Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

SUPPPORTING INFORMATION

Synthesis of Furo[3,2-*b*:4,5-*b*']diindoles and their Optical- and Electrochemical Properties

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Table of Content

General information

All used chemicals are commercially available and used without further purification. All reactions were carried out in dried pressure tubes under an argon atmosphere. Analytical TLC on Merck silica gel 60 F254 plates was visualized by fluorescence quenching. Column chromatography was performed on Merck Geduran Si 60 (0.063-0.200 mm). ^{1}H NMR and ^{13}C NMR spectra were carried out on a Bruker Advance DRX-500 MHz, 300 MHz or 250 MHz. Chemical shifts in ppm were corrected by residual solvent. Multiplicities: s = singlet, d = doublet, dd = doublet of doublets, t = triplet, td = triplet of doublets, tt = triplet of triplets, m = multiplet, q = quartet. Nicolet 550 FT – IR spectrometer was used with ATR sampling technique for solids. Signal characterization: w = weak, m = medium, s = strong. Gas chrmatography - mass analysis was performed on an Agilent HP-5890 instrument with an Agilent HP-5973 Mass Selective Detector (EI) and HP-5 capillary column using helium carrier gas. Agilent 1969A TOF mass spectrometer was used for ESI HR-MS measurements. High Resolution MS (HRMS) was performed on a Finnigan MAT 95 XP. Single crystal X-Ray structure determination was carried out on a Bruker X8Apex diffractometer with CCD camera (Mo Kα radiation and graphite monochromator, a = 0.071073 Å). Melting points were determined on a Micro-Hot-Stage GalenTM III Cambridge Instruments. The melting points are not corrected. All electrochemical studies were performed with an Autolab (PGSTAT 302N, Metrohm) at 22 °C in dried dimethylformamide under an Argon atmosphere. 0.1 M tetrabutylammonium hexafluorophosphate (Fluka) was used as conducting support. The working electrode was a glassy carbon disk electrode (d = 2 mm), a Pt-electrode as the counter electrode, an Ag/AgCl/ LiCl sat. in EtOH-system as the reference electrode (all electrodes: Metrohm) and the ferrocenium/ferrocene as internal reference system (potential of Fc^{+} /Fc: 0.51 V [vs. Ag/AgCl/LiCl sat. in EtOH]. The CV scans were repeated three times at a scan rate of 40 $mV{\cdot}s^{-1}$. The DPV measurements in oxidative and anodic directions were performed with a step potential of 5 mV, modulation amplitude of 0.025 V, modulation time of 0.05 s and an interval time of 0.5 s. The measurements were performed at a compound concentration of 0.1mM diluted in the electrolyte solution. Density functional theory (DFT) calculations were performed on **3a**, **3c**, **3e** and **3l** using the B3LYP hybrid functional with a 6-311G(d,p) basis set. The calculations were performed with Gaussian09, Revision E.01. Additionally, the geometry optimization was realized without symmetry constraints using the Berny algorithm.

Chemical protocols

General procedure for the preparation of 3,4-dibromo-2,5-bis(2-bromophenyl)furan 2: Tetrabromofuran **1**, 2.2 equiv. 2-bromophenyl boronic acid, $Pd(PPh_3)_4$ (5 mol%) and 5.0 equiv. K_3PO_4 were added to a 250 mL Schlenk flask under Argon atmosphere. To the mixture 70 mL 1,4-dioxane and 10 mL distilled water were added. The reaction was heated at 90°C for 8h. The mixture was allowed to reach room temperature, diluted with water and extracted with dichloromethane. The organic layer was dried over Na_2SO_4, filtered and the solvent was evaporated *in vacuo*. The brown residue was purified by column chromatography (silica gel, heptane/ethylacetate (20:1)) to yield 3,4-dibromo-2,5-bis(2-bromophenyl)furan **2**.

