Supporting Information

A Practical Method for Transforming Alkynes into α-Diketones

Zhonghui Wan, Chauncey D. Jones, David Mitchell, John Y. Pu, and Tony Y. Zhang*

Chemical Process R & D, Eli Lilly and Company, Lilly Corporate Cente, Indianapolis, IN 46285, USA

wanzh@lilly.com

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General Consideration: All reactions were carried out under nitrogen unless otherwise noted. Solvents and chemicals were used from vendors without further purification. Flash chromatography[1] was performed on silica gel 60 (Merck, 230-400). **^{1}H NMR** were recorded on 500 MHz spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CHCl_3$: δ 7.27 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet), coupling constants (Hz), integration. **^{13}C NMR** spectra were recorded on 125 MHz spectrometers with complete proton decoupling. Chemical shifts are reported in ppm from tetramethylsilane with the solvent as the internal standard ($CDCl_3$: δ 77.23 ppm). **HRMS** was recorded on LCT-TOF mass spec using APcI (+) ionization.

Experimental

General Procedure for Oxidation of Alkynes to α-Dicarbonyl Compounds: The alkyne substrate 2.0 mmol was mixed with 2.0 mL of 88% formic acid, 2.0 mmol (4.0 mmol if there is a basic N in the molecule) of methanesulfonic acid, 12.0 mmol of DMSO, and 0.20 mmol of 48% HBr in a 10 mL flask. The reactions were heated at 105~110 °C using a short path to distill off the volatiles (mostly dimethyl sulfide generated from the reaction, and some solvents) until complete conversion (usually 5-10 hours). After completion, the reaction was cooled down to room temperature. The crude product was extracted into ethyl acetate after aqueous workup. Flash chromatography on silica gel afforded the pure product.

Benzil (2a):[2] General procedure was followed employing 355 mg (2.0 mmol) of diphenylacetylene. Purification by flash chromatography (10% ethyl acetate in hexane) gave 318.2 mg (82%) of the title compound.

1-(4-Methoxy-phenyl)-2-p-tolyl-ethane-1,2-dione (2b): General procedure was followed employing 470 mg (2.2 mmol) of 1-(4-methoxy-phenyl)-2-p-tolyl-ethyne. Purification by flash chromatography (50% dichloromethane in hexane) gave 320 mg (56%) of the title compound. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 2.43 (s, 3H), 3.89 (s, 3H,), 6.97 (d, *J* = 8.5 Hz, 2H), 7.30 (d, *J* = 8.5 Hz, 2H), 7.87 (d, *J* = 8.5 Hz, 2H), 7.94 (d, *J* = 8.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ 21.9, 55.6, 114.3, 126.2, 129.9, 130.8, 132.3, 146.0, 164.9, 193.4, 194.6. **HRMS** $(M+H)^+$ calcd for $C_{16}H_{15}O_3$ 255.1021, found 255.1028. **IR** (KBr, cm^{-1}): 1670, 1665, 1600.

1-(6-Methoxy-2-naphthyl)-2-p-tolyl-ethane-1,2-dione (2c): General procedure was followed employing 550 mg (2.0 mmol) of 1-(6-methoxy-naphthyl)-2-p-tolyl-ethyne. Purification by flash chromatography (10% ethyl acetate in hexane) gave 405 mg (66%) of the title compound. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 2.44 (s, 3H), 3.95 (s, 3H,), 7.17 (d, *J* = 3.0 Hz, 1H), 7.20 (dd, *J* = 8.5, 3.0 Hz, 1H), 7.32 (d, *J* = 9.0 Hz, 2H), 7.80 (d, *J* = 8.5 Hz, 1H), 7.82 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 9.0 Hz, 2H), 8.05 (dd, *J* = 9.0, 1.5 Hz, 1H), 8.32 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ 21.9, 55.5, 106.0, 120.0, 124.6, 127.7, 127.76, 128.570, 129.7 (2C), 130.1 (2C), 130.8, 131.5, 133.2, 138.3, 146.1, 160.6, 194.6 (2C). **HRMS** $(M+H)^+$ calcd for $C_{20}H_{17}O_3$ 305.1178, found 305.1188. **IR** (KBr, cm^{-1}): 1660, 1625, 1603.

2-Bromo-3,3-dimethyl-1-p-tolyl-butan-1-one (2d): General procedure was initially followed employing 505 mg (2.9 mmol) of 1-(3,3-Dimethyl-but-1-ynyl)-4-methyl-benzene, but the reaction stopped after formation of about 10% of bromoketone as indicated by LC-MS. Another 3.0 mmol of 48% HBr and 3 mL of DMSO were added. The reaction was continued until complete conversion. Purification by flash chromatography (5% dichloromethane in hexane) gave 590 mg (75%) of the title compound. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 1.21 (s, 3H), 2.37 (s, 3H), 5.14 (s, 1H), 7.23 (d, *J* = 8.5 Hz, 2H), 7.87 (d, *J* = 8.5 Hz, 2H).. **^{13}C NMR** (125 MHz, $CDCl_3$): δ 21.7, 27.4, 35.1, 57.7, 128.7, 129.5, 133.6, 144.4, 193.8. **HRMS** $(M+H)^+$ calcd for $C_{13}H_{18}BrO$ 269.0541, found 269.0523. **IR** (KBr, cm^{-1}): 1669, 1604.

3,3-Dimethyl-1-(4-trifluoromethyl-phenyl)-butane-1,2-dione (2e): General procedure was followed employing 501 mg (2.2 mmol) of 1-(3,3-Dimethyl-but-1-ynyl)-4-trifluoromethyl-benzene. Purification by flash chromatography (5% dichloromethane in hexane) gave 450 mg (79%) of the title compound. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 1.30 (s, 9H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.94 (d, *J* = 8.0 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ 26.0, 42.7, 122.2, 124.4, 125.9 (d), 129.8, 135.5 (t), 193.8, 209.7. **HRMS** $(M+H)^+$ calcd for $C_{13}H_{14}F_3O_2$ 259.0946, found 259.0942. **IR** (KBr, cm^{-1}): 1690, 1686.

1-(4-Methoxy-phenyl)-2-(4-trifluoromethyl-phenyl)-ethane-1,2-dione (2f): General procedure was followed employing 499 mg (1.81 mmol) of 4-(4-trifluoromethyl-phenylethynyl)-anisole. Purification by flash chromatography (45% dichloromethane in

hexane) gave 320 mg (57%) of the title compound. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 6.9 (d, *J* = 9.0 Hz, 2H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.93 (d, *J* = 9.0 Hz, 2H), 8.08 (d, *J* = 8.0 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ 55.6, 114.5, 122.3, 124.5, 125.6, 125.9, 130.2, 132.5, 135.8, 165.3, 191.9, 193.3. **HRMS** $(M+H)^+$ calcd for $C_{16}H_{12}F_3O_3$ 309.0739, found 309.0746. **IR** (KBr, cm^{-1}): 1680, 1654, 1601.

1-(4-Chloro-phenyl)-2-phenyl-ethane-1,2-dione (2g):[3] General procedure was followed employing 497 mg (2.3 mmol) of 1-chloro-4-phenylethynyl-benzene. Purification by flash chromatography (45% dichloromethane in hexane) gave 458 mg (80%) of the title compound. **^{1}H NMR (**500 MHz, $CDCl_3$**):** d 7.45 (d, *J* = 8.0 Hz, 2H), 7.48 (t, *J* = 8.0 Hz, 2H), 7.63 (t, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 8.5 Hz, 2 H), 7.94 (d, *J* = 7.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$**):** d 129.1, 129.4, 129.9, 131.2, 131.4, 132.8, 135.1, 141.5, 193.0, 193.8. **IR** (KBr, cm^{-1}): 1668, 1587.

1-(4-Methanesulfonyl-phenyl)-2-phenyl-ethane-1,2-dione (2h): General procedure was followed employing 255 mg (1.0 mmol) of 1-methanesulfonyl-4-phenylethynyl-benzene. Purification by flash chromatography (60% dichloromethane in hexane) gave 190 mg (66%) of the title compound. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 3.07 (s, 3H), 7.52 (t, *J* = 7.5 Hz, 2H), 7.68 (t, *J* = 8.0 Hz, 1H), 7.96 (d, *J* = 7.5 Hz, 2H), 8.07 (d, *J* = 8.5 Hz, 2H), 8.15 (d, *J* = 8.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ 44.2, 128.1, 129.2, 130.0,

130.7, 132.4, 135.4, 136.8, 145.6, 192.5, 193.1. **HRMS** $(M+H)^+$ calcd for $C_{15}H_{13}O_4S$ 289.0534, found 289.0522. **IR** (KBr, cm^{-1}): 1683, 1675, 1596.

1-(4-Fluoro-phenyl)-2-(4-trifluoromethyl-phenyl)-ethane-1,2-dione (2i): General procedure was followed employing 530 mg (2.0 mmol) of (4-fluoro-phenyl)-ethynyl-4-trifluoromethyl-benzene. Purification by flash chromatography (15% ethyl acetate in hexane) gave 552 mg (93%) of the title compound. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.22 (m, 2H), 7.80 (d, *J* = 7.5 Hz, 2H), 8.04 (m, 2H), 8.10 (d, *J* = 7.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ 116.5(d), 126.1, 130.3, 132.8, 132.9, 135.5, 166.0, 168.0, 191.5, 192.5, **HRMS** $(M+H)^+$ calcd for $C_{15}H_9F_4O_2$ 297.0539, found 297.0547. **IR** (KBr, cm^{-1}): 1670, 1664, 1598.

1-(Pyridin-3-yl)-2-*p*-tolyl-ethane-1,2-dione (2j): General procedure was followed employing 200.0 mg (1.03 mmol) of 1-(3-pyridinyl)-2-p-tolyl-ethyne. Purification by flash chromatography (30% ethyl acetate in hexane) gave 178.0 mg (76%) of the title compound. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 2.40 (s, 3H), 7.28 (d, *J* = 7.5 Hz, 2H), 7.43 (dd, *J* = 6.0, 5.0 Hz, 1H), 7.84 (d, *J* = 7.5 Hz, 2H), 8.24 (dd, *J* = 6.0, 2.5 Hz, 1H), 8.80 (dd, *J* = 5.0, 1.5 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ 21.9, 123.8, 128.7, 129.8, 130.0, 130.1, 136.8, 146.7, 151.3, 154.7, 192.6, 193.0. **HRMS** $(M+H)^+$ calcd for $C_{14}H_{12}NO_2$ 226.0868, found 226.0871. **IR** (KBr, cm^{-1}): 1666, 1604, 1582.

1-(Isoquinolin-7-yl)-2-*p*-tolyl-ethane-1,2-dione (2k): General procedure was followed employing 490 mg (2.0 mmol) of 7-(*p*-tolyl-ethynyl)-isoquinoline. Purification by flash chromatography (20% ethyl acetate in hexane) gave 458 mg (83%) of the title compound. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 2.46 (s, 3H); 7.34 (d, *J* = 8.5 Hz, 2H), 7.72 (d, *J* = 4.5 Hz, 1H), 7.93 (d, *J* = 8.5 Hz, 2H), 7.97 (d, *J* = 9.0 Hz, 1H), 8.32 (d, *J* = 9.0 Hz, 1H), 8.55 (s, 1H), 8.68 (d, *J* = 5.5 Hz, 1H), 9.33 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ 22.0, 120.4, 127.7, 127.8, 128.1, 129.8, 130.2, 130.4, 131.7, 132.8, 138.6, 146.2, 146.6, 154.2, 193.5, 193.6. **HRMS** $(M+H)^+$ calcd for $C_{18}H_{14}NO_2$, 276.0124, found 276.0124. **IR** (KBr, cm^{-1}): 1672, 1628, 1603.

1-Isoquinolin-7-yl-2-(4-trifluoromethyl-phenyl)-ethane-1,2-dione (2l): General procedure was followed employing 498 mg (1.68 mmol) of 7-(4-trifluoromethyl-phenylethynyl)-isoquinoline. Purification by flash chromatography (30% ethyl acetate in hexane) gave 291 mg (53%) of the title compound. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.81 (d, *J* = 6.0 Hz, 1H), 7.83 (d, *J* = 7.5 Hz, 2H), 8.04 (d, *J* = 9.0 Hz, 1H), 8.18 (d, *J* = 7.5 Hz, 2H), 8.38 (d, *J* = 9.0 Hz, 1H), 8.62 (s, 1H), 8.71 (d, *J* = 6.0 Hz, 1H), 9.39 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ 20.9, 120.4, 126.1, 126.1, 127.6, 128.0, 128.1, 130.4, 131.2, 133.09, 135.5, 138.8, 146.4, 154.2, 192.1, 192.3. **HRMS** $(M+H)^+$ calcd for $C_{18}H_{11}F_3NO_2$ 330.0742, found 330.0744. **IR** (KBr, cm^{-1}): 1678, 1656, 1626.

1-(3-Amino-phenyl)-2-p-tolyl-ethane-1,2-dione (2m): General procedure was followed employing 497 mg (2.4 mmol) of 3-*p*-tolylethynyl-phenylamine. Purification by flash chromatography (10% dichloromethane in hexane) gave 340 mg (59%) of the title compound. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 2.39 (s, 3H), 3.89 (brs, 2H), 6.88 (d, *J* = 7.5 Hz, 1H), 7.18-7.27 (m, 5H), 7.82 (d, *J* = 8.0 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ 21.9, 114.7, 120.3, 121.4, 129.7, 129.8, 129.9, 130.6, 133.9, 146.2, 147.3, 194.8, 195.4. **HRMS** $(M+H)^+$ calcd for $C_{15}H_{14}NO_2$ 240.1024, found 240.1017. **IR** (KBr, cm^{-1}): 3463, 3376, 1666, 1603.

4-[2-(2-Chloro-phenyl)-2-oxo-acetyl]-benzoic acid (2n): General procedure was initially followed employing 515 mg (2.0 mmol) of 4-(2-chloro-phenylethynyl)-benzoic acid. Purification by flash chromatography (5% dichloromethane in hexane) gave 435 mg (75%) of the title compound. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.60 (ddd, *J* = 7.5, 7.5, 2.0 Hz, 1H), 7.64 (dd, *J* = 7.5, 2.0 Hz, 1H), 7.75 (ddd, *J* = 7.5, 7.5, 2.0 Hz, 1H), 7.93 (dd, *J* = 7.5, 2.0 Hz, 1H), 8.12 (d, *J* = 7.5 Hz, 2H), 8.14 (d, *J* = 7.5 Hz, 2H), 13.48 (br, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ 128.7, 130.5, 130.6, 131.2, 132.7, 133.0, 133.4, 135.2, 136.4, 136.6, 166.8, 191.9, 193.4. **HRMS** $(M-H)^-$ calcd for $C_{15}H_{18}ClO_4$ 287.0117, found 287.0122. **IR** (KBr, cm^{-1}): 1685, 1680, 1583.

Phenylglyoxal (2o):[4] General procedure was initially followed employing 1.0 g (10.0 mmol) of phenylacetylene. The crude product was extracted into dichloromethane, purified by chromatography using 15~20% ethyl acetate in hexanes afforded the title compound 740 mg, 48% yield. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.05 (dd, *J* = 7.5, 1.0 Hz,

2H), 7.62 (dt, *J* = 1.0, 7.5 Hz, 1H), 7.50 (dd, *J* = 7.5, 7.5 Hz, 2H), 6.72 (d, *J* = 7.0 Hz, 2H), 5.67 (t, *J* = 7.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ 196.6, 134.1, 133.7, 129.8, 128.9, 89.6. **IR** (KBr, cm^{-1}): 3406, 1697, 1597.

References

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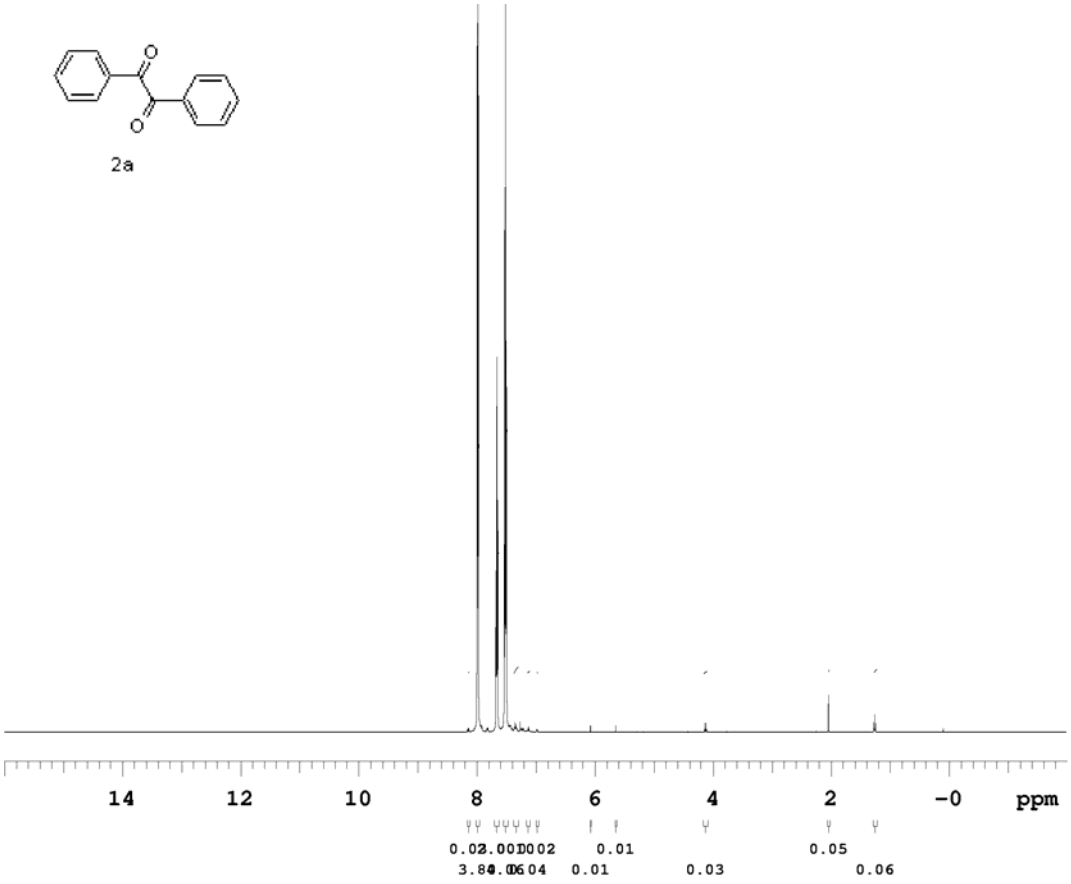
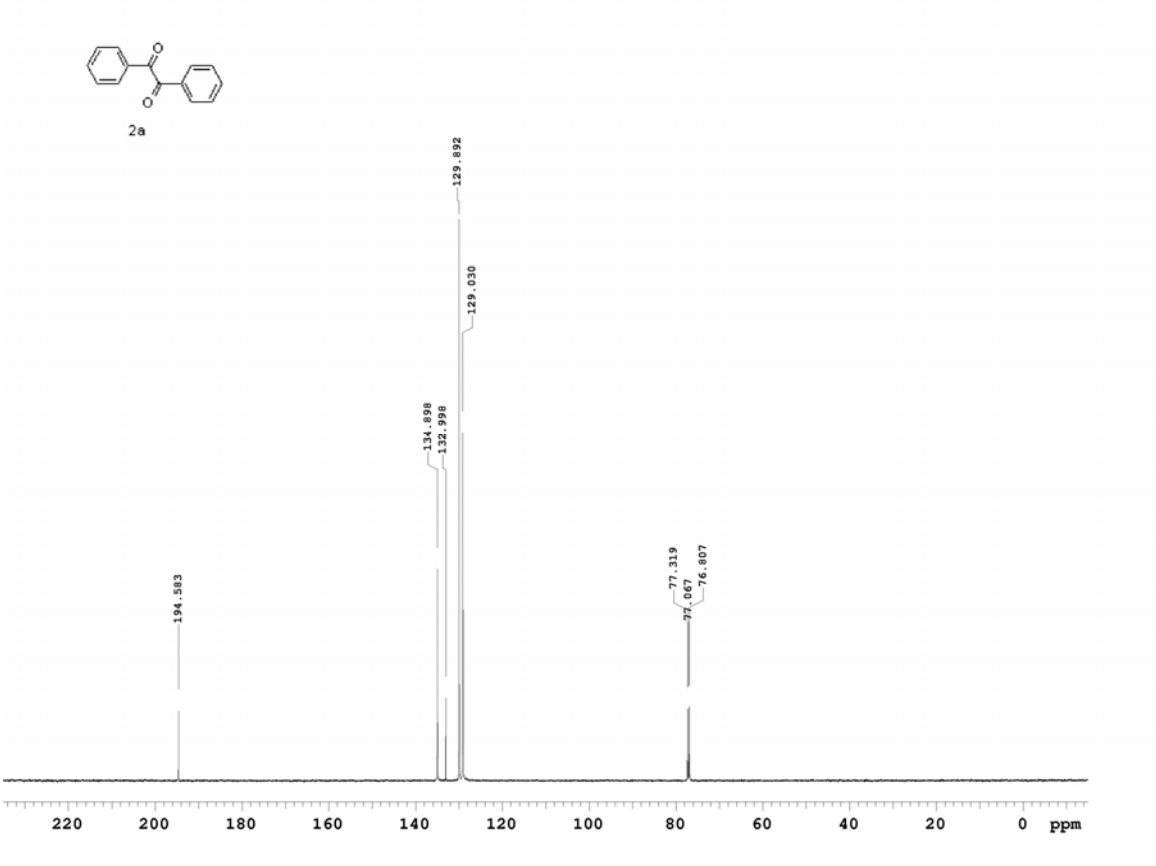
4. Meester, Johan W. G. De; Plas, Henk C. van der; Middelhoven, Wouter J.; *J. Heterocycl. Chem.* **1987**, *24*, 441-451.

