549,7.81
66762497\C,0,-3.545264734,-1.2389948068,7.6129373999\C,0,-3.2672565336
,-2.6925327705,7.2619391674\C,0,-5.0436424407,-1.4238552595,7.40853214
12\C,0,-4.7273928564,-2.7863718367,6.7232034221\H,0,-3.1056632574,-3.3
201182974,8.1488430927\H,0,-2.4563824721,-2.8851460484,6.5532561973\H,
0,-5.5983100491,-1.5554256055,8.3470577037\H,0,-5.558670855,-0.6581846
821,6.8173260923\H,0,-5.3182915219,-3.6480974506,7.0468144521\H,0,-4.7
702393235,-2.7190443934,5.6320440398\C,0,-3.2542797274,1.1937552765,8.
0571408948\C,0,-4.4656635529,1.4275549485,8.7335005335\C,0,-2.52745577
44,2.3123010865,7.6074593057\C,0,-4.941602461,2.7230188729,8.931703350
8\H,0,-5.0263655515,0.5881328435,9.1306358553\C,0,-3.0046570215,3.6072
834091,7.8040499048\H,0,-1.5851250898,2.162211726,7.0897462992\C,0,-4.
2161636693,3.8204335184,8.4651621065\H,0,-5.878008324,2.8746457323,9.4
628049504\H,0,-2.4244588029,4.4524786001,7.4421937792\H,0,-4.585880490
9,4.8301099179,8.6227856727\\Version=ES64L-G16RevA.03\State=3-A\HF=-14
98.3820202\S2=2.059369\S2-1=0.\S2A=2.00173\RMSD=3.365e-09\Dipole=1.501
4838,-1.1082545,-0.2025631\Quadrupole=-1.6917751,-1.5443595,3.2361346,

-0.3959669,-19.4776514,5.7282529\PG=C01 [X(C36H30N2)]\\@

^{3}IntB'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\31-Mar-2020\0\\#p
M06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti
tle Card Required\\0,3\C,0,0.3609173579,-0.3115825482,1.236753481\C,0,
0.0035173157,0.3186108189,0.011416175\C,0,0.1743032084,1.7197035685,-0
.0434788098\C,0,0.6277602896,2.4536324882,1.046338961\C,0,0.9432110743
,1.8095244716,2.2477586436\C,0,0.8144427127,0.426911252,2.3368908054\H
,0,-0.0869705526,2.2295502648,-0.965058209\H,0,0.725249118,3.532476768
8,0.9636675288\H,0,1.2972417479,2.3760815074,3.1038466549\H,0,1.078229
7201,-0.1038661592,3.2458974728\N,0,0.3247011397,-1.6909416417,1.35678
66736\C,0,0.3050311342,-2.8660299643,1.4643048275\C,0,-0.5137421161,-0
.4202913273,-1.1483303713\C,0,0.0003398626,-0.1101018837,-2.4802933964
\C,0,-0.8231067817,-0.1976897024,-3.6284171628\C,0,1.3433152555,0.2948
82335,-2.6719447088\C,0,-0.3265218825,0.094733789,-4.8946597847\H,0,-1
.8676910319,-0.470992208,-3.5087466571\C,0,1.8338845462,0.587601532,-3
.9400054528\H,0,2.0049049834,0.3576514335,-1.8134189247\C,0,1.00451192
,0.4881243343,-5.0613197363\H,0,-0.9858929495,0.0286572487,-5.75648977
11\H,0,2.8724387122,0.8868379306,-4.0563107005\H,0,1.3897005256,0.7171
608085,-6.0511129894\C,0,-1.5949538704,-1.3791692968,-0.9706136292\C,0
,-2.5072191456,-1.1497531395,-0.0152312153\N,0,-3.4441376509,-0.861623
8516,0.7126255461\C,0,-3.662488224,-1.1436678793,2.0845992525\C,0,-4.5
377028962,-0.3036353887,2.8021048956\C,0,-3.05670005,-2.2476568763,2.7
047438656\C,0,-4.7487589479,-0.5861063122,4.1600351893\C,0,-3.30331245
65,-2.517093042,4.0465151228\H,0,-2.3847254072,-2.8782489418,2.1303101
972\C,0,-4.150117009,-1.6811963195,4.7792654837\H,0,-5.4043501884,0.06
75671043,4.7286804985\H,0,-2.8306022208,-3.3737347974,4.5188611134\H,0
,-4.3456345411,-1.8842118177,5.8286389754\C,0,-5.2174699858,0.88010703
32,2.1801416424\C,0,-6.2362324026,0.6850494077,1.3257752703\C,0,-6.844

0924782,-0.5674434022,0.7141350257\C,0,-7.058335723,1.5894123458,0.416
7152547\C,0,-7.4038456467,0.3294273067,-0.4317348981\H,0,-7.6398202929
,-0.9997012164,1.3357863905\H,0,-6.1532837161,-1.3679030118,0.43372041
97\H,0,-7.9458183906,2.0094273217,0.9083337537\H,0,-6.5242924984,2.410
7967988,-0.0743109044\H,0,-8.4551600522,0.1899221702,-0.6992975851\H,0
,-6.795841759,0.2637867768,-1.338590864\C,0,-4.725247025,2.2297926221,
2.5640919254\C,0,-5.5932771007,3.3319592032,2.6699309964\C,0,-3.360099
4921,2.4406107589,2.8331122408\C,0,-5.1133160004,4.5961152229,3.009508
3595\H,0,-6.6570292389,3.1906840334,2.5102712147\C,0,-2.8803241006,3.7
050936497,3.1683712943\H,0,-2.6669857788,1.6074302011,2.7677474352\C,0
,-3.7534112803,4.7910740539,3.25706466\H,0,-5.8071654324,5.4291312945,
3.0908819564\H,0,-1.8186426015,3.8396998478,3.3587942917\H,0,-3.380028
496,5.7763277209,3.5235694757\C,0,-1.6555610296,-2.7057530564,-1.73500
83762\C,0,-3.081815891,-3.2367119701,-2.0434665189\C,0,-3.8813142444,-
2.379891345,-2.9680212273\H,0,-1.1223239302,-3.4606878676,-1.139164337
3\H,0,-1.0964008523,-2.5964130199,-2.6674416823\H,0,-2.9661989227,-4.2
420969024,-2.4689944591\H,0,-3.6190004208,-3.3617869356,-1.0924152405\
H,0,-3.843561194,-2.529761844,-4.0428185059\H,0,-4.4413904246,-1.52704
13263,-2.5977794127\\Version=ES64L-G16RevA.03\State=3-A\HF=-1498.40680
01\S2=2.03408\S2-1=0.\S2A=2.000765\RMSD=9.350e-09\Dipole=-0.2599694,1.
0454115,-0.0172301\Quadrupole=1.6122127,-6.5948225,4.9826098,8.6652442
,-0.0795158,2.2743248\PG=C01 [X(C36H30N2)]\\@

^{3}TS3'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\01-Apr-2020\0\\#p
M06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti
tle Card Required\\0,3\C,0,0.022587583,-0.0796887186,0.0616284992\C,0,
0.0438148875,-0.0559984347,1.4599311491\C,0,1.2635398873,-0.0089954012
,2.1252379397\C,0,2.4625796394,0.026376109,1.3993989958\C,0,2.47074583
54,0.0355940612,-0.0197642713\C,0,1.213312169,-0.0393238965,-0.6551019