General procedure for double C-N coupling – Synthesis of furo[3,2-*b*:4,5-*b*']diindole 3a-o. 3.0 equiv. of amine was added to a pressure tube charged with **2**, $Pd_2(dba)_3$ (5 mol%), dppf (10 mol%) and 5.0 equiv. of NaO*t*Bu under Argon. The mixture was dissolved in anhydrous toluene (10 mL). The tube was sealed with a Teflon valve and stirred at 110°C for 20h. The mixture was allowed to reach room temperature, worked up with water and extracted with dichloromethane. The combined organic layers were dried over sodium sulfate and concentrated under vacuum. The crude material was purified by flash column chromatography on silica gel to yield furo[3,2-*b*:4,5-*b*']diindole 3**a-o**.

Crystal Data

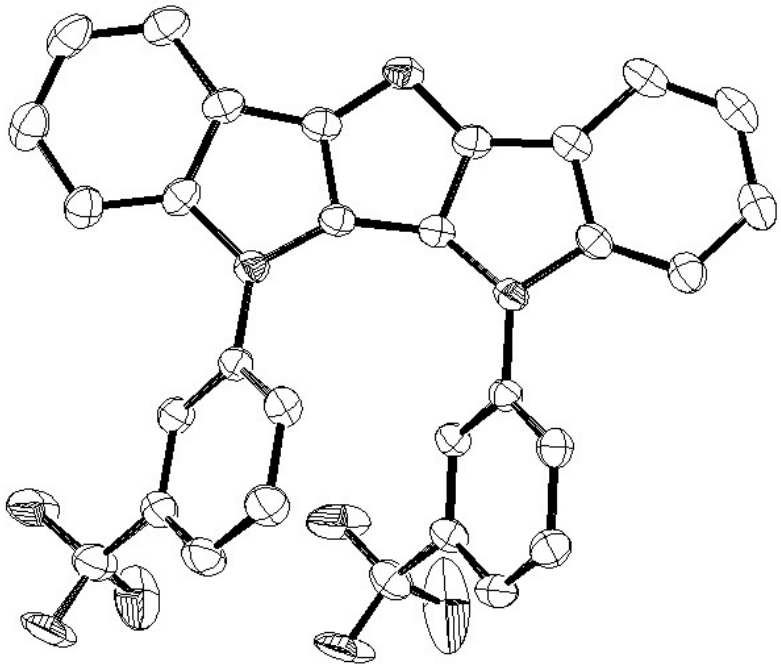

Figure 1. Crystal structure of compound **3d** in monoclinic form.

Chemical formula moiety	'$C_{30}H_{16}F_6N_2O$'
Chemical formula weight	534.45
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Symmetry space group name H-M	'P 21/n'
Symmetry space group name Hall	'-P 2yn'
Symmetry Int Tables number	14
Cell length a	12.3782(3)
Cell length b	12.3739(3)
Cell length c	15.7294(4)
Cell angle alpha	90.00
Cell angle beta	99.4790(10)
Cell angle gamma	90.00
Cell volume	2376.32(10)
Cell formula units Z	4
Exptl crystal description	block
Exptl crystal colour	colourless
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Exptl crystal size mid	0.15
Exptl crystal size min	0.14
Exptl crystal density diffrn	1.494
Exptl crystal F 000	1088