NMR and IR Spectra

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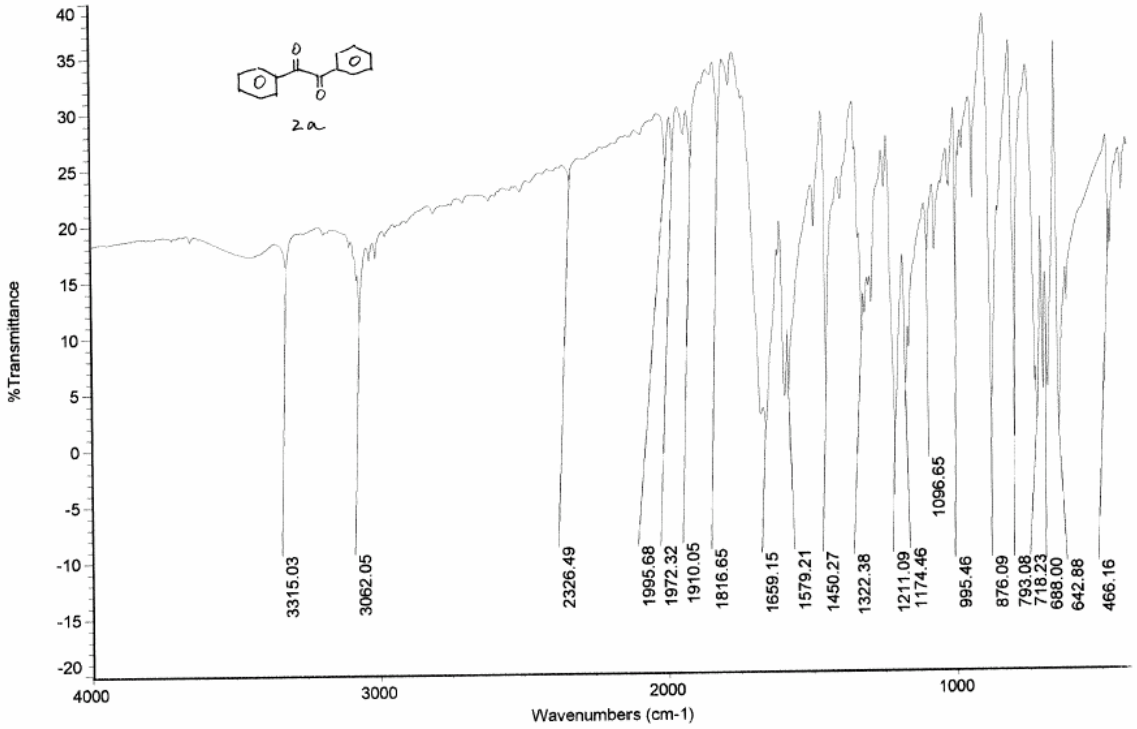
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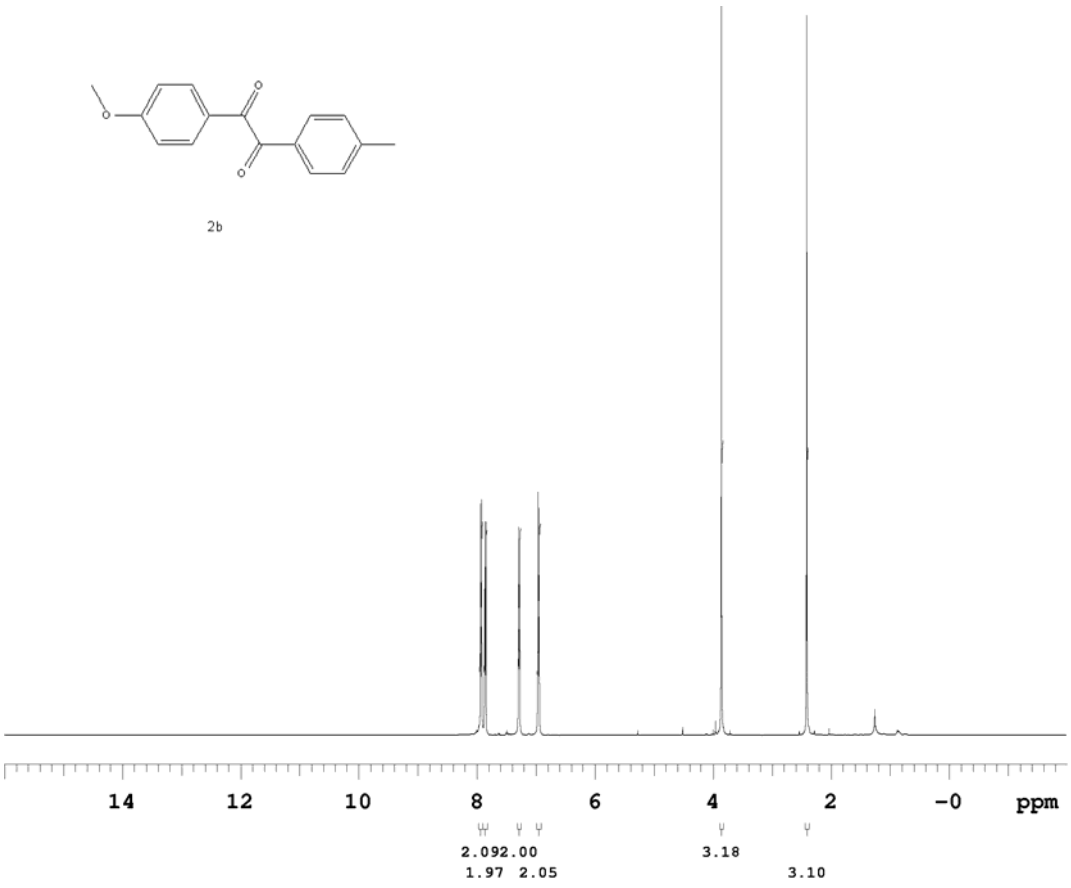
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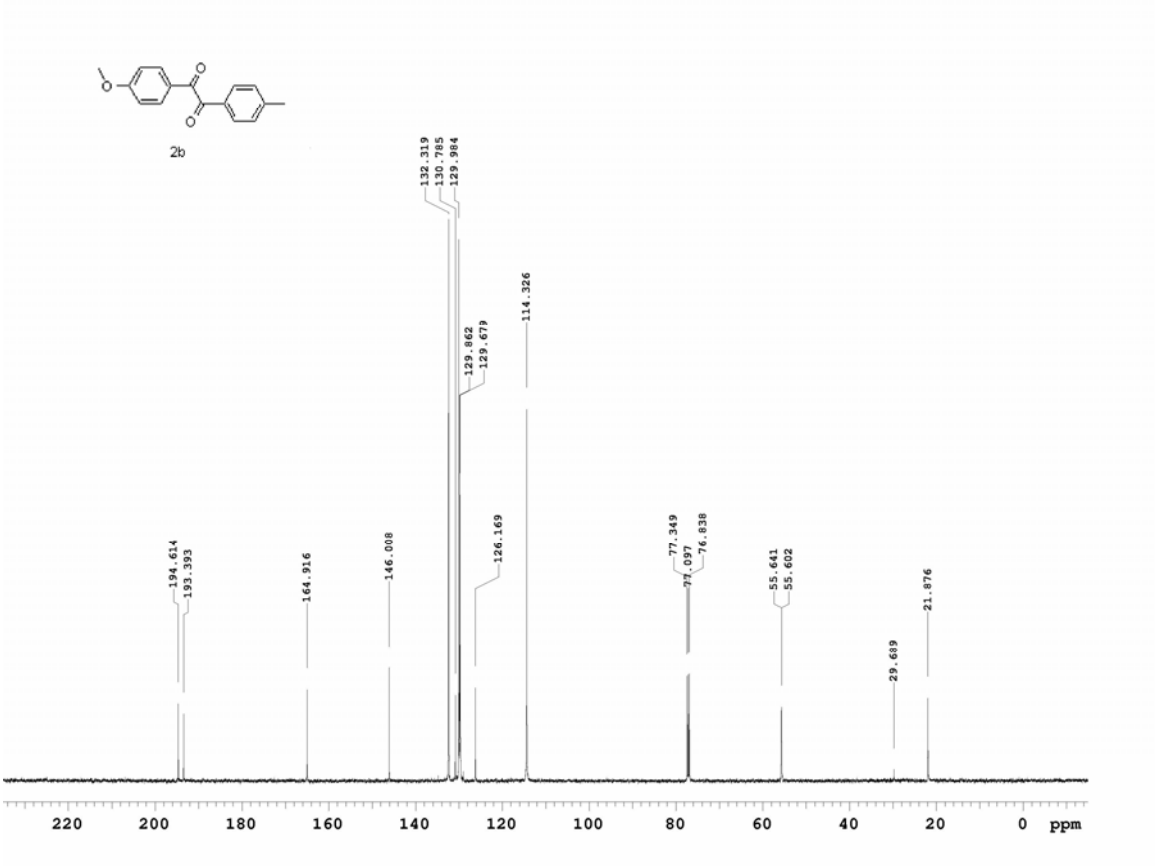
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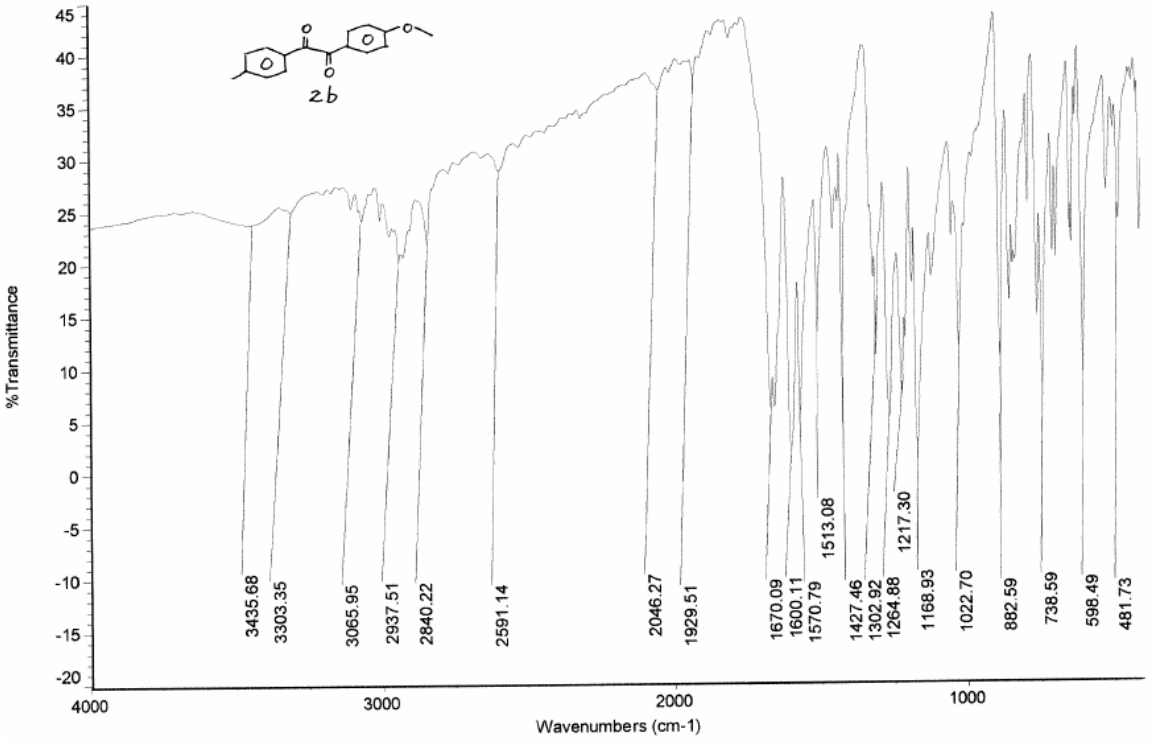
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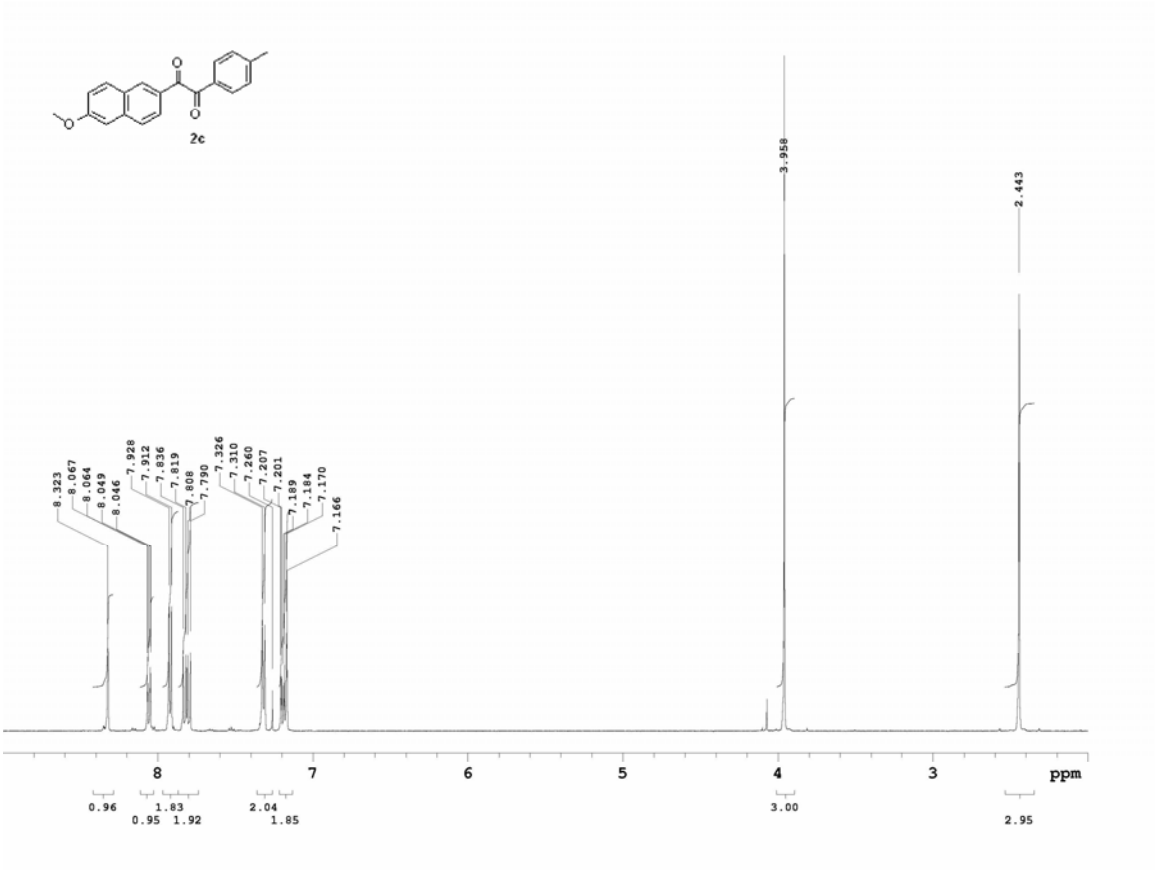
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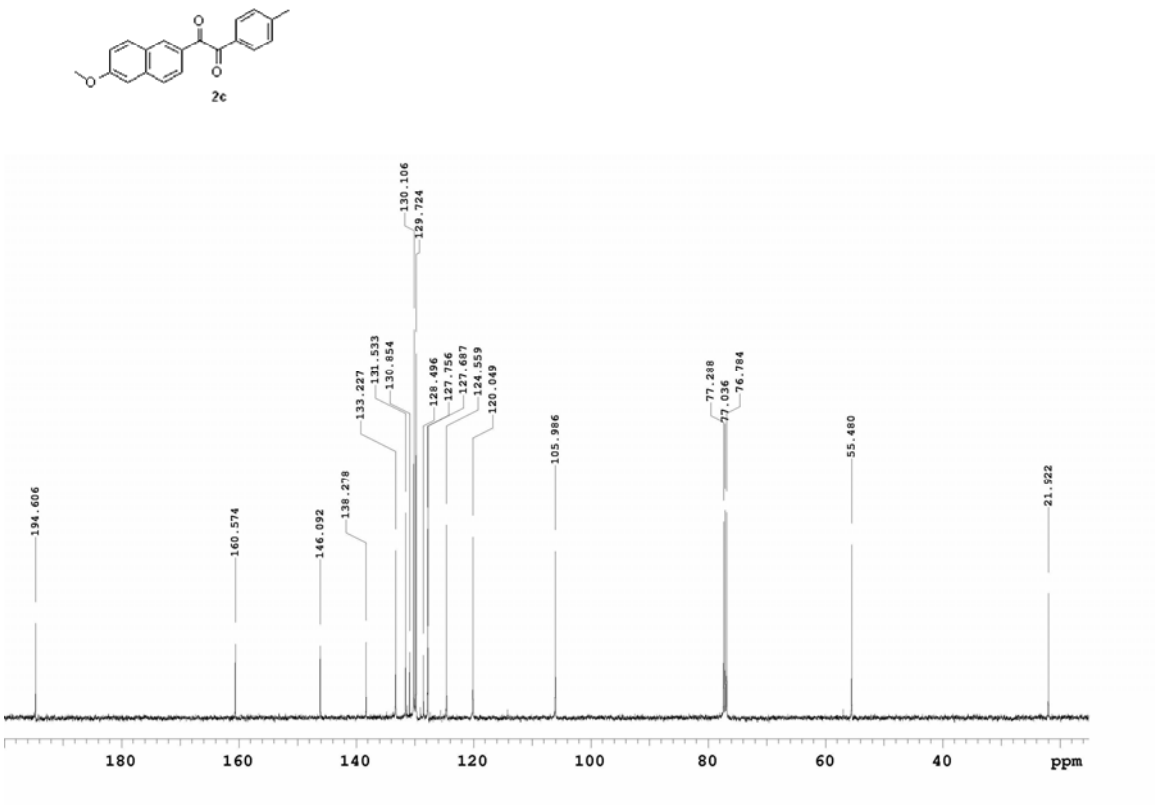