543\H,0,-0.9242550176,-0.1207399271,-0.4695528568\H,0,-0.8814623379,-0
.0831861972,2.0277044335\H,0,1.312556689,-0.0168464452,3.2093408676\H,
0,1.1903203561,-0.0469256021,-1.7404430786\C,0,3.7029109153,0.10195510
93,-0.8290551873\C,0,3.8915883251,-0.8914785173,-1.8875708359\C,0,3.36
97758864,-2.2010108616,-1.7532509255\C,0,4.5883876255,-0.5949585702,-3
.0834464627\C,0,3.5507239326,-3.1576925071,-2.7462866784\H,0,2.8388728
657,-2.4674936398,-0.8447951852\C,0,4.7652447478,-1.5551247979,-4.0753
332576\H,0,4.9585997132,0.4115933516,-3.2492595424\C,0,4.252364175,-2.
8450978334,-3.9144266558\H,0,3.149551594,-4.1579357913,-2.603934185\H,
0,5.292953948,-1.2879416753,-4.9875410567\H,0,4.3921150874,-3.59360160
28,-4.6894138581\C,0,4.6559983061,1.1556447959,-0.5960030335\C,0,4.278
8996165,2.4889130446,0.0678538145\C,0,5.9355684848,1.0910089994,-0.997
3912665\C,0,5.4450194247,3.4948997056,0.1806896531\H,0,3.900789301,2.2
976096106,1.0769567533\H,0,3.4519733459,2.9326189756,-0.5027022297\C,0
,5.9803513238,4.0161639244,-1.1387897365\H,0,5.0972790316,4.3394185672
,0.7884215064\H,0,5.7288728059,3.4565445834,-2.0376140491\C,0,8.216611
3085,3.9760985709,-1.4605945576\N,0,7.129284653,1.1562968429,-1.207182
1788\C,0,7.8864041409,1.5435168615,-2.3347493104\C,0,8.4300121855,2.84
54218578,-2.4515155584\C,0,8.1790064663,0.5425924009,-3.2724152432\C,0
,9.3136699989,3.0489673808,-3.528121075\C,0,9.0184779902,0.8041581921,
-4.3497170952\H,0,7.7412744968,-0.4404164839,-3.131267774\C,0,9.601466
3258,2.0645478331,-4.4705988157\H,0,9.8097009649,4.0092522809,-3.60455
59388\H,0,9.231006507,0.0208107353,-5.0719941721\H,0,10.2916164431,2.2
793844806,-5.2815247343\H,0,5.8637418698,5.086802525,-1.2896530923\C,0
,8.7737277633,3.7464273994,-0.0767893117\C,0,9.7235879837,2.7391593355
,0.1637966174\C,0,8.4102840475,4.5667153738,1.0063605509\C,0,10.291201
4566,2.5661894115,1.4262245998\H,0,10.032726975,2.0884168493,-0.646902
8319\C,0,8.9780465209,4.3974089607,2.2680767655\H,0,7.6583298505,5.335
1020426,0.8655532409\C,0,9.9244938197,3.3952384005,2.4857735354\H,0,11
.0236490394,1.7776835204,1.5783250334\H,0,8.6713822027,5.0459954582,3.

0847637998\H,0,10.363417772,3.257782689,3.4702345875\C,0,8.2909240371,
5.2814380804,-1.9739142302\C,0,7.9095130425,5.910010952,-3.3059084602\
C,0,8.5113460157,6.6412492148,-1.3375151006\C,0,8.4377591314,7.2688475
788,-2.760341898\H,0,6.8192985417,5.9150791985,-3.4639660327\H,0,8.362
9766452,5.5268243211,-4.2257017433\H,0,7.6822101894,6.9759868814,-0.69
54852081\H,0,9.4386110497,6.7779439679,-0.7667312372\H,0,7.777463633,8
.1328831657,-2.8783284705\H,0,9.4242687213,7.5245052509,-3.1581109037\
N,0,3.6502000291,0.0026268649,2.1124535104\C,0,4.6472659873,-0.0366618
218,2.7456856282\H,0,6.2438429732,3.0265605565,0.772540285\\Version=ES
64L-G16RevA.03\State=3-A\HF=-1498.3776973\S2=2.092244\S2-1=0.\S2A=2.00
3648\RMSD=4.745e-09\Dipole=-1.2375361,0.7308101,-1.277255\Quadrupole=7
.4250654,-0.3957381,-7.0293272,4.9286174,-9.8099352,6.9900675\PG=C01 [
X(C36H30N2)]\\@

^{3}IntC'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\01-Apr-2020\0\\#p
M06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti
tle Card Required\\0,3\C,0,5.6560425923,-1.4686958736,-1.8949282656\C,
0,5.5714305077,-2.8165042133,-1.5283550733\C,0,4.5615062598,-3.2262119
297,-0.6663451787\C,0,3.6284224546,-2.3009365413,-0.1755252069\C,0,3.6
709386544,-0.9309426331,-0.5531965558\C,0,4.7283756743,-0.5544308112,-
1.4124617415\H,0,6.4415587704,-1.1337335076,-2.5666154675\H,0,6.290024
3619,-3.5390225334,-1.903473495\H,0,4.4848325432,-4.259203966,-0.34264
14843\H,0,4.7931996744,0.4863347796,-1.7132198808\C,0,2.7109800656,0.0
823186001,-0.0926975721\C,0,3.2380444084,1.3785779325,0.3660850922\C,0
,4.4465581317,1.450699626,1.0949333356\C,0,2.5614132307,2.5907685775,0
.1084965296\C,0,4.9403458291,2.6672233012,1.5552895976\H,0,4.985525968
4,0.534600589,1.3163206281\C,0,3.0591868893,3.8076038417,0.5692908562\
H,0,1.6572539187,2.5800541992,-0.4922215\C,0,4.2488280797,3.8547462822
,1.298788773\H,0,5.8655850011,2.6884492491,2.1254210782\H,0,2.52272261

6,4.7256549003,0.3424771563\H,0,4.6357794005,4.8042658993,1.6583067743
\C,0,1.3047953566,-0.1635993759,-0.1077732786\C,0,0.6071827364,-1.2309
570923,-0.9714229901\C,0,0.3878119547,0.5896732561,0.5338070924\C,0,-0
.4120225875,-0.6098365042,-1.9779119152\H,0,0.1291277909,-1.9790864019
,-0.3352709213\H,0,1.384936858,-1.7540767354,-1.5334343267\C,0,-1.9280
662169,-0.8520928597,-1.7956978354\H,0,-0.2244059235,0.4667367835,-2.0
650560647\H,0,-0.1849717464,-1.0201476464,-2.9705537973\H,0,-2.3929018
96,-0.4744298449,-2.7151629989\C,0,-2.7781358823,-0.2169073474,-0.6348
013049\N,0,-0.6279970563,1.1211054558,0.9426347166\C,0,-1.5157956138,1
.9288224861,0.1764173554\C,0,-2.5409810927,1.313002274,-0.5771632243\C
,0,-1.3703469179,3.3188044821,0.2236486082\C,0,-3.3418458126,2.1698438
06,-1.3477099307\C,0,-2.2026814509,4.1356734928,-0.5374706835\H,0,-0.5
892482808,3.7395441873,0.8496052898\C,0,-3.1829086061,3.5554313863,-1.
34088655\H,0,-4.1125318241,1.7272361345,-1.9708652397\H,0,-2.077830381
5,5.2145745878,-0.5065709062\H,0,-3.8315564552,4.1757061851,-1.9530257
908\H,0,-2.1160737332,-1.9315034487,-1.8070570165\C,0,-2.6447151263,-0
.9165219679,0.7434753054\C,0,-3.0888839613,-0.2647698335,1.9087241778\
C,0,-2.2447274137,-2.2557422465,0.8690173351\C,0,-3.1007441086,-0.9100
697287,3.1428424694\H,0,-3.4143031122,0.7693599227,1.8516797268\C,0,-2
.2465400854,-2.9032992688,2.106958528\H,0,-1.9172477186,-2.8165383791,
0.0010387103\C,0,-2.6735349081,-2.2348820424,3.25220134\H,0,-3.4378588
409,-0.3703391714,4.024251646\H,0,-1.9028268693,-3.9320927538,2.169193
4632\H,0,-2.6709734034,-2.7361732701,4.2160959769\C,0,-4.2317197864,-0
.5090405829,-0.9895121627\C,0,-4.8476720831,-1.7373707235,-1.623629835
8\C,0,-5.537328083,-0.0814544838,-0.3520581094\C,0,-6.2414514085,-1.20
71304955,-1.1689337743\H,0,-4.5630318138,-2.6851744327,-1.1390307112\H
,0,-4.7045020382,-1.8710109055,-2.7053341231\H,0,-5.5751658318,-0.2431
383472,0.7356106839\H,0,-5.8757997345,0.9469738076,-0.5372877556\H,0,-
6.8437592071,-1.9076342653,-0.583740532\H,0,-6.849471132,-0.828327995,
-1.9955985382\N,0,2.6924919721,-2.7621681318,0.7352927343\C,0,1.925357