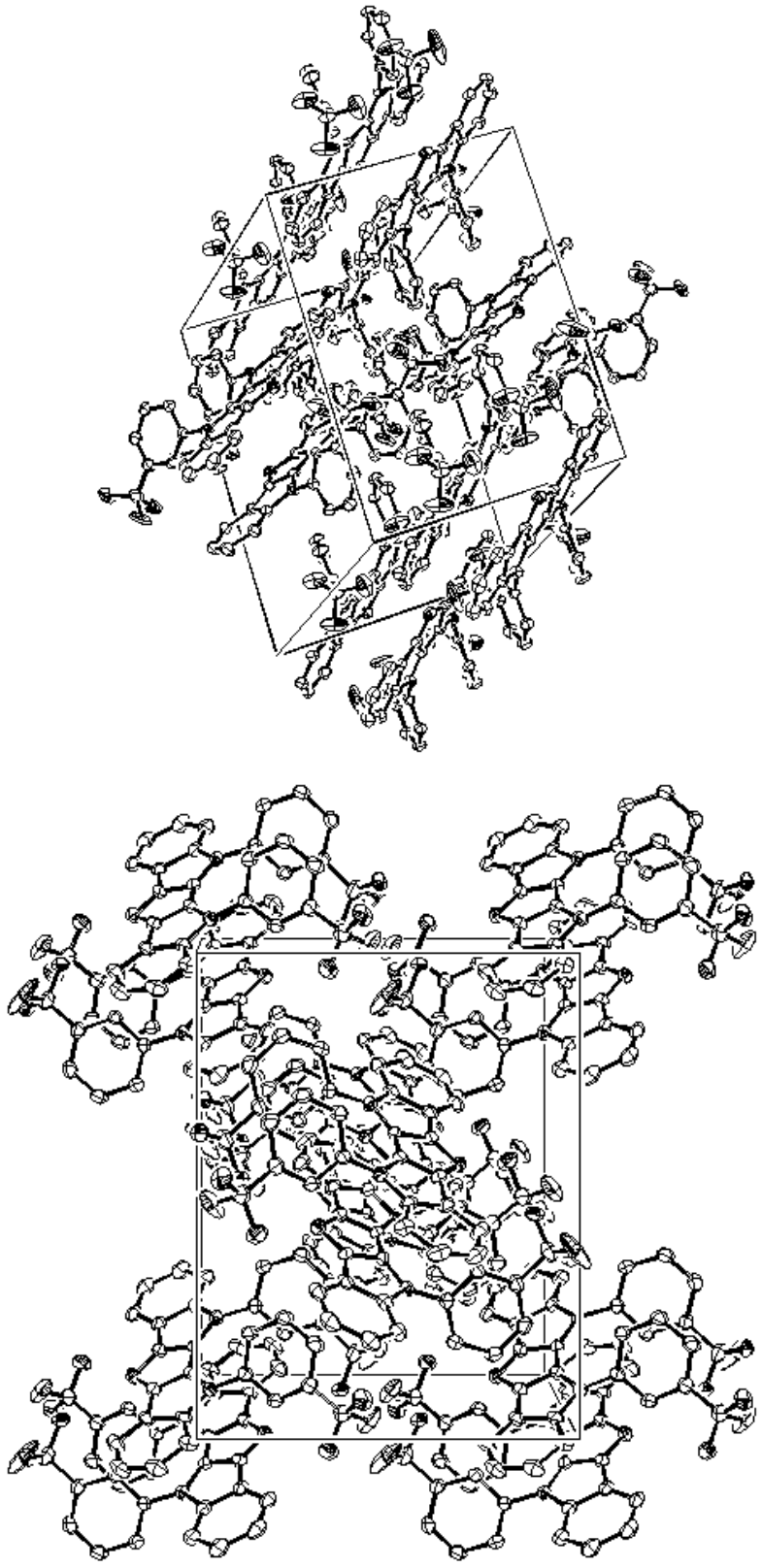

Figure 2. Crystal lattice of compound **3d** in monoclinic form.