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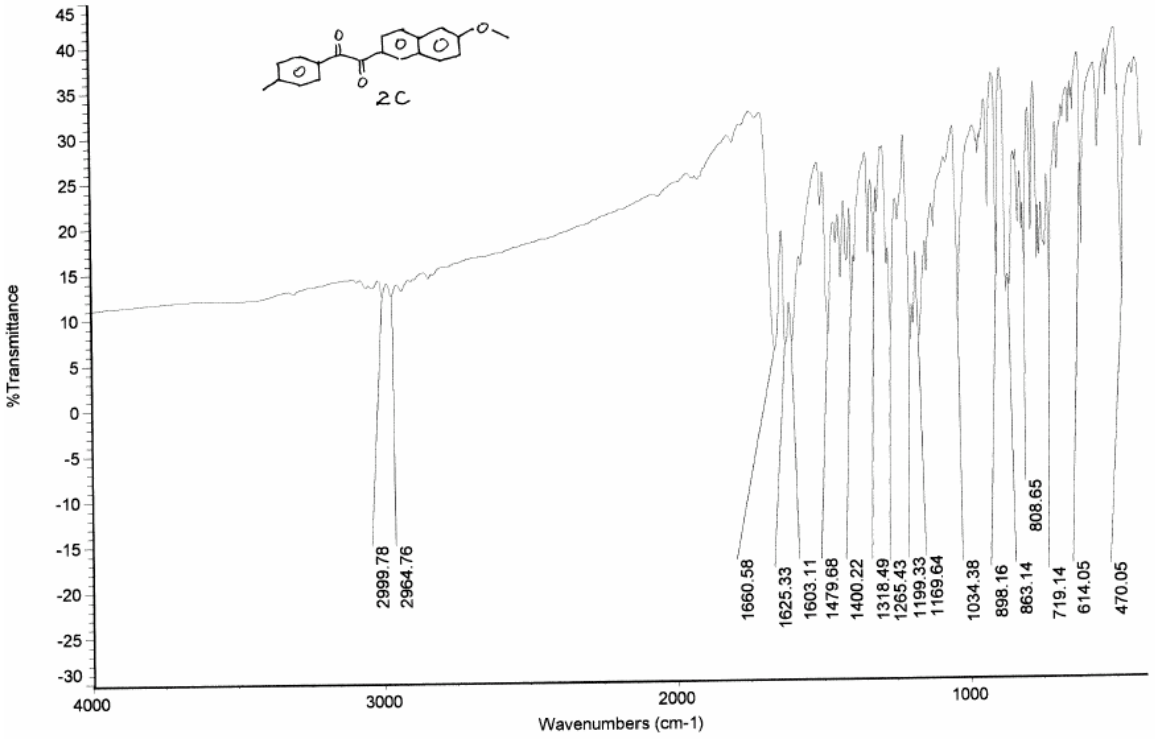
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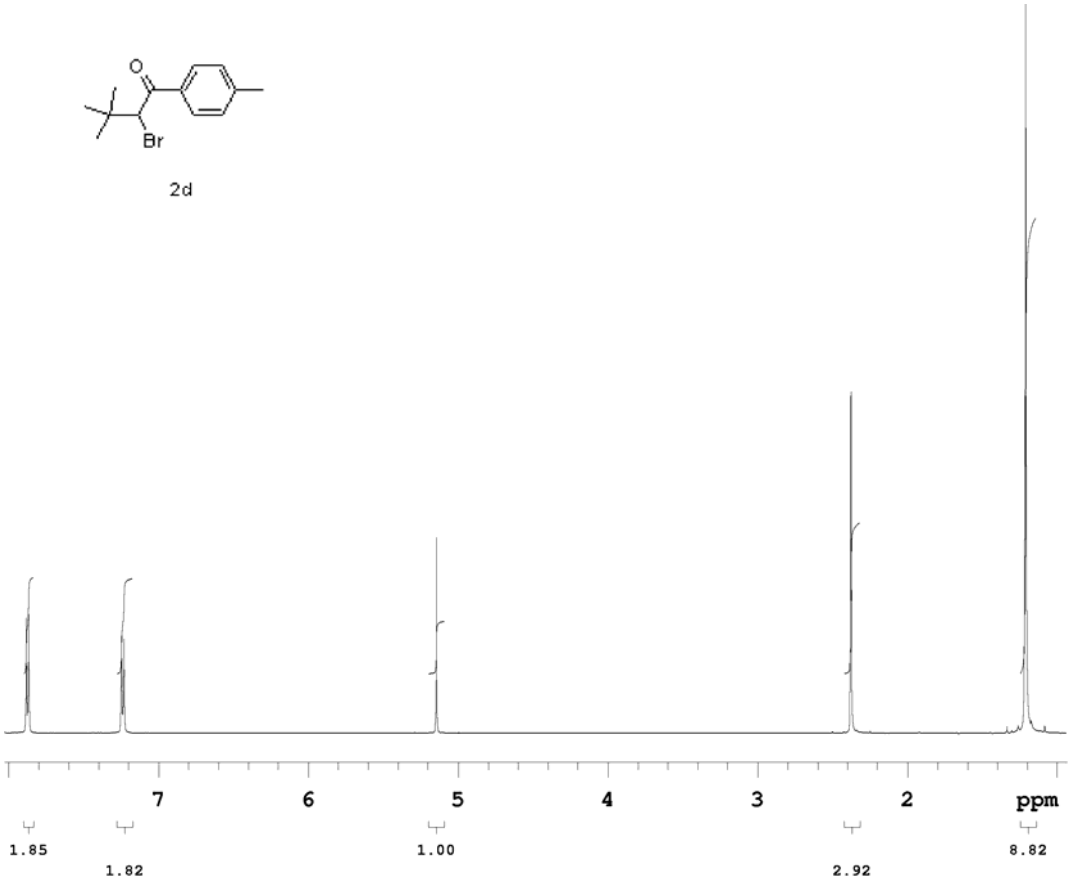
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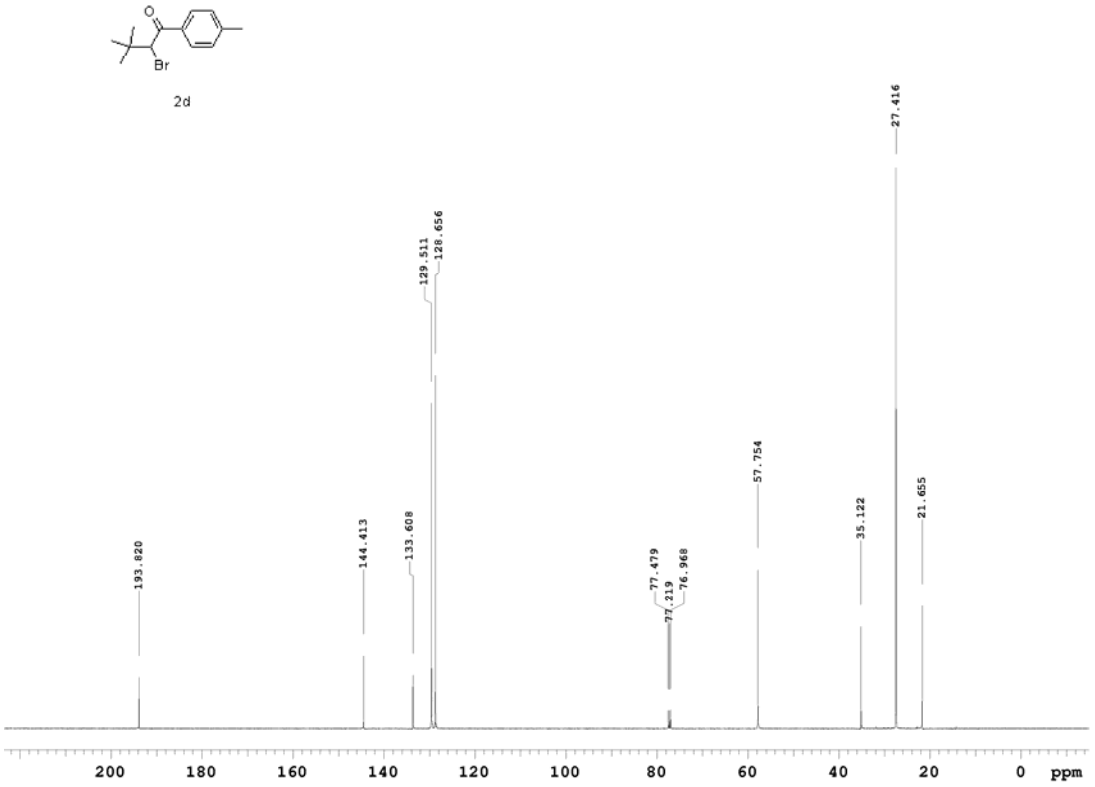
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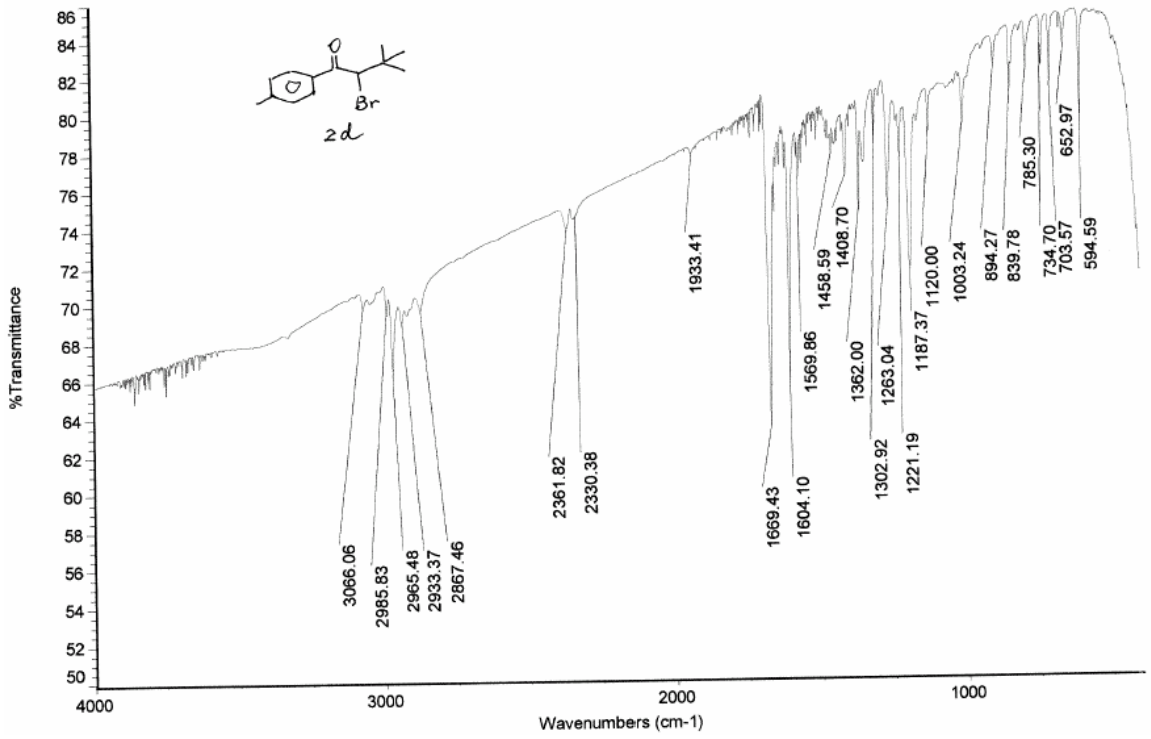
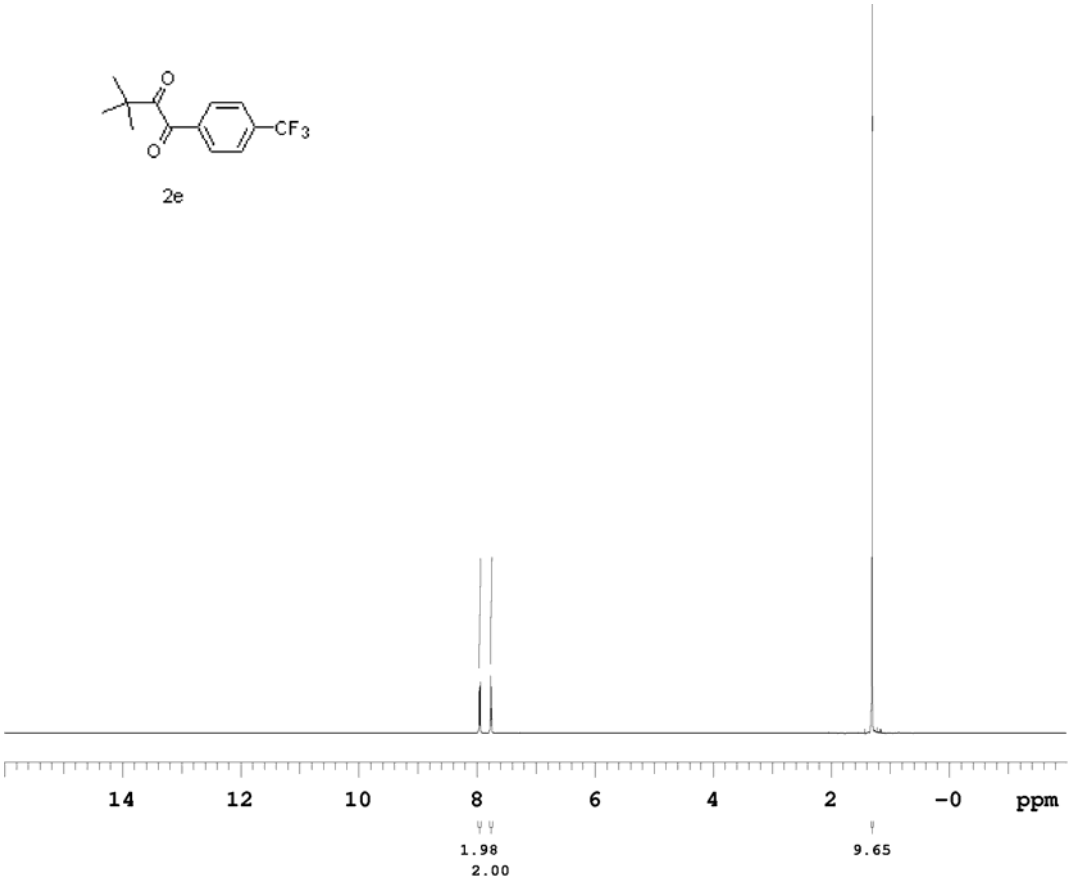
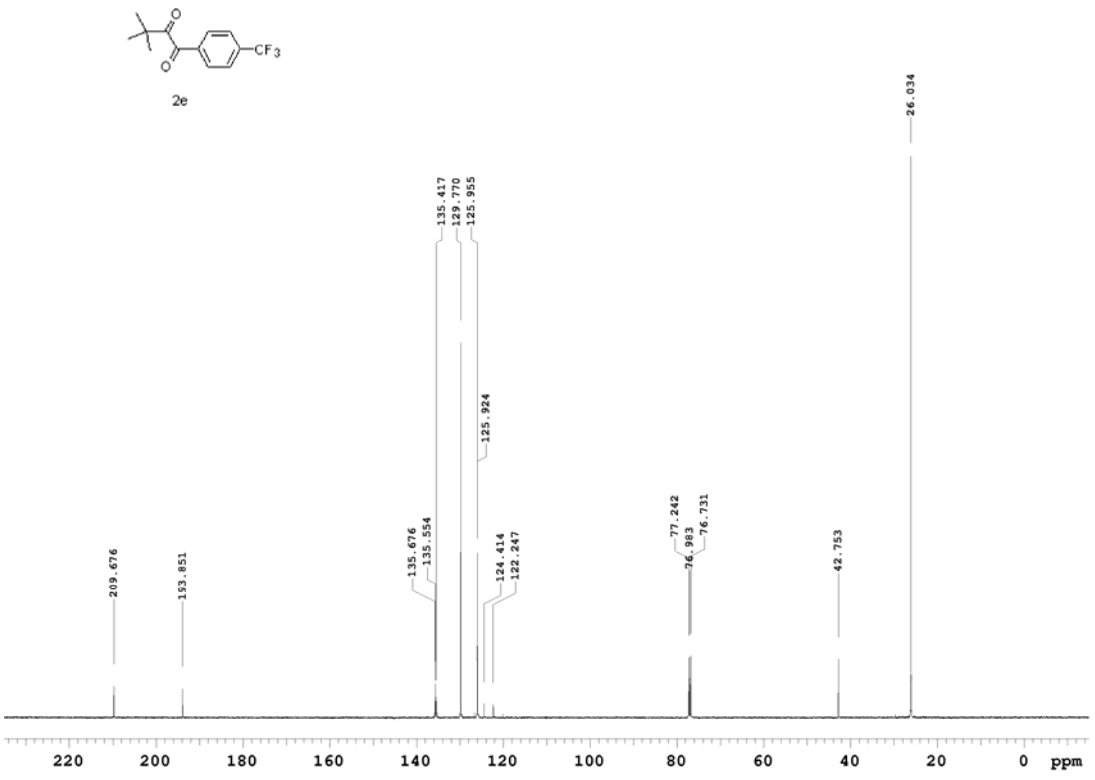
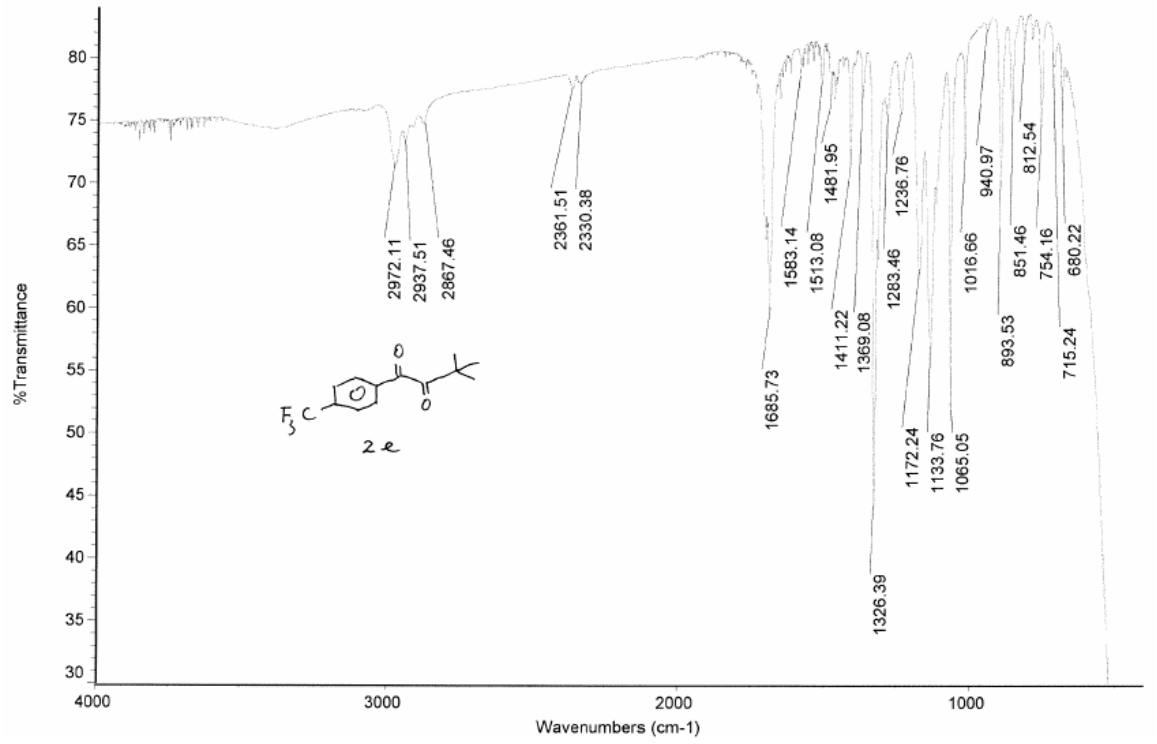
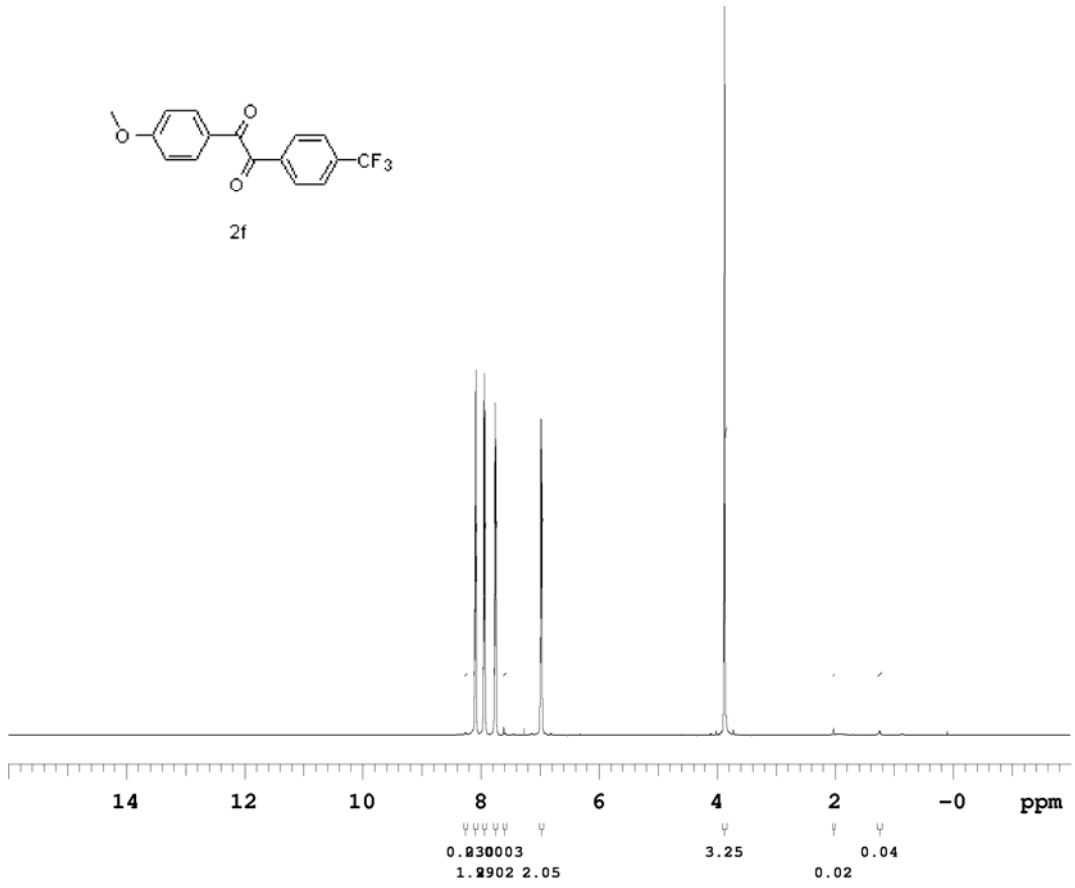
ppm