3634,-3.2069660739,1.5159841777\\Version=ES64L-G16RevA.03\State=3-A\HF
=-1498.4145068\S2=2.034123\S2-1=0.\S2A=2.000734\RMSD=6.598e-09\Dipole=
0.5341848,0.6468932,-1.7151844\Quadrupole=8.9810463,0.8855946,-9.86664
08,-3.6396246,-1.4567001,6.8749256\PG=C01 [X(C36H30N2)]\\@

^{3}TS4'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\01-Apr-2020\0\\#p
M06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti
tle Card Required\\0,3\C,0,5.8102510496,-1.3394482264,-1.5163726372\C,
0,5.8242118892,-2.6728340135,-1.0905601304\C,0,4.7853830039,-3.1434268
79,-0.2969915337\C,0,3.7285562862,-2.2959001614,0.0657499607\C,0,3.670
5407149,-0.9426305276,-0.3738362589\C,0,4.761757979,-0.5021056938,-1.1
602856061\H,0,6.6158124232,-0.9563385444,-2.1367165947\H,0,6.638995418
2,-3.3352103921,-1.3669460933\H,0,4.7789748953,-4.1642285551,0.0715246
556\H,0,4.7544323581,0.5254143489,-1.5085785631\C,0,2.5838869974,-0.01
17790431,-0.0459647397\C,0,2.9634285055,1.3716410889,0.3015073174\C,0,
4.0608454529,1.6306890895,1.1500731567\C,0,2.2688033427,2.4790783806,-
0.2256003624\C,0,4.4375799312,2.9337391561,1.4641370905\H,0,4.60915533
37,0.794892774,1.5747671912\C,0,2.651126346,3.7824668091,0.0834447446\
H,0,1.4382249188,2.3110629814,-0.9035398301\C,0,3.734818715,4.01817363
45,0.9325913399\H,0,5.2796275225,3.103591304,2.1302800645\H,0,2.104769
73,4.6167369477,-0.3492462438\H,0,4.0313537462,5.0353327222,1.17434650
98\C,0,1.2106289605,-0.4513938956,-0.0612938707\C,0,0.7438028905,-1.53
03282002,-1.035271756\C,0,0.2641410954,0.2156569436,0.6514419287\C,0,-
0.2439391447,-0.9297492139,-2.0713921139\H,0,0.3006684665,-2.396167223
1,-0.5390578748\H,0,1.6216023407,-1.9006971861,-1.5703374923\C,0,-1.74
45289137,-1.0211559922,-1.7392516126\H,0,0.0417094911,0.1082534494,-2.
2806223841\H,0,-0.1189150074,-1.473645826,-3.0176953421\H,0,-2.3040246
711,-0.6419931477,-2.6035584735\C,0,-2.3163254506,-0.320657203,-0.4644
214026\N,0,-0.2862191827,1.2173728775,1.1653139877\C,0,-1.1904831127,1

.9147080937,0.3321915679\C,0,-2.0824995184,1.2145478415,-0.5192073522\
C,0,-1.1803697229,3.3186040011,0.3675965599\C,0,-2.8499498493,1.985682
5406,-1.4062053051\C,0,-1.9649971986,4.0480426356,-0.5171490516\H,0,-0
.5116964952,3.8075302572,1.0687536234\C,0,-2.7862262734,3.3768074477,-
1.4281665384\H,0,-3.5415418322,1.4793294981,-2.0740634489\H,0,-1.93171
85154,5.1341320162,-0.5024449862\H,0,-3.3957639228,3.9344637852,-2.133
6192402\H,0,-1.9785937701,-2.0879951818,-1.671503877\C,0,-1.7258298217
,-0.9715434147,0.7900786388\C,0,-2.1702285613,-0.7124877047,2.23113300
54\C,0,-1.6849958156,-2.4791347158,1.0512120081\C,0,-2.5117171259,-2.2
230173052,2.3426780283\H,0,-2.9786995701,0.00409921,2.3975419514\H,0,-
1.328445298,-0.430072272,2.8698476067\H,0,-2.1208242753,-3.1402283516,
0.293932777\H,0,-0.6778084383,-2.8413278588,1.2908116662\H,0,-3.576699
1271,-2.415046977,2.1874579238\H,0,-2.1742598322,-2.7385151315,3.24678
83906\C,0,-3.8582735872,-0.5864454925,-0.370851448\C,0,-4.4728357049,-
1.6984956925,-0.9699768497\C,0,-4.6787031587,0.2597694215,0.399805804\
C,0,-5.838137831,-1.9512638956,-0.8103068736\H,0,-3.9008924764,-2.3847
405956,-1.5825174231\C,0,-6.0388887623,0.007178917,0.5651724725\H,0,-4
.251985513,1.1432294334,0.8617369423\C,0,-6.6301194747,-1.1030637572,-
0.0402145965\H,0,-6.2779224818,-2.8180650811,-1.2970352039\H,0,-6.6383
894615,0.6868701955,1.1653013539\H,0,-7.6915158931,-1.2998095242,0.083
849212\C,0,1.9716183205,-3.2838704294,1.6521858638\N,0,2.7651358463,-2
.8128390963,0.9164672873\\Version=ES64L-G16RevA.03\State=3-A\HF=-1498.
4057708\S2=2.041257\S2-1=0.\S2A=2.001062\RMSD=4.301e-09\Dipole=0.05389
69,0.183932,-1.4390115\Quadrupole=12.7650469,-0.7906246,-11.9744223,-0
.8976382,-2.5821995,6.6804988\PG=C01 [X(C36H30N2)]\\@

^{3}IntD'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\08-Apr-2020\0\\#p
M06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti
tle Card Required\\0,3\C,0,-1.3864127008,0.6272924541,-1.1232459589\C,