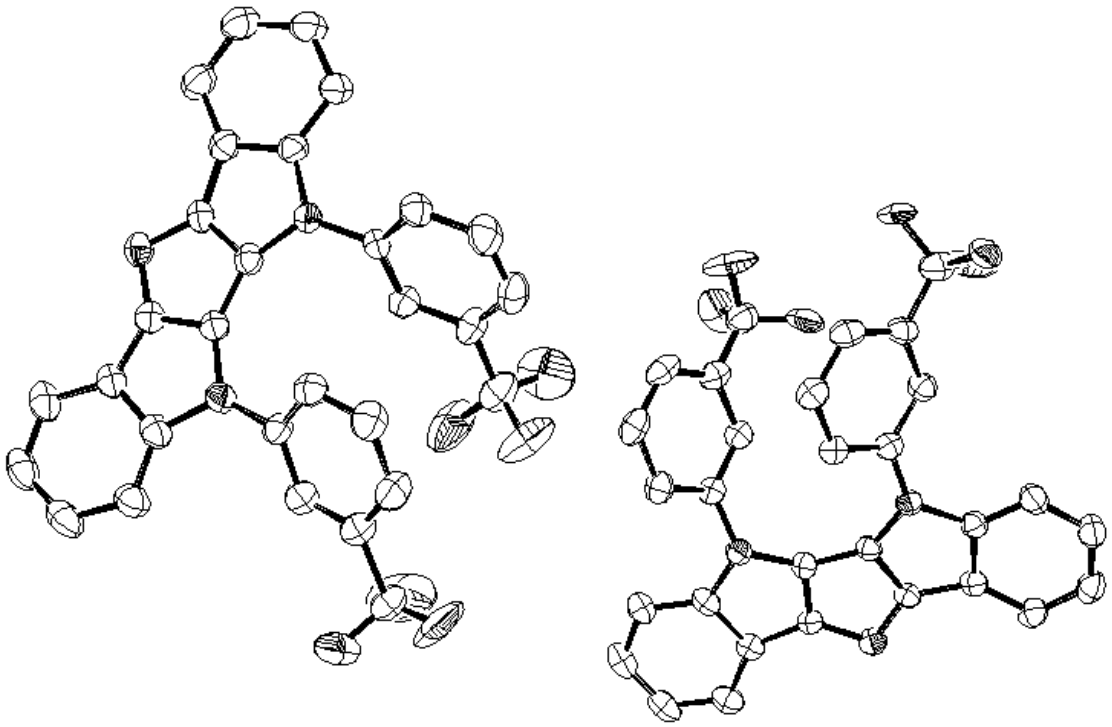

Figure 3. Crystal structure of compound **3d** in triclinic form.

Chemical formula moiety	$C_{30}H_{16}F_6N_2O$
Chemical formula weight	534.45
SymmetryCell setting	triclinic
Symmetry space group name H-M	'P -1'
Symmetry space group name Hall	'-P 1'
Symmetry Int Tables number	2
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Cell length b	14.0152(7)
Cell length c	21.8246(11)
Cell angle alpha	87.108(3)
Cell angle beta	79.954(3)
Cell angle gamma	86.606(3)
Cell volume	2418.8(2)
Cell formula units Z	4
Exptl crystal description	needle
Exptl crystal colour	colourless
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Exptl crystal density diffrn	1.468
Exptl crystal F 000	1088