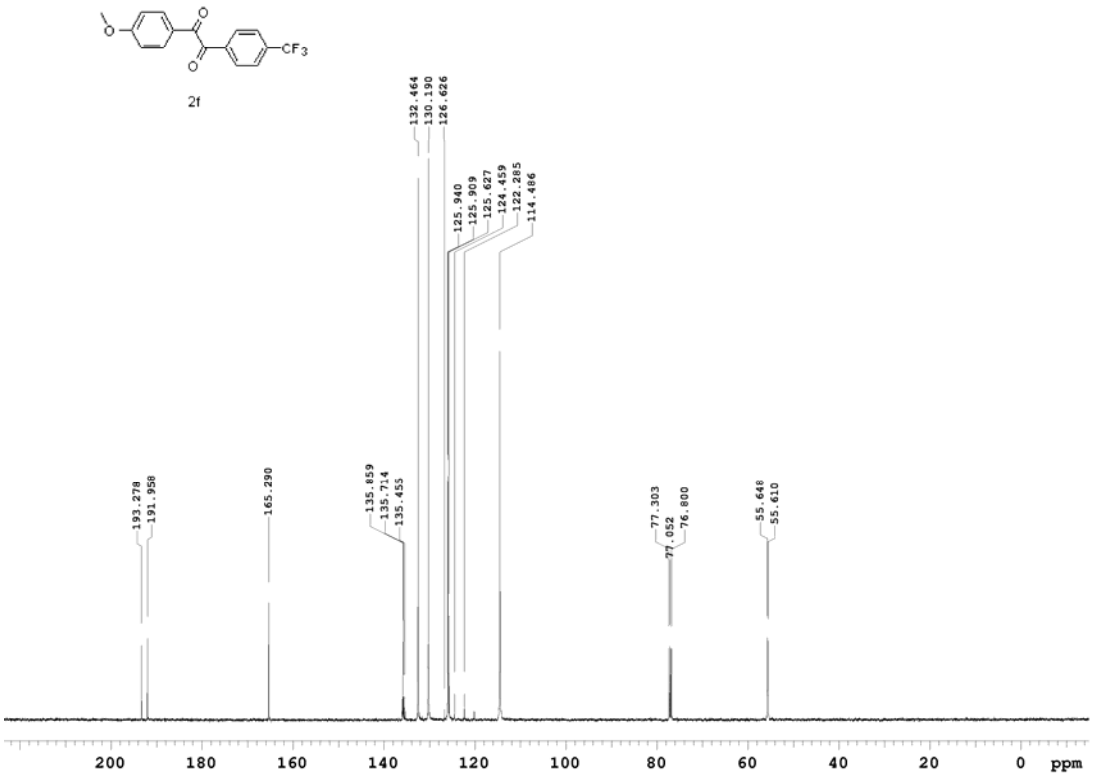

2d
%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
3066.06
2985.83
2965.48
2933.37
2867.46
2361.82
2330.38
1933.41
1669.43
1604.10
1569.86
1458.59
1408.70
1362.00
1302.92
1263.04
1221.19
1187.37
1120.00
1003.24
894.27
839.78
785.30
734.70
703.57
652.97
594.59

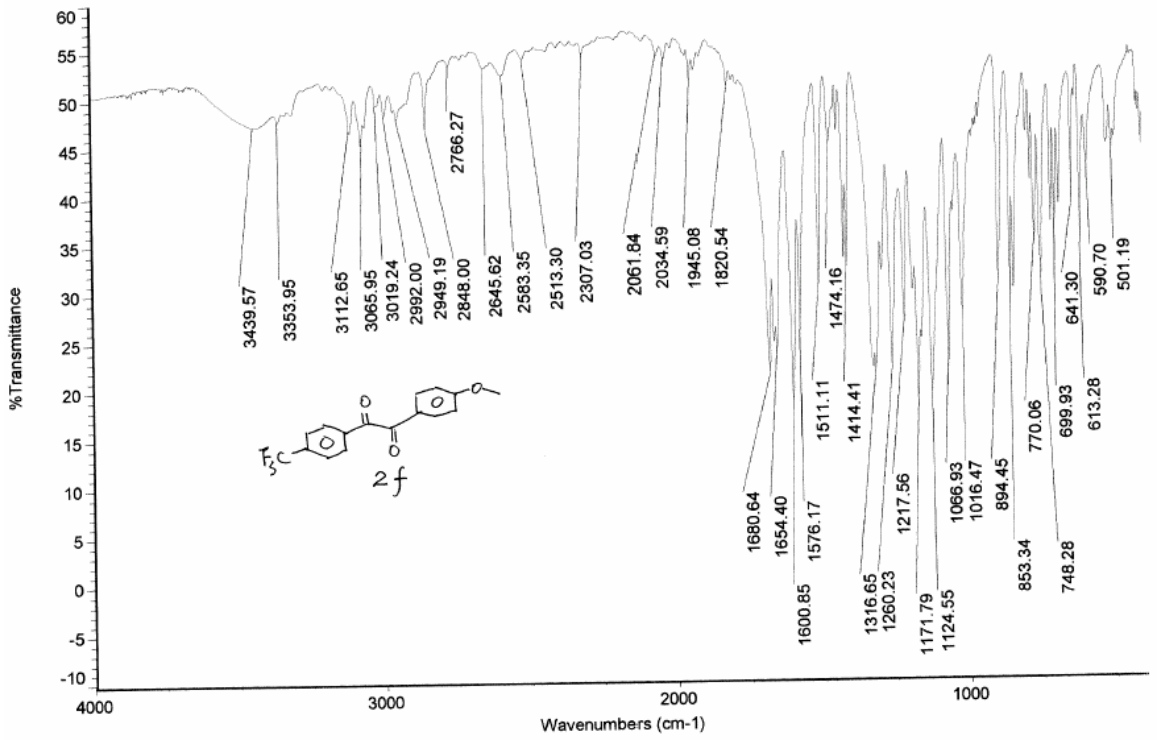

O
O
CF3
2e
14
12
10
8
6
4
2
−0
ppm
1.98
2.00
9.65

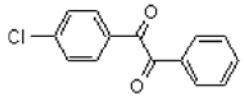

2e
209.676
153.851
135.676
135.554
135.417
129.770
125.955
125.924
124.414
122.247
77.242
76.983
76.731
42.753
26.034
220
200
180
160
140
120
100
80
60
40
20
0
ppm


%Transmittance
Wavenumbers (cm-1)
2972.11
2937.51
2867.46
2361.51
2330.38
1685.73
1583.14
1513.08
1481.95
1411.22
1369.08
1326.39
1283.46
1236.76
1172.24
1133.76
1065.05
1016.66
940.97
893.53
851.46
812.54
754.16
715.24
680.22
2e

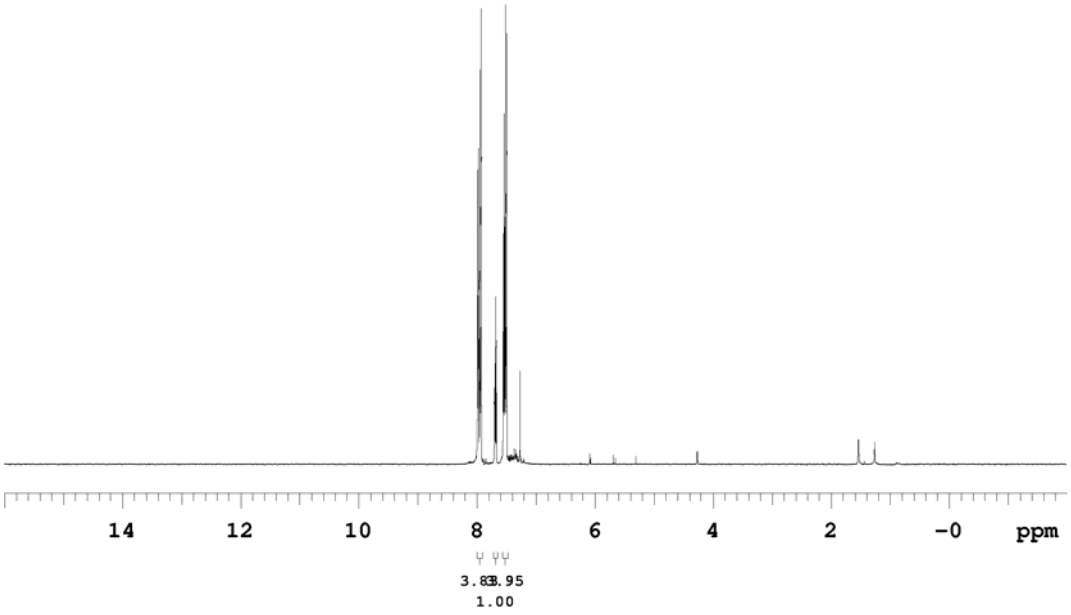

O
O
O
CF3
2f
14
12
10
8
6
4
2
−0
ppm
0.83
0.90
0.03
1.92
2.05
3.25
0.02
0.04

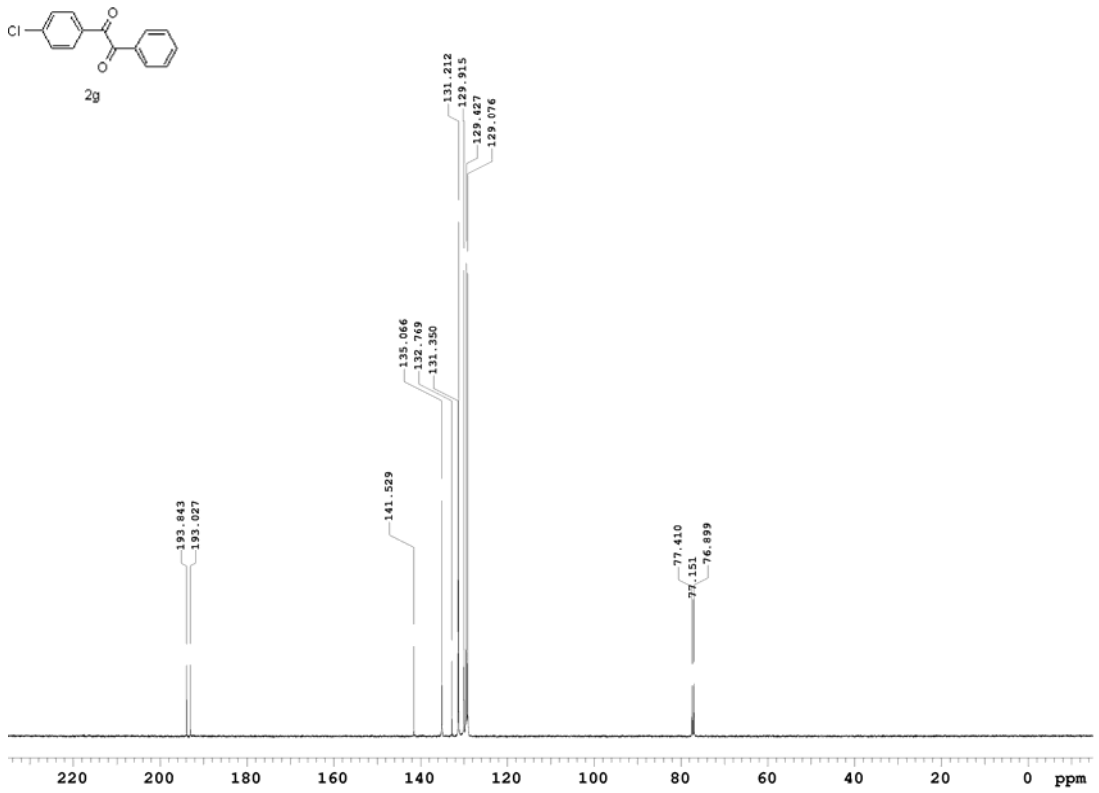

2f
193.278
191.958
165.290
135.859
135.714
135.455
132.464
130.190
126.626
125.940
125.909
125.627
124.459
122.285
114.486
77.303
77.052
76.800
55.648
55.610
200
180
160
140
120
100
80
60
40
20
0
ppm

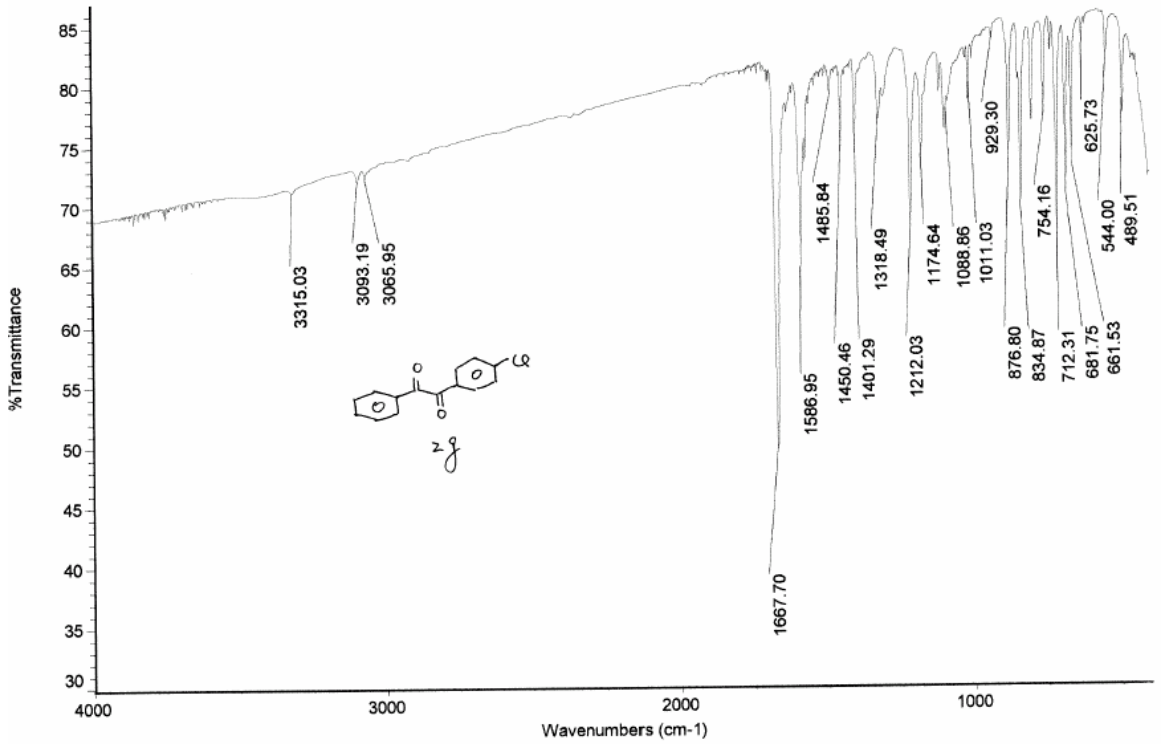

%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
3439.57
3353.95
3112.65
3065.95
3019.24
2992.00
2949.19
2848.00
2766.27
2645.62
2583.35
2513.30
2307.03
2061.84
2034.59
1945.08
1820.54
1680.64
1654.40
1600.85
1576.17
1511.11
1474.16
1414.41
1316.65
1260.23
1217.56
1171.79
1124.55
1066.93
1016.47
894.45
853.34
770.06
748.28
699.93
641.30
613.28
590.70
501.19
2f