0,-1.2459293479,1.3002441783,1.3682797725\C,0,-0.3858387893,2.5289204024,0.9826898708\C,0,0.7916266006,2.2933481461,-0.0227241213\C,0,3.5386174228,-2.7182456986,1.7041038861\C,0,-0.0201861322,0.0826945517,-0.7904912089\C,0,-2.0947529059,-0.1362742639,-2.3030803258\C,0,-2.5251369982,1.2129435005,-2.9206070499\C,0,-1.5346714976,1.9335238418,-1.9765264079\C,0,-2.1238901155,0.5568336365,0.2780357029\N,0,0.0026453761,-1.2982575278,-0.5924886796\C,0,-2.9984195299,-1.5080940878,1.5533973315\C,0,-2.9307683465,-2.8643691935,1.9035848509\C,0,-1.9366649078,-3.6904771529,1.3577862988\C,0,-0.9998740776,-3.1524873624,0.4959051713\C,0,-2.0905623424,-0.9348255464,0.6699295873\C,0,-1.0231982644,-1.7677465941,0.1561550446\C,0,-6.169352768,2.2042162636,-0.0425423114\C,0,-5.1258960129,2.9796321742,0.4590348865\C,0,-3.8420973599,2.4437660009,0.5805345562\C,0,-3.5548834266,1.1214228804,0.2028241442\C,0,-4.6260113276,0.355644641,-0.2948060111\C,0,-5.9104435636,0.8853055235,-0.416712408\H,0,-7.169972618,2.6176873153,-0.1345088385\H,0,-5.3055335076,4.0074730518,0.7636530229\H,0,-3.0599358342,3.0773162222,0.98143811\H,0,-4.4628693167,-0.6788014756,-0.5747515766\H,0,-6.7111728458,0.258999227,-0.801608747\C,0,1.0587904421,0.8339429524,-0.3723941403\N,0,3.4894321306,-2.3681693516,0.5770606562\C,0,3.4199379246,-2.0076148668,-0.7577261945\C,0,2.3672038377,0.2360535506,-0.1732702586\C,0,2.8335991883,-0.7766157332,-1.1443883019\C,0,3.8961237,-2.9205315096,-1.7075523494\C,0,3.7919179593,-2.637476518,-3.0654413376\C,0,3.2004386996,-1.4392567755,-3.4743699894\C,0,2.7306536946,-0.5346800379,-2.5275259094\C,0,4.6886616622,0.7054452362,0.644570028\C,0,5.5686598635,1.1495544007,1.6249903771\C,0,5.0876803371,1.5976689959,2.8587579615\C,0,3.7107452439,1.5901114226,3.0995161364\C,0,2.8276082598,1.1491119267,2.1200258886\H,0,5.0770518502,0.3736085598,-0.3135149793\H,0,6.6371423687,1.1503090221,1.4251746543\H,0,5.7770431552,1.9400326791,3.6255571974\H,0,3.3249885835,1.9148995859,4.0625137252\H,0,1.7649853114,1.1098398124,2.3384312987\C,0,3.2898312315,0.6986532084,0.8604066686\H,0,4.3295002305,-3.852907428,-1

.3601797515\H,0,4.1644547165,-3.3487347431,-3.7967777166\H,0,3.1141600
131,-1.2056446602,-4.532056779\H,0,2.2816250001,0.399213492,-2.8506312
472\H,0,-2.3484558275,1.3372537607,-3.9934053875\H,0,-3.5672862722,1.4
610360755,-2.7059959583\H,0,-0.6004813937,2.173765462,-2.4912790849\H,
0,-1.900060934,2.8301304726,-1.4698393759\H,0,-1.3587175919,-0.6649373
384,-2.9160493985\H,0,-2.8840105339,-0.8446355144,-2.042034784\H,0,0.0
392852527,2.893421382,1.9266082793\H,0,-1.0116953044,3.3459598446,0.60
96869542\H,0,0.5885867215,2.8470215304,-0.9446520125\H,0,1.7032977843,
2.7354127225,0.3832917525\H,0,-0.5653268918,0.5588702486,1.7977585558\
H,0,-1.9117001406,1.5851308892,2.1909116095\H,0,-3.7913607249,-0.89599
27907,1.9723081419\H,0,-3.6600077868,-3.2739752887,2.5970030414\H,0,-1
.8945063394,-4.7429145186,1.6236607943\H,0,-0.194039284,-3.7488372662,
0.0800876439\\Version=ES64L-G16RevA.03\State=3-A\HF=-1498.4668036\S2=2
.064669\S2-1=0.\S2A=2.002684\RMSD=5.147e-09\Dipole=-1.4013983,1.025646
6,-0.9646198\Quadrupole=2.0878177,0.0029817,-2.0907994,3.6337755,-10.9
155696,8.3776293\PG=C01 [X(C36H30N2)]\\@

^{3}TS5'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\01-Apr-2020\0\\#p
M06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti
tle Card Required\\0,3\C,0,0.0091340075,0.0374156575,-0.0101391148\C,0
,-0.0116351498,-0.0114192896,2.5977054505\C,0,1.5394788217,-0.01169220
27,2.5712499325\C,0,2.2059315906,-1.3107370778,2.0279048673\C,0,0.4713
279556,-1.3918305226,0.2803128393\C,0,-0.7524452541,0.1778711217,-1.38
208122\C,0,0.0997900666,1.4199191052,-1.7313741222\C,0,1.0239984554,1.
1094837158,-0.5286149083\C,0,-0.8293595993,0.3837130419,1.2893215791\N
,0,-0.4069337143,-2.2950087083,0.5462515765\C,0,-3.3079336878,-0.31967
23456,1.7092197242\C,0,-4.321783008,-1.2801225883,1.6184849791\C,0,-4.
0508569554,-2.5379846257,1.0788675298\C,0,-2.7551534001,-2.8492067793,
0.6717219306\C,0,-2.0215590913,-0.5878975488,1.2403020845\C,0,-1.73878
27797,-1.8906939514,0.7559671029\C,0,-1.8952403562,4.6313298947,1.2306

49215\C,0,-0.8177458629,4.1798959075,1.9903207094\C,0,-0.4955330584,2.
8217248849,2.0221842526\C,0,-1.2333418072,1.8684038981,1.2993179801\C,
0,-2.3139999063,2.3490597282,0.5362497065\C,0,-2.6415977235,3.70488944
41,0.5025460039\H,0,-2.1517359134,5.6869831014,1.2083274588\H,0,-0.221
2327239,4.8831241225,2.5658571711\H,0,0.3514237764,2.5121008005,2.6245
231134\H,0,-2.9242234067,1.6545779742,-0.0291131751\H,0,-3.4890138783,
4.0333250639,-0.0938285879\C,0,1.9150283405,-1.6618950521,0.573340174\
C,0,2.0309052552,-3.6654953952,-1.6880401611\C,0,2.94227492,-1.6135086
711,-0.5450961135\C,0,2.641338015,-2.3772854538,-1.7538349727\C,0,1.65
73385813,-4.3638654857,-2.837280024\C,0,1.8870335388,-3.8058023785,-4.
0913669542\C,0,2.5110606516,-2.553386322,-4.192637883\C,0,2.8870997448
,-1.8601759638,-3.0500295173\C,0,4.3814385742,0.2701430682,0.356562026
6\C,0,5.6049193042,0.9255513443,0.4156569871\C,0,6.6960248675,0.471924
923,-0.3316402159\C,0,6.5392571209,-0.6565405773,-1.1446027845\C,0,5.3
183602459,-1.3115034563,-1.2154850951\H,0,3.5535794862,0.6658982268,0.
9275460141\H,0,5.7071890537,1.803362084,1.0485008532\H,0,7.6528393476,
0.9830954096,-0.2759367655\H,0,7.3815149277,-1.036207056,-1.7171245804
\H,0,5.23156089,-2.2061274927,-1.8216183713\C,0,4.1851984585,-0.870058
0895,-0.4702608463\H,0,1.2029715766,-5.3435124037,-2.7281667396\H,0,1.
5890827936,-4.3433293148,-4.9867776295\H,0,2.6930555577,-2.1150171361,
-5.1698965421\H,0,3.3508231842,-0.8829118734,-3.1412039423\H,0,0.57799
41435,1.4126918702,-2.7156578057\H,0,-0.4482252494,2.3582063143,-1.615
7645037\H,0,1.9724715984,0.6744745492,-0.8427769362\H,0,1.2317463812,1
.9467966495,0.1418251723\H,0,-0.5503186931,-0.6772679191,-2.0340116238
\H,0,-1.8346890738,0.3133766224,-1.3343658121\H,0,1.8786012883,0.08361
18997,3.6114026583\H,0,1.9192247763,0.8746929557,2.0524018718\H,0,3.28
6381764,-1.2660072436,2.1963072422\H,0,1.8305372424,-2.1408967031,2.63
71515175\H,0,-0.3265719241,-1.0139956445,2.9006679993\H,0,-0.355061084
3,0.6487095194,3.399895629\H,0,-3.534707482,0.6529187607,2.1343807739\
H,0,-5.3204555189,-1.0405173034,1.9738601866\H,0,-4.8377605678,-3.2837