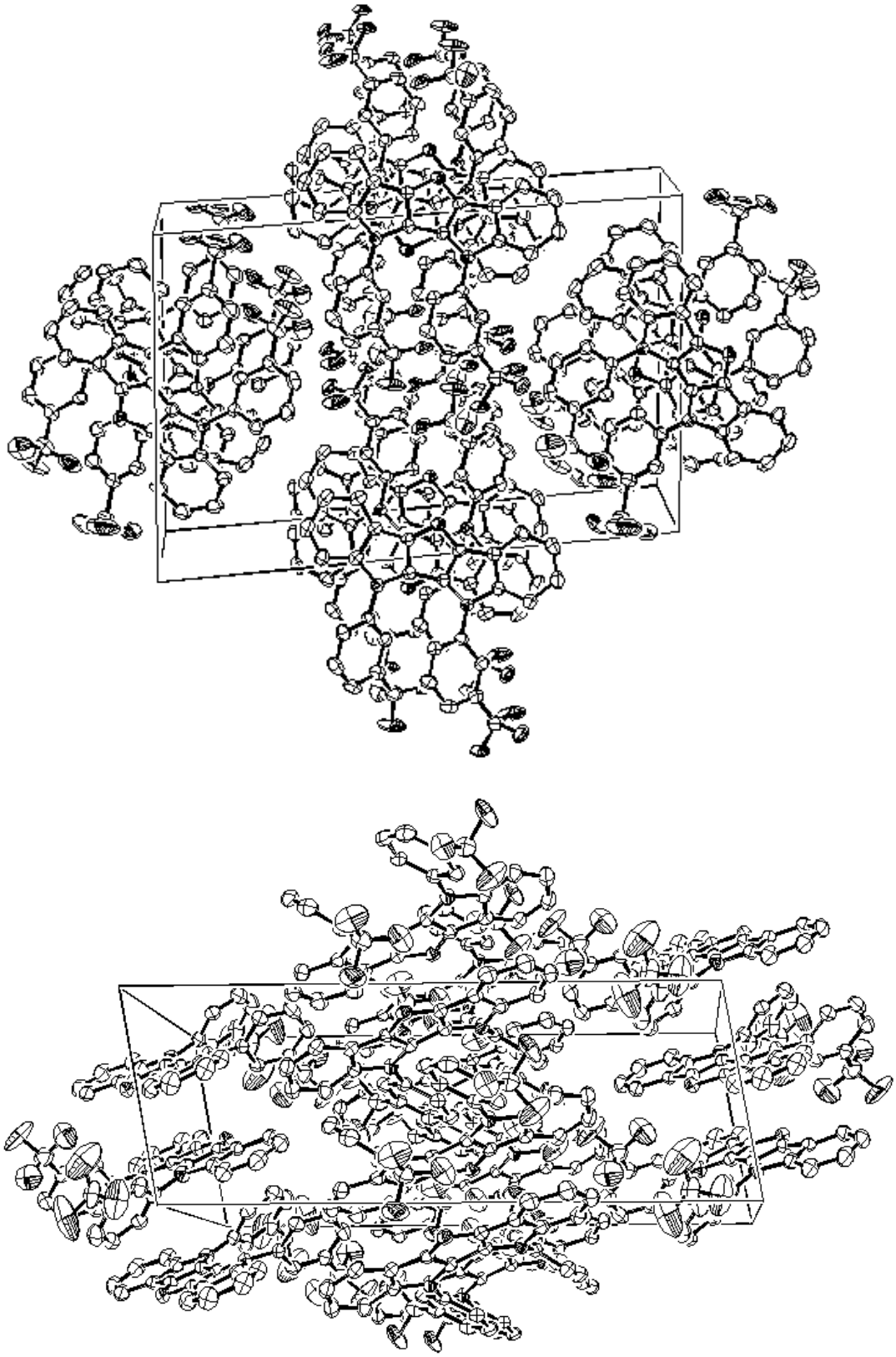


Figure 4. Crystal lattice of compound **3d** in triclinic form

Electrochemistry

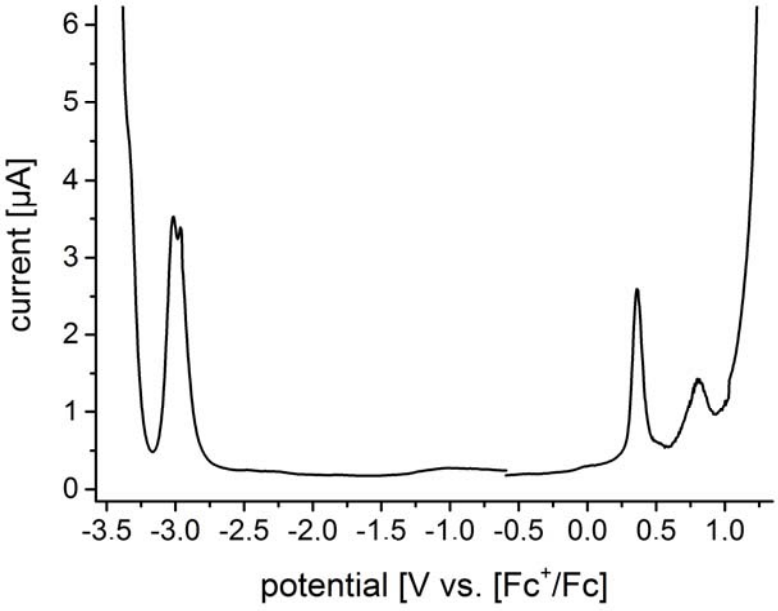


Figure 5. DPVs of selected compounds **3a** in DMF.