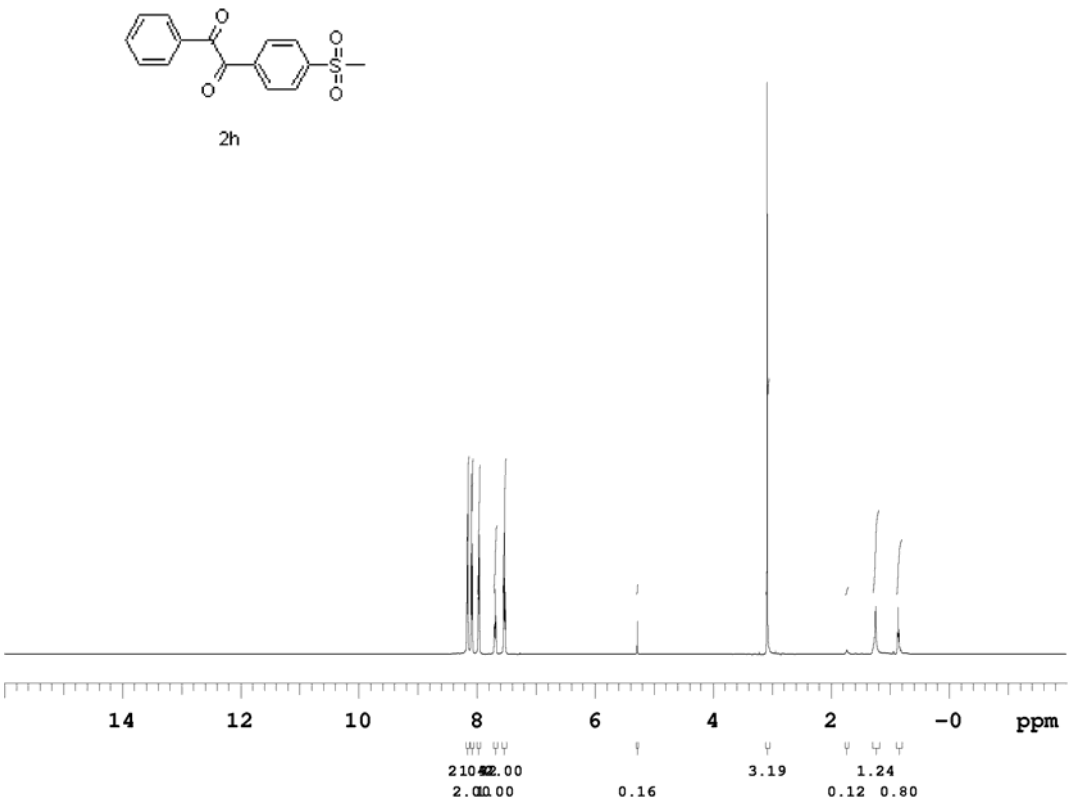


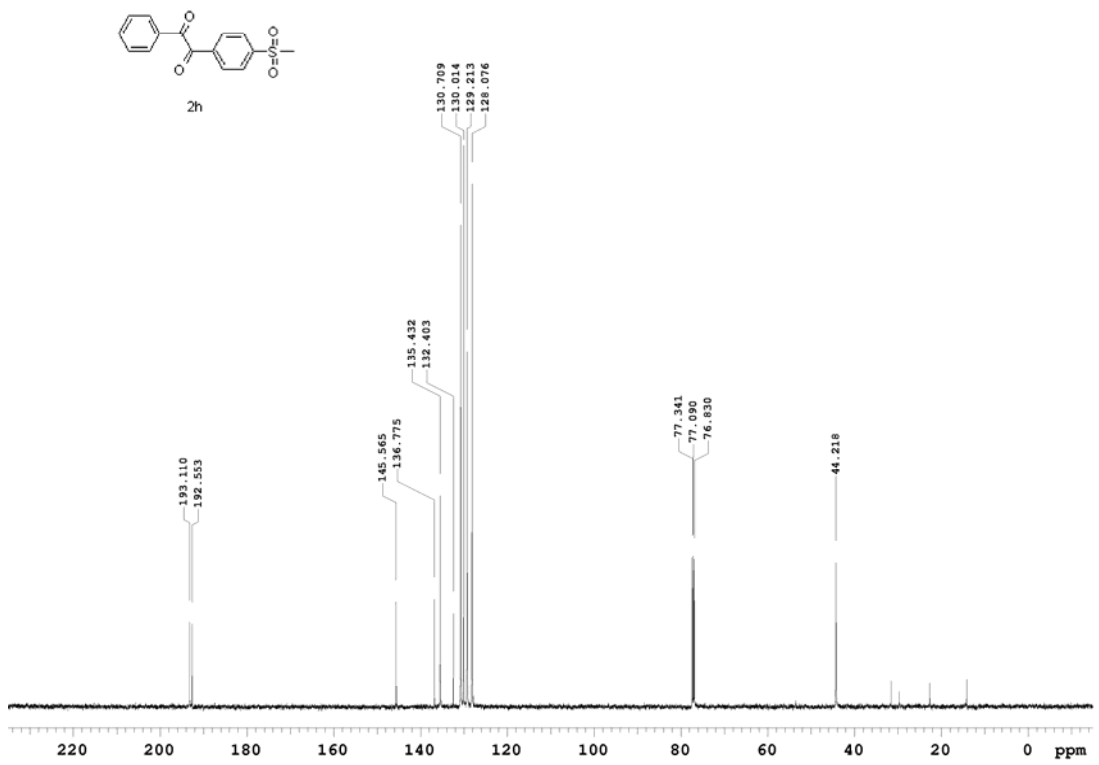
2g

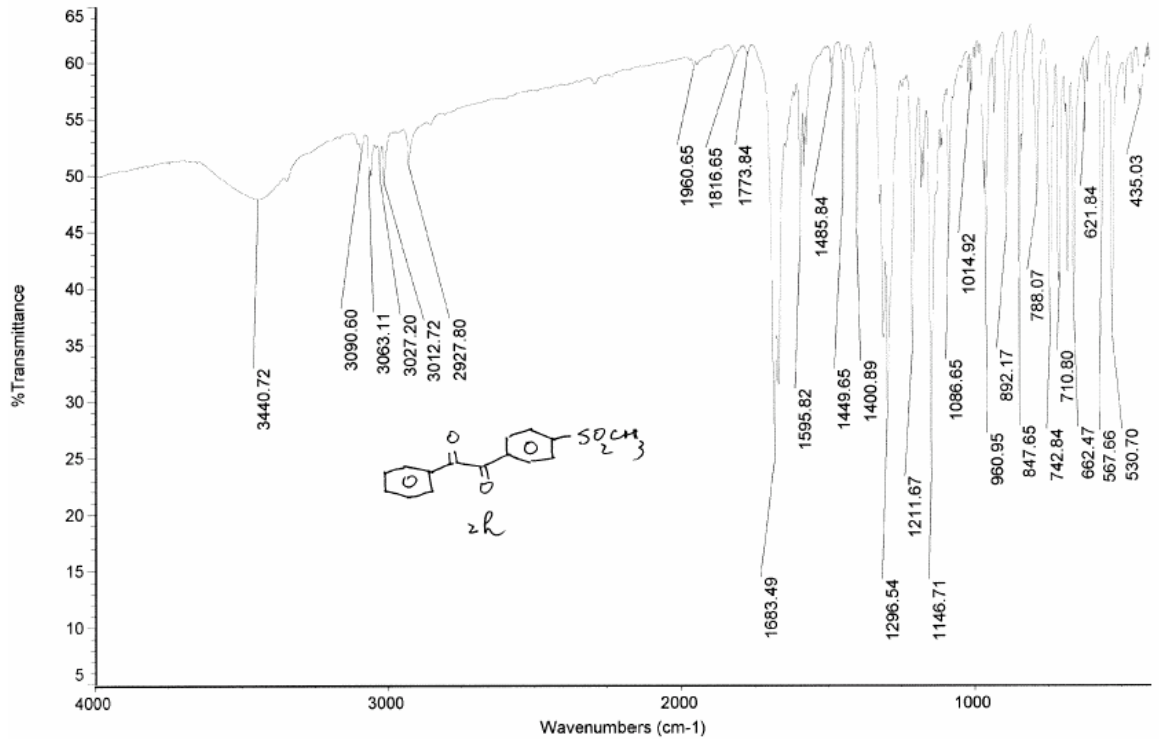


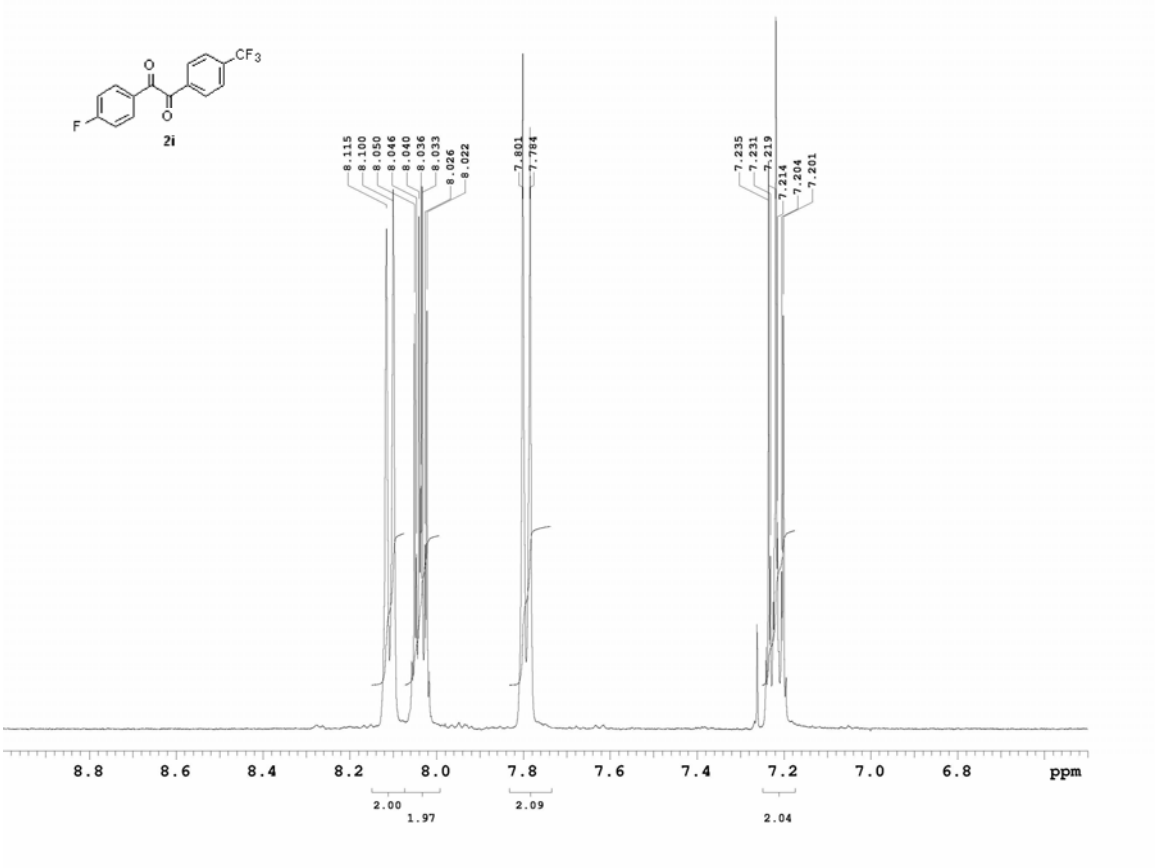

2g
193.843
193.027
141.529
135.066
132.769
131.350
131.212
129.915
129.427
129.076
77.410
77.151
76.899
220
200
180
160
140
120
100
80
60
40
20
0
ppm

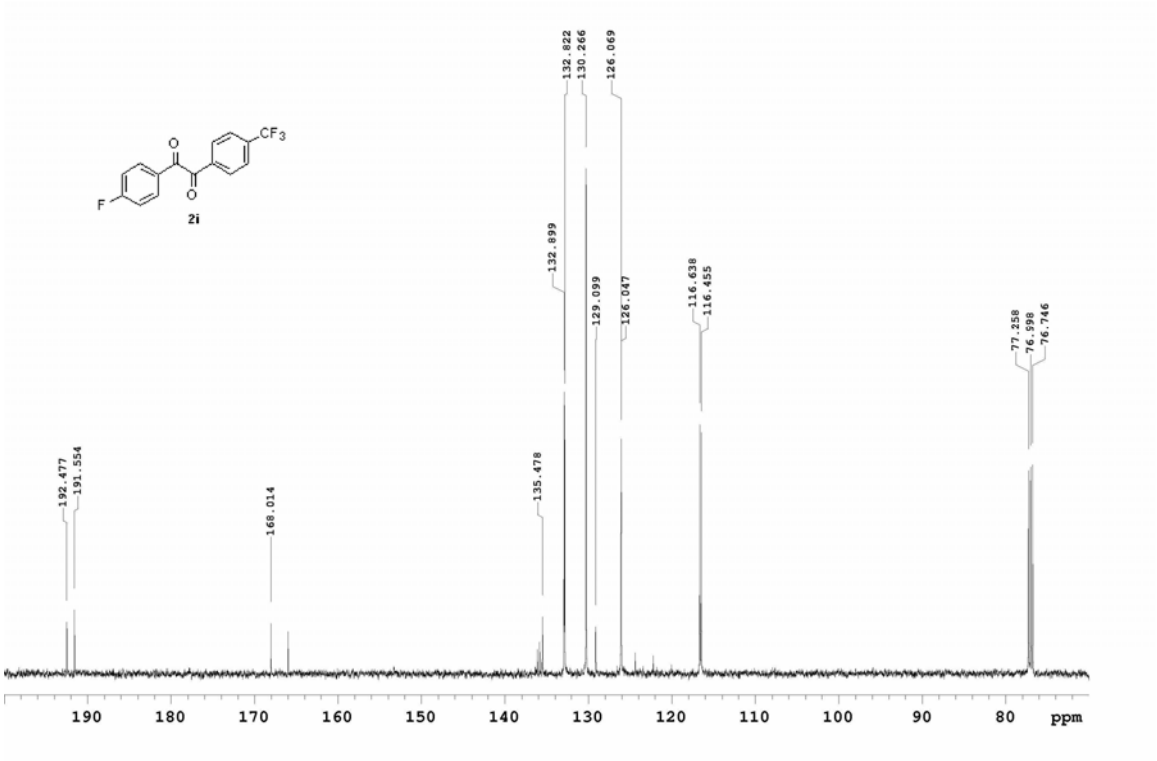

%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
3315.03
3093.19
3065.95
1667.70
1586.95
1485.84
1450.46
1401.29
1318.49
1212.03
1174.64
1088.86
1011.03
929.30
876.80
834.87
754.16
712.31
681.75
661.53
625.73
544.00
489.51
2g

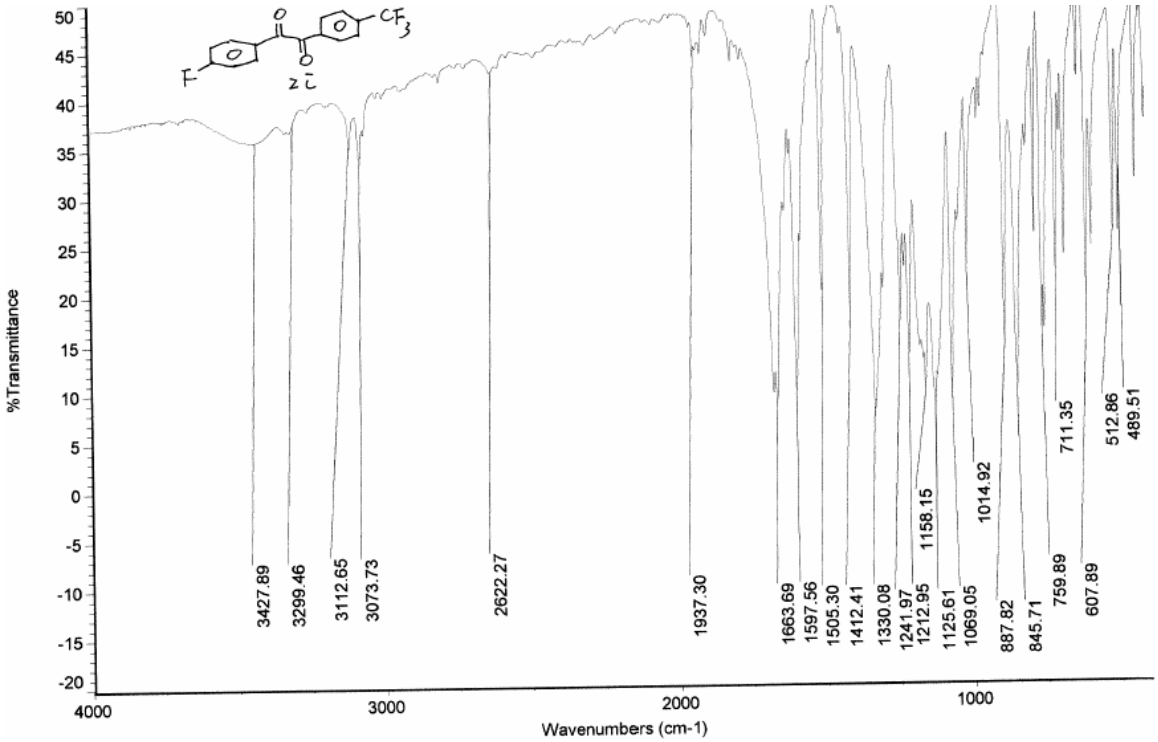

2h
14
12
10
8
6
4
2
−0
ppm
2.00
3.19
1.24
0.16
0.12
0.80

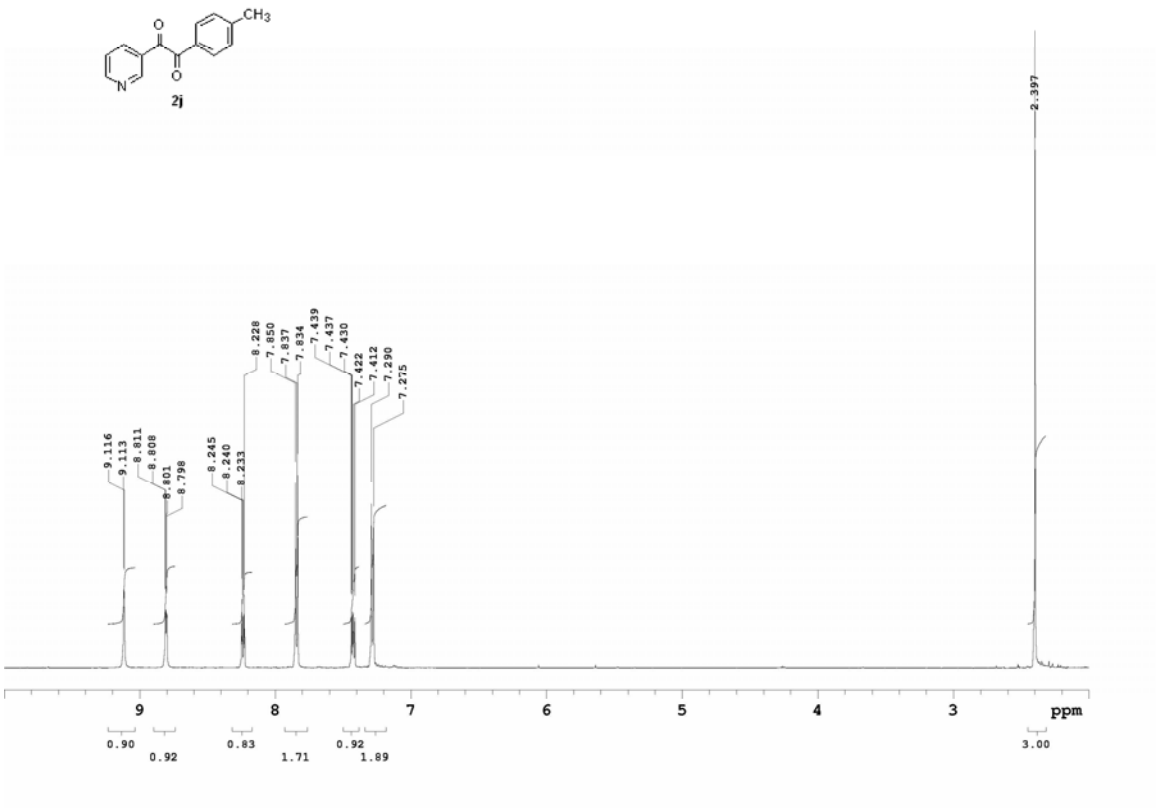

2h
193.110
192.553
145.565
136.775
135.432
132.403
130.709
130.014
129.213
128.076
77.341
77.090
76.830
44.218
220
200
180
160
140
120
100
80
60
40
20
0
ppm