618657,1.0046109207\H,0,-2.4984144877,-3.8396159872,0.3076914209\C,0,1
.9311894484,-3.9108773657,0.7285634861\N,0,1.8866097726,-4.2254873871,
-0.4313350321\\Version=ES64L-G16RevA.03\State=3-A\HF=-1498.4320695\S2=
2.038637\S2-1=0.\S2A=2.000967\RMSD=7.438e-09\Dipole=0.5309503,1.796636
1,-0.9114328\Quadrupole=5.3098414,-7.1675363,1.857695,3.7090556,-1.668
4623,12.4895981\PG=C01 [X(C36H30N2)]\\@

^{3}IntE'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\01-Apr-2020\0\\#p
M06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti
tle Card Required\\0,3\C,0,-1.0108201394,0.2130348199,-0.393098809\C,0
,-1.782395859,0.8983392835,1.9826469507\C,0,-0.4245813662,1.6344776037
,2.1170079332\C,0,0.8297574215,0.7330283725,2.2457842945\C,0,-0.131162
0711,-0.6809302852,0.4697442963\C,0,-1.3106199775,-0.434052566,-1.8003
016812\C,0,-0.979960092,0.9067862601,-2.4938833291\C,0,-0.4237239618,1
.4478410263,-1.154837156\C,0,-2.2713838119,0.4575023337,0.5374906014\N
,0,-0.6130754402,-1.7760315365,0.9377088636\C,0,-4.2630865163,-1.19386
68714,0.8764273714\C,0,-4.7312911279,-2.5022180925,1.042230447\C,0,-3.
8344728496,-3.5704854581,1.0765082236\C,0,-2.465716504,-3.3245666457,0
.9882051966\C,0,-2.9015340667,-0.934312097,0.7161677329\C,0,-1.9942355
398,-2.018318407,0.8175041265\C,0,-4.8960349228,3.4355363999,-1.312569
0053\C,0,-4.0147589929,3.8002859915,-0.2966609045\C,0,-3.194394896,2.8
434738964,0.3043135939\C,0,-3.2231617866,1.4935852556,-0.0858027309\C,
0,-4.1182707383,1.1503567963,-1.1163095421\C,0,-4.9415310958,2.1020094
852,-1.718958827\H,0,-5.5394416687,4.1769932567,-1.7783008512\H,0,-3.9
615284115,4.8335109824,0.0367254678\H,0,-2.5215616255,3.1696613117,1.0
89820095\H,0,-4.1903859255,0.1202296991,-1.4451213585\H,0,-5.624163045
7,1.7935352014,-2.5066321564\C,0,1.2204690963,-0.2321519523,1.07047312
21\C,0,2.7671326887,-2.1871128311,-0.3252152396\C,0,2.3093863678,0.219
5522289,0.0592477454\C,0,2.751235945,-0.8520322996,-0.8242131413\C,0,3

.1626458255,-3.2535354058,-1.1325913943\C,0,3.5329814726,-3.0226245981
,-2.4562338012\C,0,3.5406321957,-1.7159957947,-2.9653319396\C,0,3.1700
634035,-0.6463498082,-2.1584273674\C,0,2.4791542025,2.7377402488,0.423
4137508\C,0,3.24154515,3.9015019691,0.4331374979\C,0,4.5981699598,3.86
83992557,0.1034911588\C,0,5.1817821032,2.6453627124,-0.2384838321\C,0,
4.4231334625,1.4813972352,-0.2544408218\H,0,1.4264029737,2.8104239116,
0.6537015036\H,0,2.7675192853,4.8442768095,0.6939107182\H,0,5.19090022
33,4.7787152016,0.1161638663\H,0,6.2395652113,2.5950457227,-0.48320521
71\H,0,4.9048818962,0.5393061186,-0.4901741356\C,0,3.0395652495,1.4838
81916,0.0743357973\H,0,3.177735235,-4.2511389723,-0.7045019884\H,0,3.8
236033516,-3.8556374246,-3.090368391\H,0,3.8340586315,-1.5360297483,-3
.9958587672\H,0,3.1745495096,0.3628684845,-2.560065128\H,0,-0.26486297
25,0.8541187683,-3.3202798573\H,0,-1.8692649559,1.4431146009,-2.833910
4159\H,0,0.664954016,1.4697311739,-1.14389803\H,0,-0.7954916134,2.4279
708093,-0.8477400082\H,0,-0.5906075771,-1.2241903809,-2.0323065274\H,0
,-2.3130004821,-0.839692495,-1.9499200122\H,0,-0.4610451775,2.21344267
02,3.0494581896\H,0,-0.312516923,2.373801523,1.3195548714\H,0,1.695470
282,1.353516134,2.4980802466\H,0,0.6582855186,0.078077665,3.1069164922
\H,0,-1.7340601563,0.0053849856,2.6125419455\H,0,-2.572941144,1.513601
7511,2.422237109\H,0,-4.9741367219,-0.3741495704,0.8544520619\H,0,-5.7
982548064,-2.6801074772,1.1468525442\H,0,-4.1970771112,-4.5871616039,1
.2015280636\H,0,-1.7387792906,-4.1268444572,1.0724927565\C,0,1.8499132
424,-1.5016736285,1.6545681195\N,0,2.4634358438,-2.3875712645,1.038008
5917\\Version=ES64L-G16RevA.03\State=3-A\HF=-1498.4654022\S2=2.048701\
S2-1=0.\S2A=2.001464\RMSD=5.073e-09\Dipole=-0.4226305,1.8306291,-0.990
5983\Quadrupole=3.4136948,2.0744445,-5.4881394,4.4757499,-5.3352648,9.
0187622\PG=C01 [X(C36H30N2)]\\@

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\01-Apr-2020\0\\#p
M06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti

tle Card Required\\0,3\C,0,-0.2090846182,-0.0941244296,-0.105281699\C,
0,0.2124536123,-0.0725556052,2.4862740676\C,0,1.7094124761,-0.38800829
67,2.224847191\C,0,2.0337850485,-1.8689239249,1.8842915555\C,0,0.04953
1099,-1.5599919212,0.1029911844\C,0,-1.1700698322,0.1554597723,-1.3360
769308\C,0,-0.2212689903,1.2643101374,-1.8460314408\C,0,0.8497452177,0
.7741841825,-0.8430961576\C,0,-0.7618119117,0.369702679,1.3068589652\N
,0,-0.8046418533,-2.3480955812,0.5765934625\C,0,-3.1709159878,-0.02577
58588,2.2290601816\C,0,-4.2684825248,-0.8717217925,2.4264309144\C,0,-4
.2439432889,-2.1801532199,1.9451746862\C,0,-3.1035175795,-2.6545105518
,1.2978208529\C,0,-2.0446919231,-0.4582295381,1.5266522976\C,0,-2.0116
808105,-1.8082177839,1.0967643335\C,0,-1.283814586,4.7128540929,1.1696
901023\C,0,-0.1188909918,4.1500104845,1.6890456876\C,0,0.0279598667,2.
7635599084,1.7514774116\C,0,-0.978549899,1.892537823,1.2987214806\C,0,
-2.1410420664,2.4830519164,0.770052232\C,0,-2.2941188021,3.868901314,0
.709223346\H,0,-1.403375933,5.7919286195,1.1255829128\H,0,0.6829474651
,4.7883830152,2.0509957403\H,0,0.9503911552,2.3623777224,2.1579631847\
H,0,-2.9486157078,1.8560703903,0.4104974053\H,0,-3.2112568353,4.286052
7262,0.301303681\C,0,2.032128048,-2.3100522423,0.4145933812\C,0,2.4003
622325,-3.7224596218,-2.0174164323\C,0,3.0620176389,-1.8765259922,-0.5
048923736\C,0,3.1570225185,-2.5259769708,-1.7855199976\C,0,2.441756635
,-4.3716194342,-3.2622619578\C,0,3.234016811,-3.8735781216,-4.28296031
59\C,0,4.0253612527,-2.7288858765,-4.0605155468\C,0,3.9999981922,-2.07
93734788,-2.8406951171\C,0,4.2599626912,0.3868961654,-0.7014536288\C,0
,5.2934067886,1.2452665046,-0.3209154196\C,0,6.2116348604,0.8559948927
,0.654006686\C,0,6.0953799348,-0.4072621585,1.2358118347\C,0,5.0621134
058,-1.2624582285,0.8549552339\H,0,3.5659347936,0.7082200202,-1.469506
3532\H,0,5.379549811,2.2202039176,-0.7936858225\H,0,7.0153886546,1.524
8925759,0.9494124591\H,0,6.8157976985,-0.7345647183,1.9808739829\H,0,5
.0041361646,-2.2557721036,1.2905477869\C,0,4.1109293963,-0.8792024733,
-0.1095066903\H,0,1.8490305126,-5.2728072946,-3.3855662405\H,0,3.26116