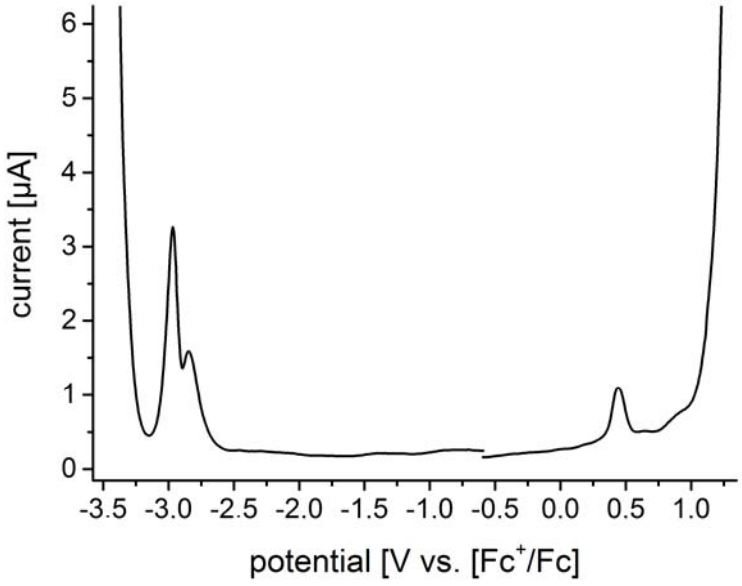


Figure 6. DPVs of selected compounds **3c** in DMF.

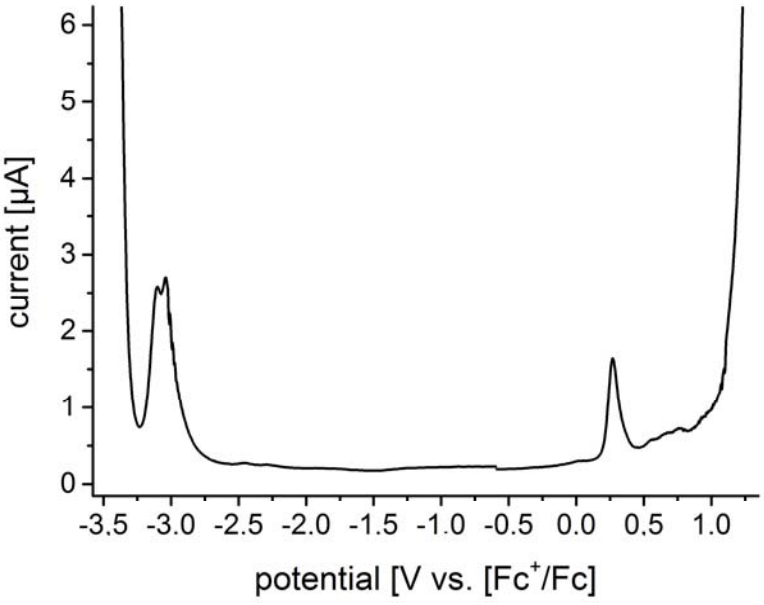


Figure 7. DPVs of selected compounds **3e** in DMF.