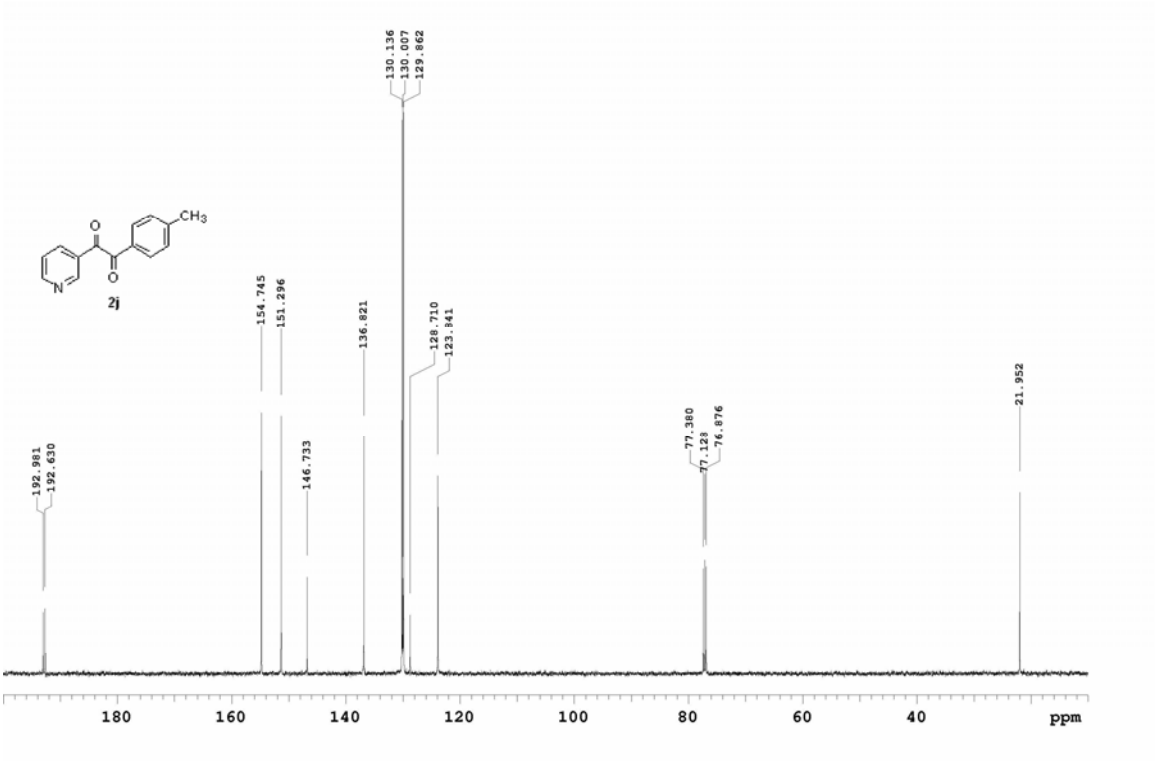

%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
3440.72
3090.60
3063.11
3027.20
3012.72
2927.80
1960.65
1816.65
1773.84
1683.49
1595.82
1485.84
1449.65
1400.89
1296.54
1211.67
1146.71
1086.65
1014.92
960.95
892.17
847.65
788.07
742.84
710.80
662.47
621.84
567.66
530.70
435.03
2k

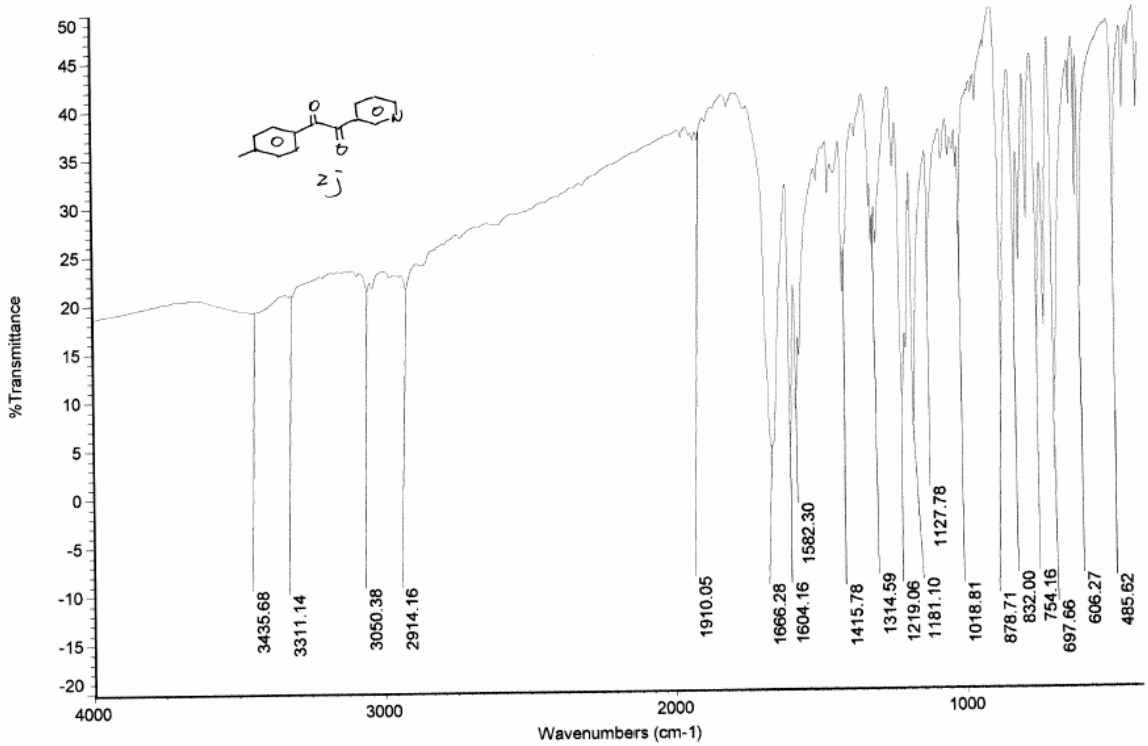

2i
8.115
8.100
8.050
8.046
8.040
8.036
8.033
8.026
8.022
7.801
7.784
7.235
7.231
7.219
7.214
7.204
7.201
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
ppm
2.00
1.97
2.09
2.04

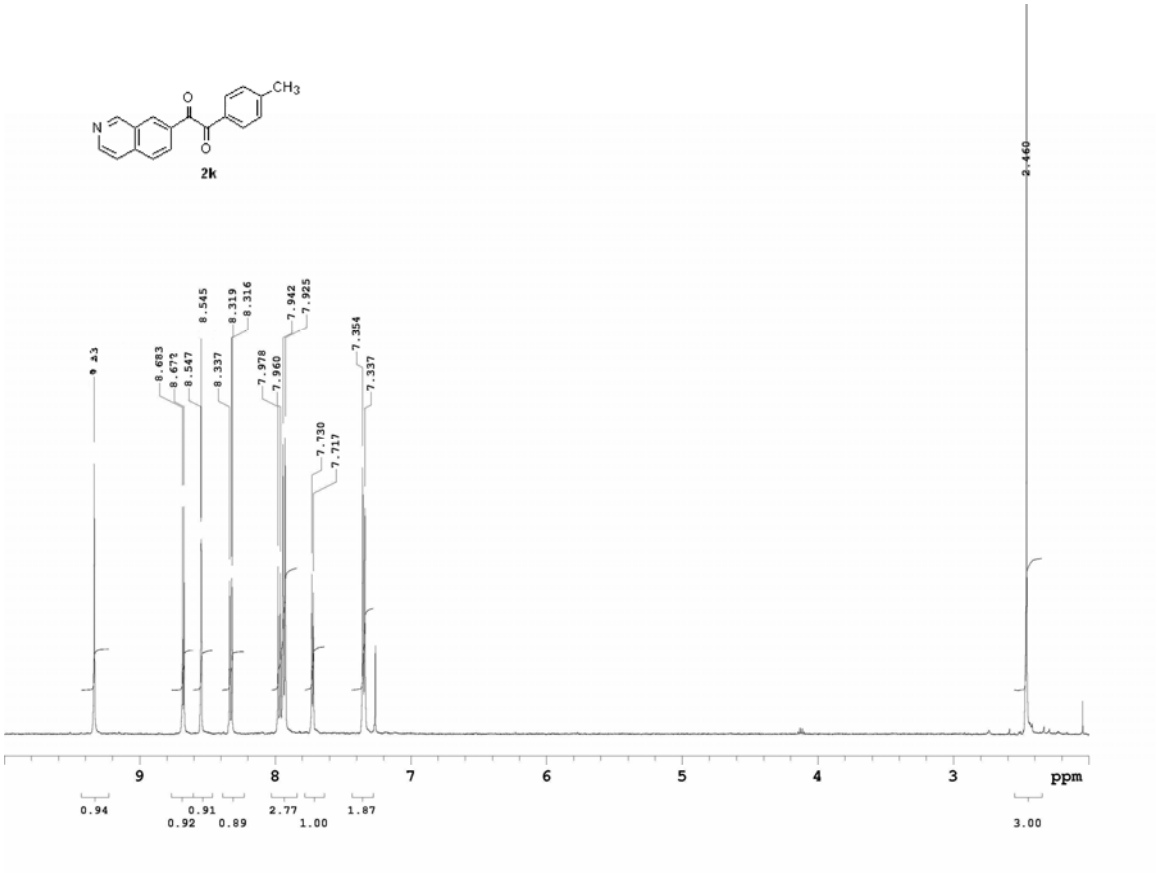

2i
192.477
191.554
168.014
135.478
132.899
132.822
130.266
129.099
126.069
126.047
116.638
116.455
77.258
76.598
76.746
190
180
170
160
150
140
130
120
110
100
90
80
ppm

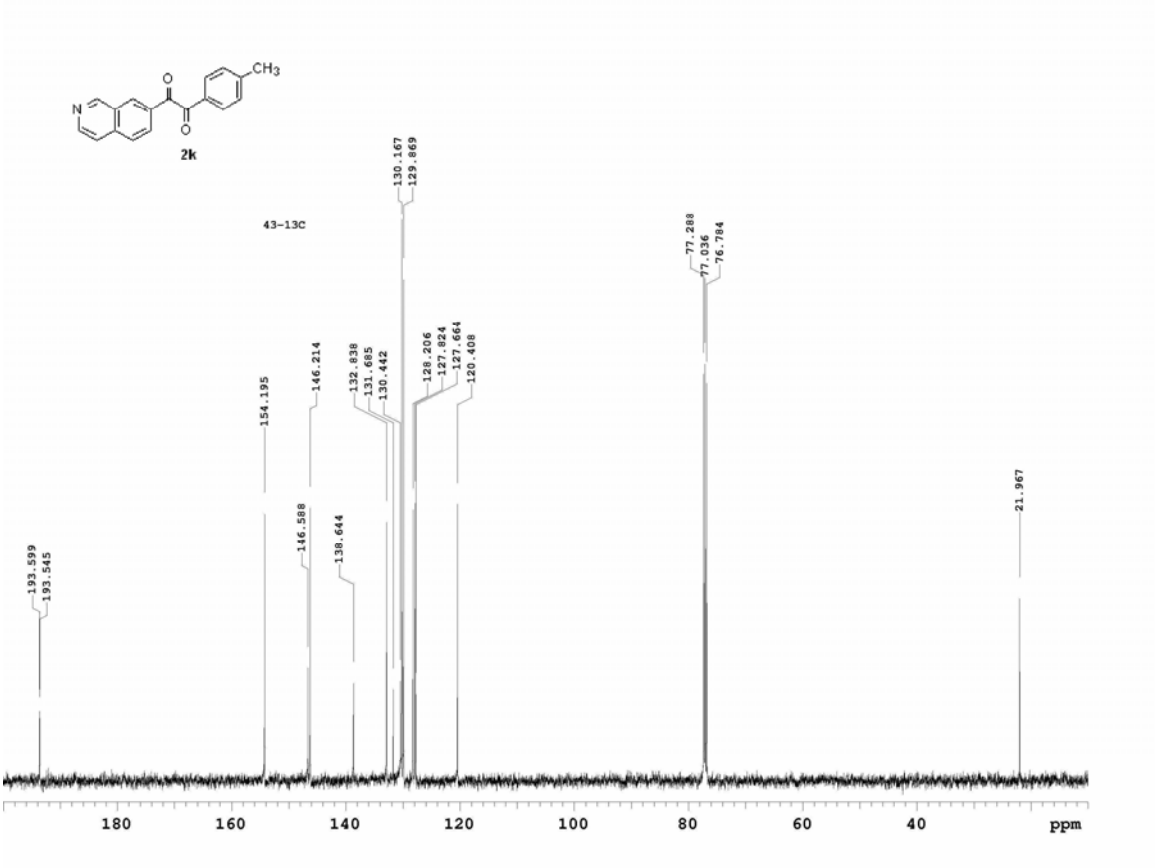

2i
%Transmittance
3427.89
3299.46
3112.65
3073.73
2622.27
1937.30
1663.69
1597.56
1505.30
1412.41
1330.08
1241.97
1212.95
1158.15
1125.61
1069.05
1014.92
887.82
845.71
759.89
711.35
607.89
512.86
489.51
4000
3000
2000
1000
Wavenumbers (cm-1)

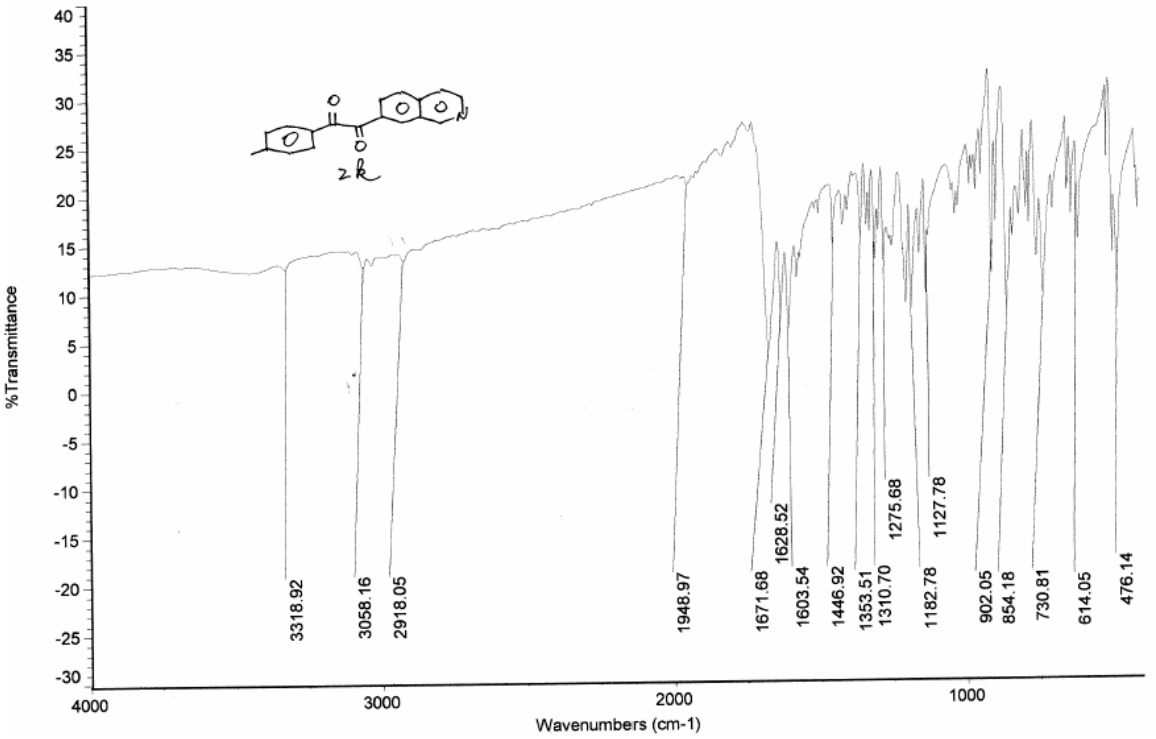

CH3
O
O
N
2j
2.397
9.116
9.113
8.811
8.808
8.801
8.798
8.245
8.240
8.233
8.228
7.850
7.837
7.834
7.439
7.437
7.430
7.422
7.412
7.290
7.275
9
8
7
6
5
4
3
ppm
0.90
0.92
0.83
1.71
0.92
1.89
3.00