29011,-4.3741854772,-5.2469119093\H,0,4.6674042977,-2.3547101221,-4.85
34629568\H,0,4.6277546721,-1.2089985818,-2.6857588589\H,0,0.0515659934
,1.2207332229,-2.9047525002\H,0,-0.5874923477,2.2680757282,-1.61782300
66\H,0,1.5789918356,0.1223881979,-1.3249794962\H,0,1.3764098745,1.5359
518626,-0.2646573529\H,0,-1.1983106997,-0.7178716971,-1.9940527908\H,0
,-2.1980295889,0.4383535605,-1.1024754289\H,0,2.2366362114,-0.16598184
36,3.1613021296\H,0,2.1484507591,0.2810307286,1.4799887514\H,0,3.02162
27289,-2.0967210658,2.2989698668\H,0,1.3289423477,-2.5180356525,2.4133
931676\H,0,-0.2193651224,-0.9615235138,2.9545533206\H,0,0.1446886041,0
.705118849,3.2526742084\H,0,-3.2035937761,0.9846683882,2.6235365772\H,
0,-5.1384189967,-0.5025223136,2.9629079003\H,0,-5.0963338354,-2.836981
9662,2.0954981291\H,0,-3.029922045,-3.6825354654,0.9562508171\C,0,1.59
70175447,-3.6609773847,0.1137820031\N,0,1.6852074924,-4.2918684934,-0.
9694983187\\Version=ES64L-G16RevA.03\State=3-A\HF=-1498.4282902\S2=2.0
72757\S2-1=0.\S2A=2.00288\RMSD=3.618e-09\Dipole=0.5516676,2.2003533,0.
109985\Quadrupole=8.1995938,-9.8480054,1.6484116,1.591025,0.3512977,0.
8582569\PG=C01 [X(C36H30N2)]\\@

^{3}TS6'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\01-Apr-2020\0\\#p
M06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti
tle Card Required\\0,3\C,0,-0.2090846182,-0.0941244296,-0.105281699\C,
0,0.2124536123,-0.0725556052,2.4862740676\C,0,1.7094124761,-0.38800829
67,2.224847191\C,0,2.0337850485,-1.8689239249,1.8842915555\C,0,0.04953
1099,-1.5599919212,0.1029911844\C,0,-1.1700698322,0.1554597723,-1.3360
769308\C,0,-0.2212689903,1.2643101374,-1.8460314408\C,0,0.8497452177,0
.7741841825,-0.8430961576\C,0,-0.7618119117,0.369702679,1.3068589652\N
,0,-0.8046418533,-2.3480955812,0.5765934625\C,0,-3.1709159878,-0.02577
58588,2.2290601816\C,0,-4.2684825248,-0.8717217925,2.4264309144\C,0,-4
.2439432889,-2.1801532199,1.9451746862\C,0,-3.1035175795,-2.6545105518

,1.2978208529\C,0,-2.0446919231,-0.4582295381,1.5266522976\C,0,-2.0116
808105,-1.8082177839,1.0967643335\C,0,-1.283814586,4.7128540929,1.1696
901023\C,0,-0.1188909918,4.1500104845,1.6890456876\C,0,0.0279598667,2.
7635599084,1.7514774116\C,0,-0.978549899,1.892537823,1.2987214806\C,0,
-2.1410420664,2.4830519164,0.770052232\C,0,-2.2941188021,3.868901314,0
.709223346\H,0,-1.403375933,5.7919286195,1.1255829128\H,0,0.6829474651
,4.7883830152,2.0509957403\H,0,0.9503911552,2.3623777224,2.1579631847\
H,0,-2.9486157078,1.8560703903,0.4104974053\H,0,-3.2112568353,4.286052
7262,0.301303681\C,0,2.032128048,-2.3100522423,0.4145933812\C,0,2.4003
622325,-3.7224596218,-2.0174164323\C,0,3.0620176389,-1.8765259922,-0.5
048923736\C,0,3.1570225185,-2.5259769708,-1.7855199976\C,0,2.441756635
,-4.3716194342,-3.2622619578\C,0,3.234016811,-3.8735781216,-4.28296031
59\C,0,4.0253612527,-2.7288858765,-4.0605155468\C,0,3.9999981922,-2.07
93734788,-2.8406951171\C,0,4.2599626912,0.3868961654,-0.7014536288\C,0
,5.2934067886,1.2452665046,-0.3209154196\C,0,6.2116348604,0.8559948927
,0.654006686\C,0,6.0953799348,-0.4072621585,1.2358118347\C,0,5.0621134
058,-1.2624582285,0.8549552339\H,0,3.5659347936,0.7082200202,-1.469506
3532\H,0,5.379549811,2.2202039176,-0.7936858225\H,0,7.0153886546,1.524
8925759,0.9494124591\H,0,6.8157976985,-0.7345647183,1.9808739829\H,0,5
.0041361646,-2.2557721036,1.2905477869\C,0,4.1109293963,-0.8792024733,
-0.1095066903\H,0,1.8490305126,-5.2728072946,-3.3855662405\H,0,3.26116
29011,-4.3741854772,-5.2469119093\H,0,4.6674042977,-2.3547101221,-4.85
34629568\H,0,4.6277546721,-1.2089985818,-2.6857588589\H,0,0.0515659934
,1.2207332229,-2.9047525002\H,0,-0.5874923477,2.2680757282,-1.61782300
66\H,0,1.5789918356,0.1223881979,-1.3249794962\H,0,1.3764098745,1.5359
518626,-0.2646573529\H,0,-1.1983106997,-0.7178716971,-1.9940527908\H,0
,-2.1980295889,0.4383535605,-1.1024754289\H,0,2.2366362114,-0.16598184
36,3.1613021296\H,0,2.1484507591,0.2810307286,1.4799887514\H,0,3.02162
27289,-2.0967210658,2.2989698668\H,0,1.3289423477,-2.5180356525,2.4133
931676\H,0,-0.2193651224,-0.9615235138,2.9545533206\H,0,0.1446886041,0

.705118849,3.2526742084\H,0,-3.2035937761,0.9846683882,2.6235365772\H,
0,-5.1384189967,-0.5025223136,2.9629079003\H,0,-5.0963338354,-2.836981
9662,2.0954981291\H,0,-3.029922045,-3.6825354654,0.9562508171\C,0,1.59
70175447,-3.6609773847,0.1137820031\N,0,1.6852074924,-4.2918684934,-0.
9694983187\\Version=ES64L-G16RevA.03\State=3-A\HF=-1498.4282902\S2=2.0
72757\S2-1=0.\S2A=2.00288\RMSD=3.618e-09\Dipole=0.5516676,2.2003533,0.
109985\Quadrupole=8.1995938,-9.8480054,1.6484116,1.591025,0.3512977,0.
8582569\PG=C01 [X(C36H30N2)]\\@