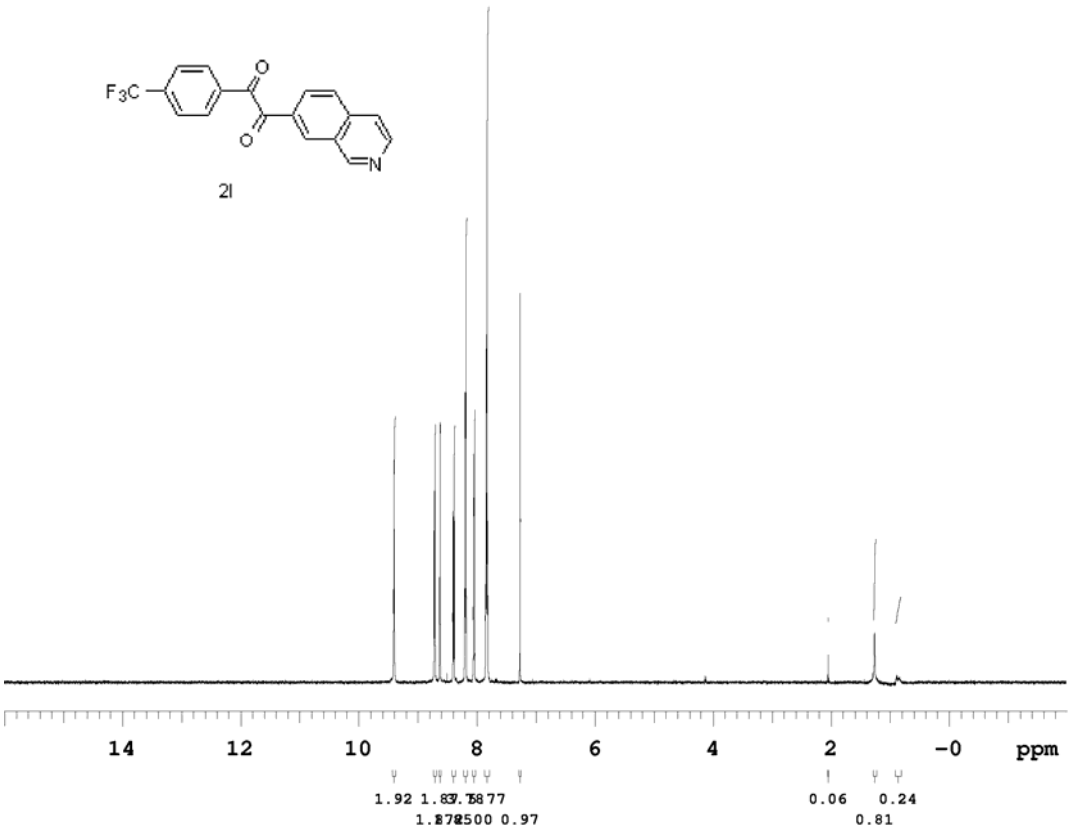

2j
192.981
192.630
154.745
151.296
146.733
136.821
130.136
130.007
129.862
128.710
123.141
77.380
77.123
76.876
21.952
180
160
140
120
100
80
60
40
ppm

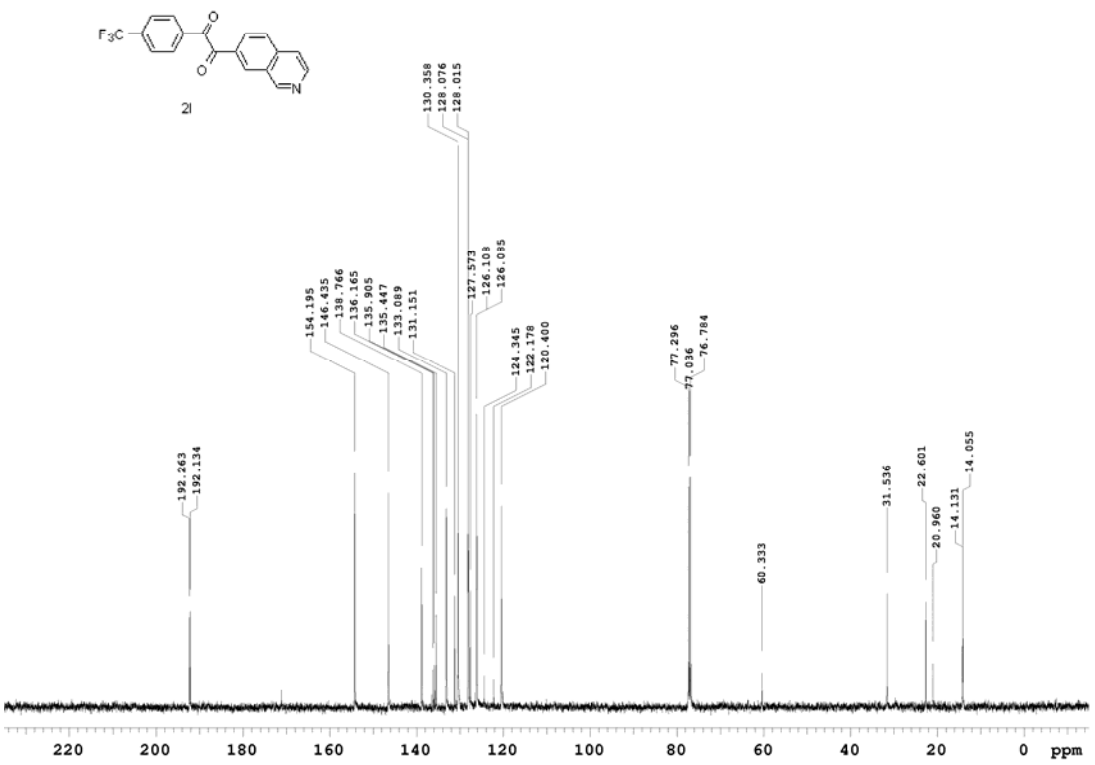

%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
3435.68
3311.14
3050.38
2914.16
1910.05
1666.28
1604.16
1582.30
1415.78
1314.59
1219.06
1181.10
1127.78
1018.81
878.71
832.00
754.16
697.66
606.27
485.62

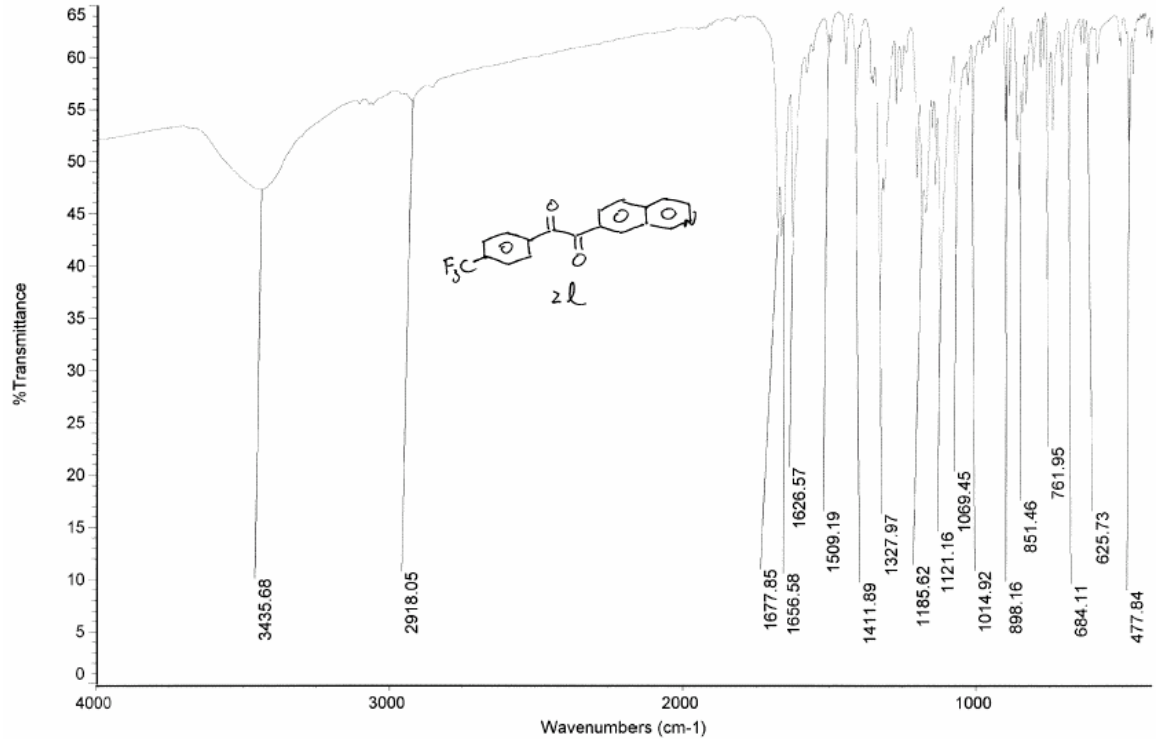

2k
9.43
8.683
8.672
8.547
8.545
8.337
8.319
8.316
7.978
7.960
7.942
7.925
7.730
7.717
7.354
7.337
2.460
9
8
7
6
5
4
3
ppm
0.94
0.92
0.91
0.89
2.77
1.00
1.87
3.00

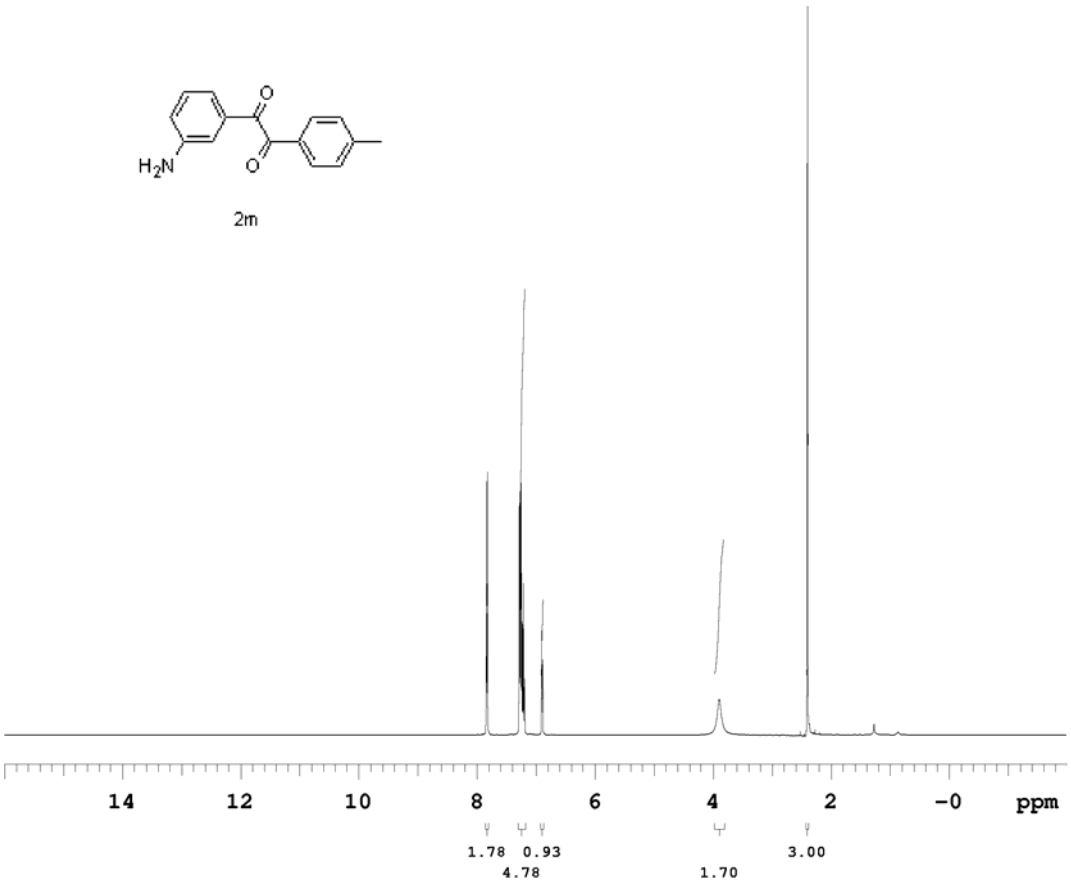

2k
43-13C
193.599
193.545
154.195
146.588
146.214
138.644
132.838
131.685
130.442
130.167
129.869
128.206
127.824
127.664
120.408
77.288
77.036
76.784
21.967
180
160
140
120
100
80
60
40
ppm

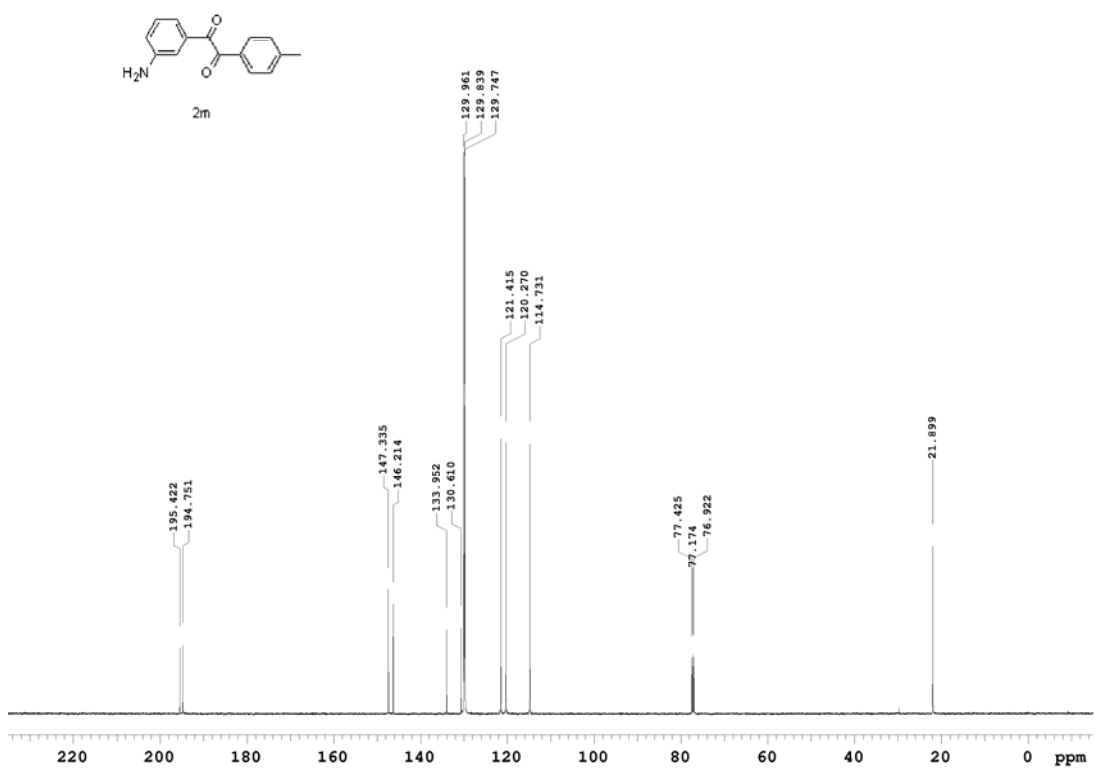

2k
%Transmittance
3318.92
3058.16
2918.05
1948.97
1671.68
1628.52
1603.54
1446.92
1353.51
1310.70
1275.68
1182.78
1127.78
902.05
854.18
730.81
614.05
476.14
4000
3000
2000
1000
Wavenumbers (cm-1)

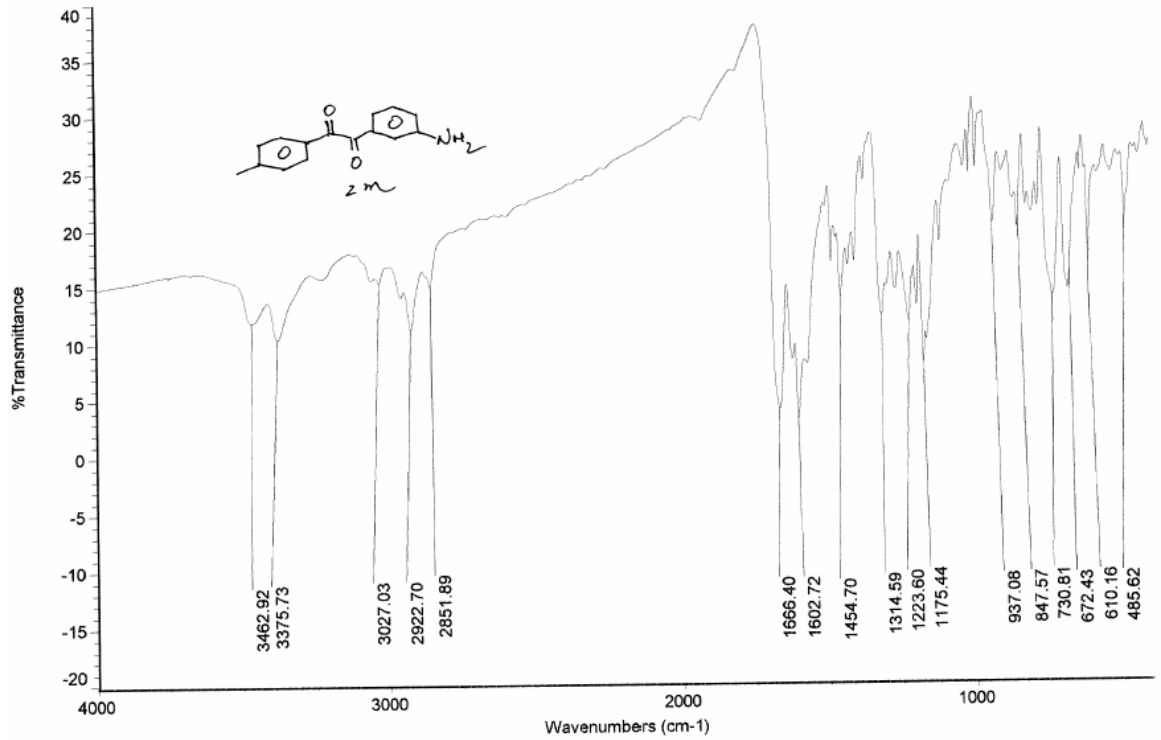

F3C
O
O
N
2l
14
12
10
8
6
4
2
−0
ppm
1.92
0.06
0.24
0.81
0.97

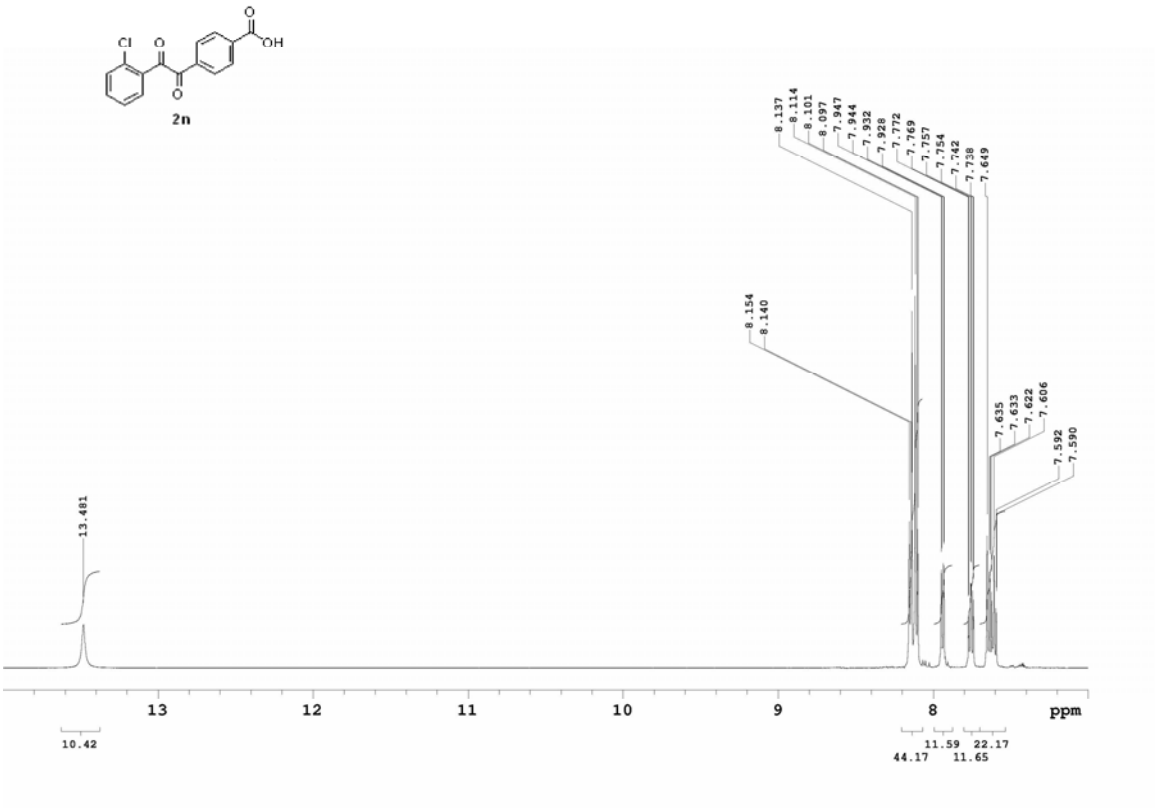

2l
130.358
128.076
128.015
127.573
126.108
126.085
154.195
146.435
138.766
136.165
135.905
135.447
133.089
131.151
124.345
122.178
120.400
77.296
77.036
76.784
192.263
192.134
60.333
31.536
22.601
20.960
14.131
14.055
220
200
180
160
140
120
100
80
60
40
20
0
ppm

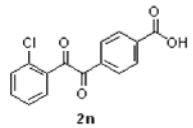

%Transmittance
65
60
55
50
45
40
35
30
25
20
15
10
5
0
3435.68
2918.05
1677.85
1656.58
1626.57
1509.19
1411.89
1327.97
1185.62
1121.16
1069.45
1014.92
898.16
851.46
761.95
684.11
625.73
477.84
4000
3000
2000
1000
Wavenumbers (cm-1)
2l


O
O
H_2N
2m
14
12
10
8
6
4
2
−0
ppm
1.78
0.93
4.78
1.70
3.00

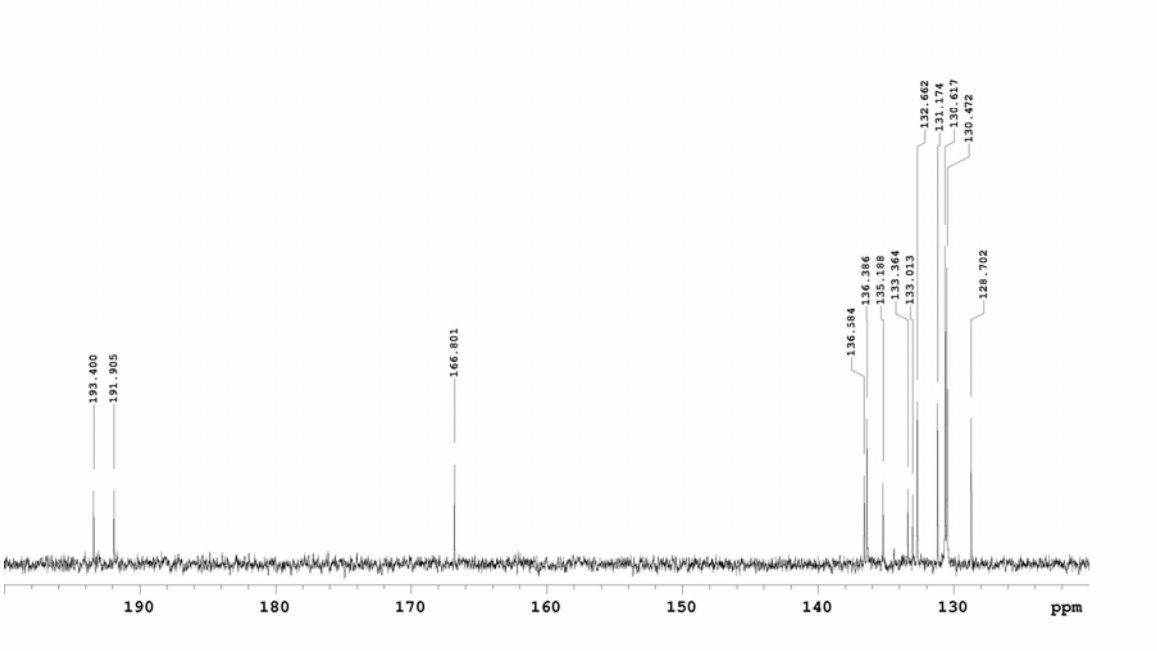

2m
195.422
194.751
147.335
146.214
133.952
130.610
129.961
129.839
129.747
121.415
120.270
114.731
77.425
77.174
76.922
21.899
220
200
180
160
140
120
100
80
60
40
20
0
ppm

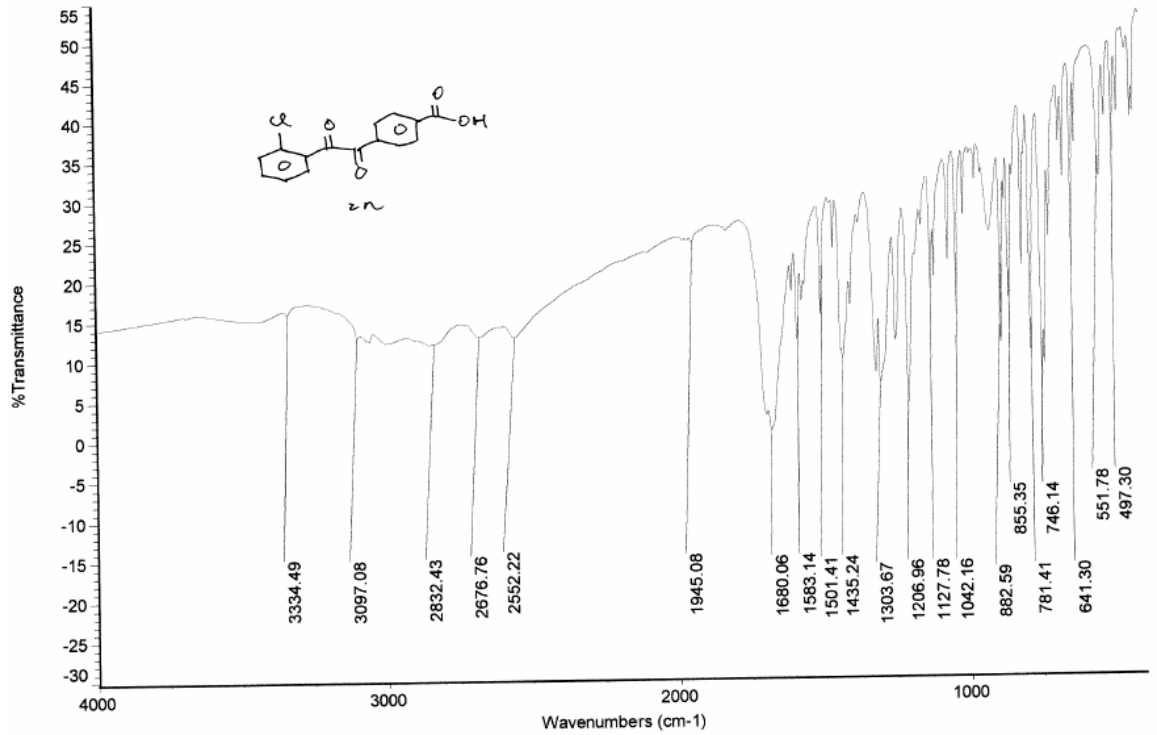

2m
%Transmittance
3462.92
3375.73
3027.03
2922.70
2851.89
1666.40
1602.72
1454.70
1314.59
1223.60
1175.44
937.08
847.57
730.81
672.43
610.16
485.62
4000
3000
2000
1000
Wavenumbers (cm-1)

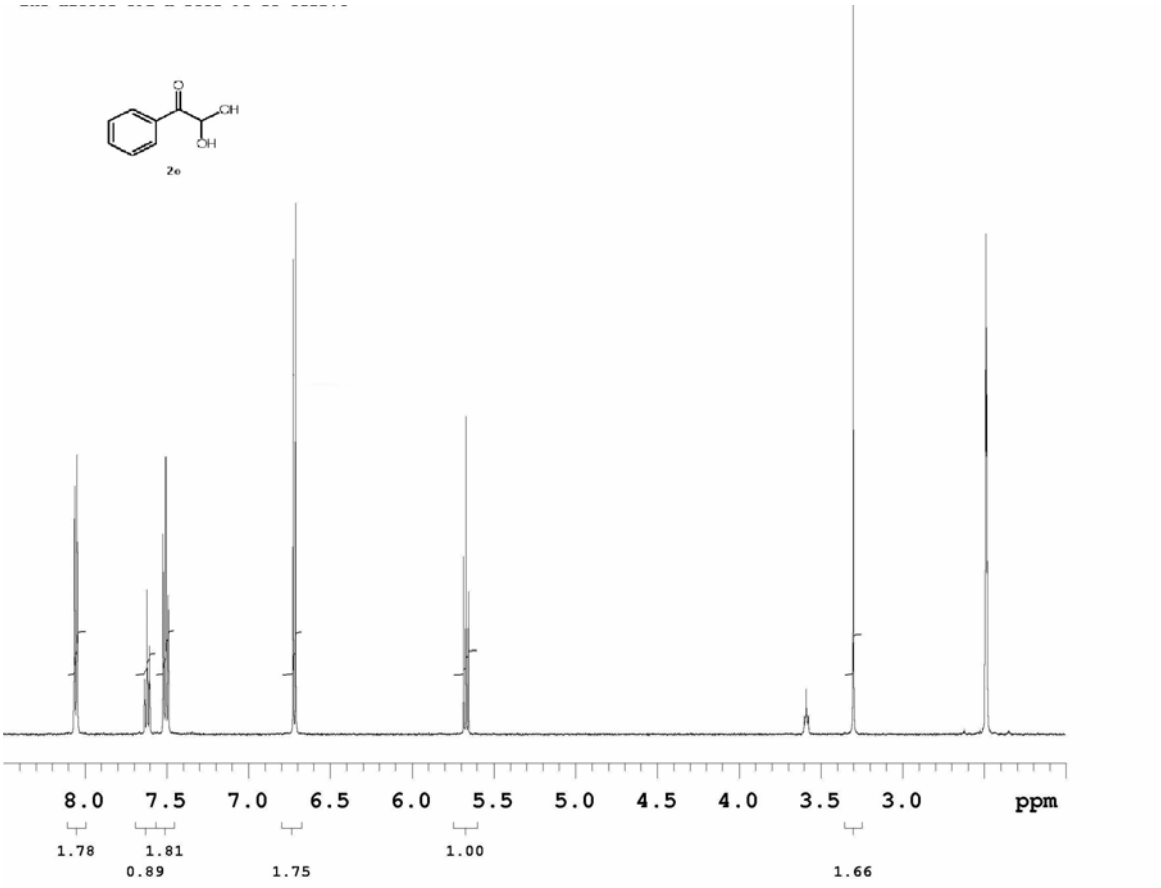

Cl
O
O
O
OH
2n
8.137
8.114
8.101
8.097
7.947
7.944
7.932
7.928
7.772
7.769
7.757
7.754
7.742
7.738
7.649
8.154
8.140
7.635
7.633
7.622
7.606
7.592
7.590
13.481
13
12
11
10
9
8
ppm
10.42
44.17
11.59
11.65
22.17

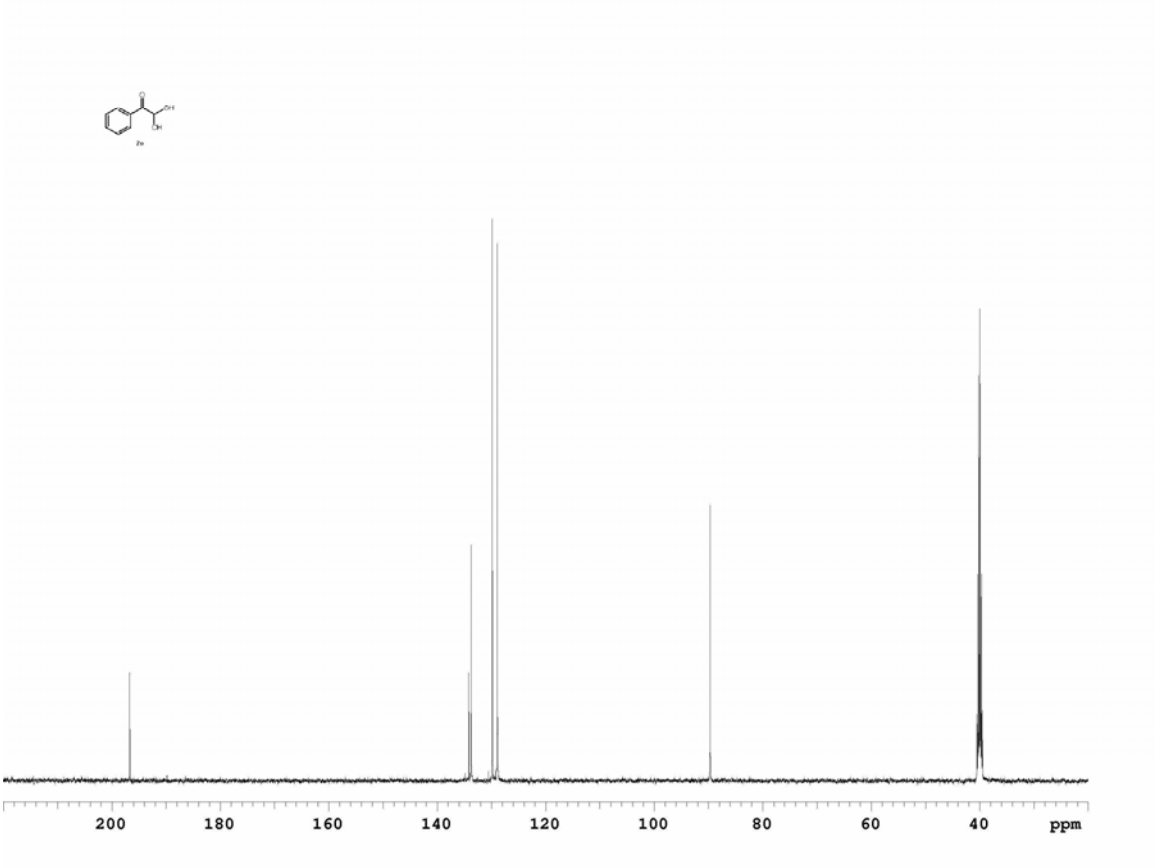

Cl
O
O
O
OH

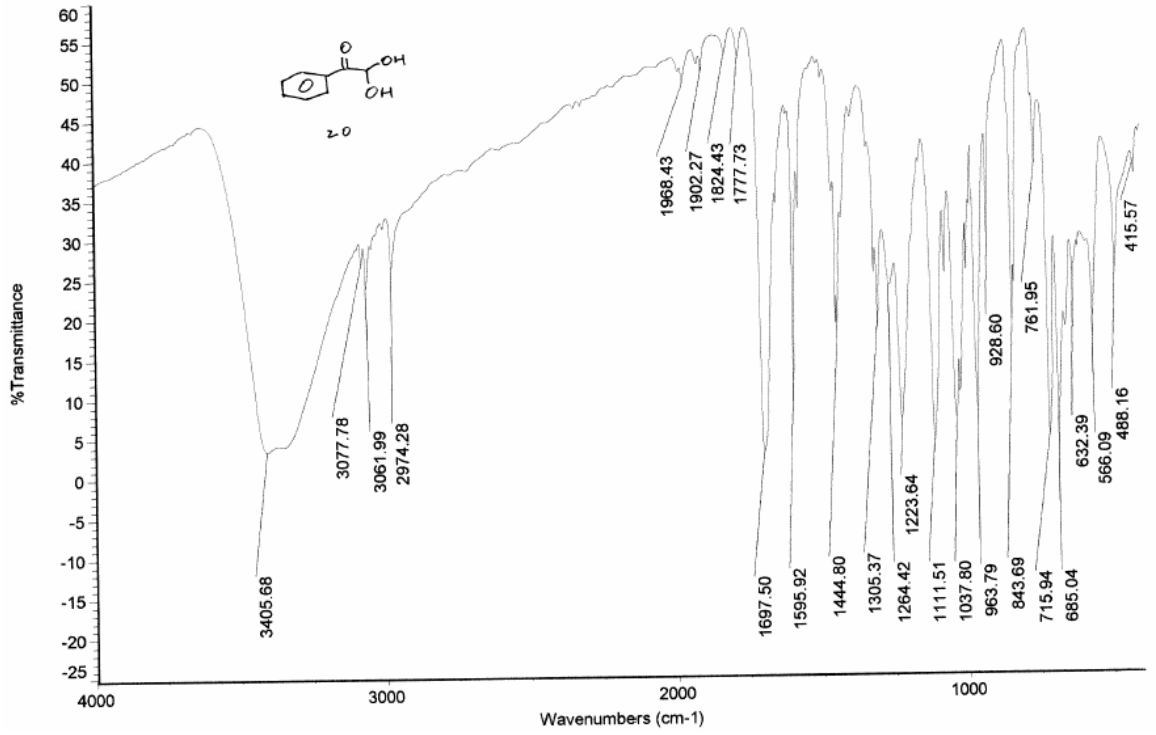
2n


193.400
191.905
166.801
136.584
136.386
135.188
133.364
133.013
132.662
131.174
130.617
130.472
128.702
190
180
170
160
150
140
130
ppm


%Transmittance
55
50
45
40
35
30
25
20
15
10
5
0
-5
-10
-15
-20
-25
-30
3334.49
3097.08
2832.43
2676.76
2552.22
1945.08
1680.06
1583.14
1501.41
1435.24
1303.67
1206.96
1127.78
1042.16
882.59
855.35
781.41
746.14
641.30
551.78
497.30
4000
3000
2000
1000
Wavenumbers (cm-1)


O
OH
OH
2e
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
ppm
1.78
1.81
0.89
1.75
1.00
1.66


200
180
160
140
120
100
80
60
40
ppm


%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
3405.68
3077.78
3061.99
2974.28
1968.43
1902.27
1824.43
1777.73
1697.50
1595.92
1444.80
1305.37
1264.42
1223.64
1111.51
1037.80
963.79
928.60
843.69
761.95
715.94
685.04
632.39
566.09
488.16
415.57