^{3}IntF'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\01-Apr-2020\0\\#p
M06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti
tle Card Required\\0,3\C,0,1.5910507331,0.7881734782,-0.6078371685\C,0
,1.4893265995,-0.7644148242,1.5037988919\C,0,0.1246995064,-1.411911474
,1.1427900379\C,0,-1.0783162077,-0.5307159726,1.5479898656\C,0,-2.7988
834458,-1.0933855564,-0.2320911618\C,0,1.0609281399,1.9285379978,0.220
6006311\C,0,2.2758246163,1.4607260273,-1.8627647313\C,0,0.9425465255,1
.2924647001,-2.6280126105\C,0,0.544619466,0.2007858954,-1.6078002844\C
,0,2.415127936,-0.1351649605,0.3891409767\N,0,1.6485024272,2.524746970
3,1.1375660803\C,0,4.5906801934,0.3389350622,1.7211135705\C,0,5.369631
7379,1.1651143014,2.5365373226\C,0,4.9296785858,2.4478272577,2.8631945
136\C,0,3.6984735648,2.8927013479,2.3856482867\C,0,3.3701793893,0.7759
146512,1.1968162291\C,0,2.9257426267,2.0655922323,1.5684824186\C,0,4.5
804638279,-3.1579135047,-1.923038372\C,0,3.4289583004,-3.5031145532,-1
.2195012764\C,0,2.7424669172,-2.5449889214,-0.468679455\C,0,3.17969375
33,-1.2128079744,-0.4006583992\C,0,4.353546861,-0.8902095052,-1.109226
9694\C,0,5.0425133311,-1.8425343762,-1.8587495178\H,0,5.1156515777,-3.
9026673477,-2.5058015019\H,0,3.0572834251,-4.524203551,-1.2463133007\H
,0,1.8587218195,-2.8590959599,0.0722992005\H,0,4.7517369413,0.11732278
21,-1.0516359121\H,0,5.9473346045,-1.5539946429,-2.3874729059\C,0,-2.4

00422042,-1.1281591113,1.1323916256\N,0,-3.8490027717,-1.5621047328,-0
.7617692972\C,0,-4.7664917914,-2.2036851963,0.0428804683\C,0,-3.294265
7801,-1.7726737217,1.9808012815\C,0,-4.5126505013,-2.3253543679,1.4445
925613\C,0,-5.9489962499,-2.7322836824,-0.5192579812\C,0,-6.8705020575
,-3.3693521341,0.2857289566\C,0,-6.6360896694,-3.4932862748,1.67339842
02\C,0,-5.4860778456,-2.98378391,2.2410767455\C,0,-2.4520762647,-3.079
8338275,3.9620087873\C,0,-2.1811614109,-3.1988804087,5.3260190636\C,0,
-2.4646327095,-2.1416505102,6.1923414286\C,0,-3.021615894,-0.964936138
4,5.6882219346\C,0,-3.2924529823,-0.8448372857,4.3244547937\H,0,-2.233
0495523,-3.9051345695,3.2895956452\H,0,-1.7480320342,-4.1183968691,5.7
107485224\H,0,-2.2529609042,-2.2341408075,7.2541076132\H,0,-3.24630722
22,-0.1377985318,6.3562786167\H,0,-3.7267319746,0.0716604813,3.9341354
147\C,0,-3.0081178359,-1.9001368479,3.4451645475\H,0,-6.1008353616,-2.
6177406655,-1.5879675471\H,0,-7.7810902211,-3.7761351886,-0.1456384446
\H,0,-7.3697716691,-3.9933430716,2.2996998446\H,0,-5.3160953209,-3.081
8255323,3.3081756967\H,0,0.3058230766,2.1780077869,-2.5406527694\H,0,1
.0048939596,1.0001577354,-3.6801392406\H,0,-0.4991231789,0.1576453566,
-1.2864030727\H,0,0.8563040624,-0.7896644217,-1.9523941827\H,0,2.68491
71065,2.4661929489,-1.7274956226\H,0,3.0452869632,0.8097549015,-2.2801
828212\H,0,0.0344756992,-2.3693460056,1.67251073\H,0,0.0476651707,-1.6
490120613,0.0794571269\H,0,-1.0559699444,-0.373473126,2.6305394808\H,0
,-0.9735230618,0.4580173246,1.0834436665\H,0,1.29229498,0.0215007424,2
.2393142806\H,0,2.1159961601,-1.4941578233,2.0282149075\H,0,4.94614902
86,-0.6589724638,1.4850951089\H,0,6.3185970684,0.7984524574,2.91851941
6\H,0,5.5339869336,3.0927070961,3.495282454\H,0,3.3113068995,3.8753023
167,2.637534462\\Version=ES64L-G16RevA.03\State=3-A\HF=-1498.4599152\S
2=2.018742\S2-1=0.\S2A=2.000205\RMSD=3.994e-09\Dipole=0.5068086,-1.311
2908,0.9580673\Quadrupole=6.926678,-7.6197181,0.6930401,4.6314978,-9.2
253968,-0.4916873\PG=C01 [X(C36H30N2)]\\@

^{3}TS7'

1\1\GINC-OM103\SP\UM06\6-311+G(d,p)\C36H30N2(3)\WEIY\01-Apr-2020\0\\#p
M06/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Ti
tle Card Required\\0,3\C,0,-0.0639940237,-0.034997905,-0.044928972\C,0
,0.0067455287,-0.0317911774,2.5677843303\C,0,1.54866078,-0.004628196,2
.7014867109\C,0,2.1080767817,-1.3373172651,3.2272254357\C,0,1.50915128
58,-2.5367027391,0.9866432948\C,0,-0.1887268728,-1.5383357161,0.006541
4262\C,0,-0.6457245764,0.4017703362,-1.4447920342\C,0,0.7931395716,0.3
764254005,-2.0106089299\C,0,1.3226500871,0.4624534259,-0.5594722821\C,
0,-0.7275226094,0.527243675,1.2939337578\N,0,-1.2660634238,-2.13813669
58,0.3365464221\C,0,-3.1907196245,0.4910970186,2.0980729444\C,0,-4.391
5680415,-0.1891860373,2.3260872125\C,0,-4.5449062828,-1.5093075595,1.8
944064988\C,0,-3.4924243832,-2.144719146,1.2465168058\C,0,-2.125011877
9,-0.1142545446,1.4287491143\C,0,-2.2826071506,-1.4669121774,1.0172002
086\C,0,-0.8454510028,4.8964951807,1.0915083842\C,0,0.1498214129,4.250
9327669,1.8220938683\C,0,0.1789332901,2.856346903,1.9010308649\C,0,-0.
7807293606,2.0614695919,1.2544430912\C,0,-1.7789304377,2.7363065358,0.
5250216701\C,0,-1.8134614269,4.1278108557,0.4437532573\H,0,-0.87055512
86,5.9811614978,1.0306845688\H,0,0.9107634185,4.8298388724,2.339426302
3\H,0,0.9669527478,2.3928478028,2.4805499078\H,0,-2.5567920555,2.16424
27682,0.0305456351\H,0,-2.6042213887,4.610165002,-0.1251855147\C,0,2.2
57746813,-2.4512079705,2.2043942833\N,0,1.6796328136,-3.4054611527,0.0
682079074\C,0,2.6219395631,-4.3887150913,0.1945256874\C,0,3.2091505866
,-3.4568126163,2.3867972476\C,0,3.4107861281,-4.4607211666,1.381004136
2\C,0,2.7950781668,-5.3360469567,-0.8412901241\C,0,3.7250010513,-6.343
4898133,-0.7026517603\C,0,4.5032429335,-6.4362547636,0.4749440968\C,0,
4.3509054944,-5.5204087474,1.49450225\C,0,5.3814060269,-3.0792000973,3
.6110190063\C,0,6.1549422161,-3.1177387518,4.7720713172\C,0,5.60400726
77,-3.5839513096,5.9671395464\C,0,4.2749536645,-4.010425577,5.99542704
26\C,0,3.499386681,-3.9665223937,4.8362910903\H,0,5.8133099395,-2.7184

970238,2.6812200199\H,0,7.1890646611,-2.7848576048,4.7413070964\H,0,6.
2071593509,-3.6160408005,6.8704319996\H,0,3.8399713227,-4.3789861635,6
.9206554557\H,0,2.4659664417,-4.3020589353,4.8601714286\C,0,4.04259031
77,-3.499593817,3.6303430896\H,0,2.1735914215,-5.2416260963,-1.7261150
519\H,0,3.8589197709,-7.0745810416,-1.4952856602\H,0,5.2264870003,-7.2
406565373,0.577811796\H,0,4.9495654196,-5.6036995595,2.3953379576\H,0,
1.0353444568,-0.5860665716,-2.4695907086\H,0,1.0724433388,1.1826168139
,-2.6957013209\H,0,2.1884910022,-0.1562358992,-0.3107916248\H,0,1.5136
76946,1.4968898712,-0.2588495769\H,0,-1.396629999,-0.2545098981,-1.892
8427997\H,0,-1.0303193737,1.4223437238,-1.4112330991\H,0,1.8444807947,
0.7721531726,3.416782506\H,0,2.0429743893,0.247243159,1.762388329\H,0,
3.0931824533,-1.1598609903,3.671047349\H,0,1.4766641011,-1.6807167333,
4.0604764561\H,0,-0.3035827194,-1.0757921945,2.6571941431\H,0,-0.44243
20873,0.4729443224,3.4318605313\H,0,-3.0868873066,1.5113050765,2.45377
64101\H,0,-5.2019270513,0.3146330688,2.8460718753\H,0,-5.4775739797,-2
.0390780566,2.0689178967\H,0,-3.5698056077,-3.1719900478,0.9035511944\
\Version=ES64L-G16RevA.03\State=3-A\HF=-1498.4419468\S2=2.022901\S2-1=
0.\S2A=2.000297\RMSD=9.425e-09\Dipole=1.2485755,0.5509369,1.2652094\Qu
adrupole=3.038046,1.4191794,-4.4572253,-8.6986957,3.1681823,-2.8469648
\PG=C01 [X(C36H30N2)]\\@

[1]P

1\1\GINC-OM103\SP\RM06\6-311+G(d,p)\C36H30N2\WEIY\01-Apr-2020\0\\#p M0
6/6-311+g(d,p) geom=check scrf=(iefpcm,SMD,solvent=1,4-Dioxane)\\Title
Card Required\\0,1\C,0,-3.5949359942,-1.8826259889,-2.8524252133\C,0,
-3.3645964891,-3.8174471174,-1.1159747792\C,0,-2.6278364558,-2.8712663
948,-0.1267629963\C,0,-1.1068529487,-2.6457100554,-0.4053197564\C,0,-1
.1143926138,-1.1881070534,-2.5071044408\C,0,-2.1145282241,-2.142772005
8,-3.0841534386\C,0,-4.2497990711,-1.2471827649,-4.1439485015\C,0,-4.8
695420159,-0.1221335882,-3.2838222578\C,0,-4.0219604364,-0.5894440263,

-2.0752120376\C,0,-4.1845814536,-3.2564169852,-2.3576826583\N,0,-1.694
7273373,-3.1574792908,-3.7474296645\C,0,-4.6969956861,-5.3506914218,-3
.8193897984\C,0,-4.3266196886,-6.2409022639,-4.8333757334\C,0,-3.12627
36086,-6.0616022278,-5.5202497862\C,0,-2.2825205483,-5.0108046553,-5.1
651804831\C,0,-3.8950576092,-4.2555243585,-3.4929440738\C,0,-2.6513031
694,-4.1138614314,-4.1569894371\C,0,-8.4217595442,-2.7143991195,-1.391
1551222\C,0,-7.4549610237,-2.694581502,-0.3874589327\C,0,-6.1086525848
,-2.8910884335,-0.7002572815\C,0,-5.6799723857,-3.111131112,-2.0205839
446\C,0,-6.6737756916,-3.1247636284,-3.0165742665\C,0,-8.0211824925,-2
.9314570021,-2.7093479371\H,0,-9.4710025638,-2.5668057208,-1.150230071
5\H,0,-7.7437067278,-2.5277959799,0.6471565751\H,0,-5.3861356811,-2.86
70769332,0.1085380223\H,0,-6.3985795574,-3.3086349484,-4.0485596595\H,
0,-8.7585219343,-2.9562880794,-3.5076825468\C,0,-0.6811420108,-1.39491
47208,-1.156443374\N,0,-0.7535039127,-0.1814298026,-3.2736649987\C,0,0
.1110687481,0.7388426508,-2.7554008618\C,0,0.182063934,-0.4526917643,-
0.6110182393\C,0,0.6028142685,0.6569453661,-1.4164546162\C,0,0.5118622
806,1.8170447593,-3.5857302744\C,0,1.3653957763,2.7861342991,-3.108938
6391\C,0,1.8474102688,2.7160136096,-1.7802446711\C,0,1.4753665485,1.67
88704644,-0.9525733277\C,0,-0.1096421506,-0.1759925647,1.8769919118\C,
0,0.3666713194,-0.2747861182,3.1851333949\C,0,1.6502446784,-0.76630414
54,3.4289746094\C,0,2.4555742245,-1.1565554695,2.3574444199\C,0,1.9803
657191,-1.0555013913,1.0491136399\H,0,-1.108265559,0.2098043419,1.6894
50894\H,0,-0.2657159272,0.0340593556,4.0133373804\H,0,2.0209396332,-0.
844148522,4.4474699487\H,0,3.4558936393,-1.5408739661,2.5385229734\H,0
,2.6093260306,-1.3598256736,0.216788555\C,0,0.6900600093,-0.5677089863
,0.7931787079\H,0,0.1192654991,1.8423109312,-4.5974799769\H,0,1.669207
714,3.6097378869,-3.7494375585\H,0,2.5158425086,3.4884818082,-1.409553
4199\H,0,1.8482141149,1.6342247128,0.0651878595\H,0,-4.6850728894,0.89
88628176,-3.630685698\H,0,-5.9433525207,-0.2497410851,-3.1234246135\H,
0,-3.1808192742,0.0738482664,-1.8624225733\H,0,-4.5786934083,-0.750344

6142,-1.1497851281\H,0,-3.4806804034,-0.8822093785,-4.8302859425\H,0,-
4.9364965366,-1.8814462042,-4.7073564257\H,0,-2.6860994665,-3.35037696
,0.8585685615\H,0,-3.1349636354,-1.9093245154,-0.0134002442\H,0,-0.587
8520251,-2.6472545495,0.5553842129\H,0,-0.7272978221,-3.5173844957,-0.
9550459258\H,0,-2.6119638719,-4.5086119886,-1.5047396477\H,0,-4.057633
9263,-4.4510925635,-0.5539689402\H,0,-5.6292478664,-5.5117174498,-3.28
7671916\H,0,-4.9780801384,-7.0758769944,-5.0775061467\H,0,-2.836581206
3,-6.7497110476,-6.3097971127\H,0,-1.3187000169,-4.87009247,-5.6452758
459\\Version=ES64L-G16RevA.03\State=1-A\HF=-1498.6008307\RMSD=5.363e-0
9\Dipole=-0.3762731,0.2924243,1.6259911\Quadrupole=4.5447152,-5.417802
1,0.8730869,5.7450268,7.1844476,1.9425058\PG=C01 [X(C36H30N2)]\\@

(J) References

(1) Kim, J. M. Beebe, Y. Jun, X. Y. Zhu, C. D. Frisbie, *J. Am. Chem. Soc.* **2006**, *128*, 4970.

(2) X. Fan, R. Liu, Y. Wei, M. Shi, *Org. Chem. Front*. **2019**, *6*, 2667.

(3) (a) K. Chen, Z. Zhang, Y. Wei, M. Shi, *Chem. Commun.* **2012**, *48*, 7696; (b) K. Chen, R. Sun, Q. Xu, Y. Wei, M. Shi, *Org. Biomol. Chem.* **2013**, *11*, 3949.