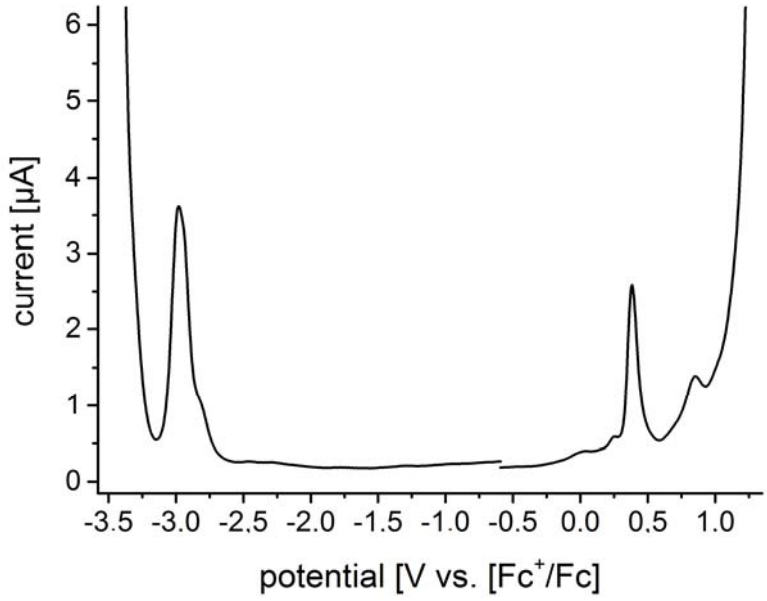


Figure 8. DPVs of selected compounds **3f** in DMF.

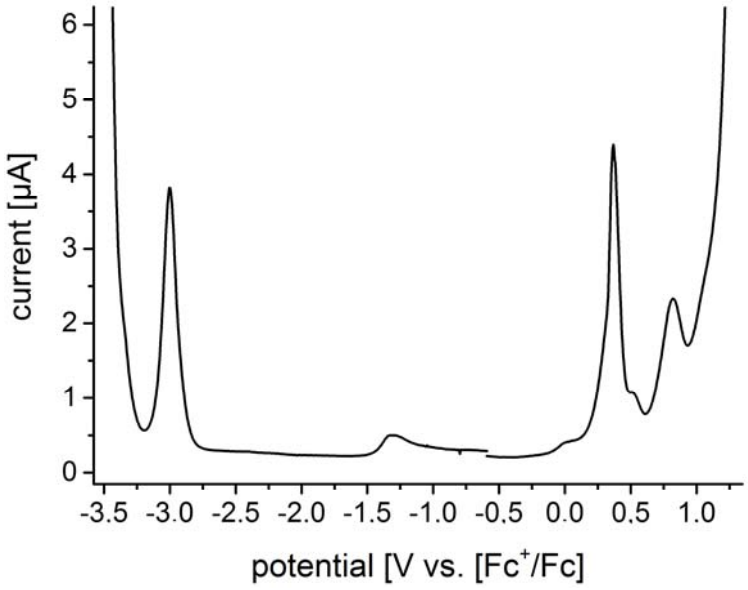
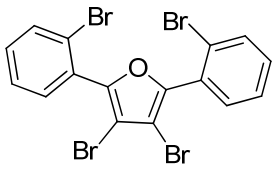


Figure 9. DPVs of selected compounds **3l** in DMF.

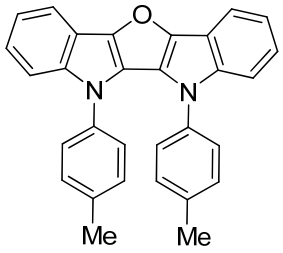
Analytical Data

3,4-Dibromo-2,5-bis(2-bromophenyl)furan (2)



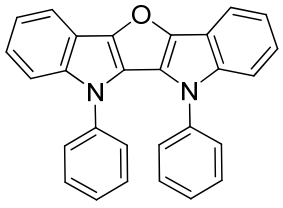
White solid, 78 %, M.p. 64 – 65 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.70 (dd, ^{3}J = 8.0 Hz, ^{4}J = 1.2 Hz, 2H, CH_{Ar}), 7.56 (dd, ^{3}J = 7.7 Hz, ^{4}J = 1.7 Hz, 2H, CH_{Ar}), 7.47 – 7.38 (m, 2H, CH_{Ar}), 7.36 – 7.28 (m, 2H, CH_{Ar}). ^{13}C NMR (63 MHz, $CDCl_3$) δ = 149.8 ($2C_{Ar}$), 133.6, 132.7, 131.4 ($2CH_{Ar}$), 130.3 ($2C_{Ar}$), 127.3 ($2CH_{Ar}$), 123.8, 104.3 ($2C_{Ar}$). IR (ATR, cm^{-1}): ṽ = 3064 (w), 3053 (w), 2949 (m), 2937 (m), 2918 (m), 2868 (w), 2850 (m), 1543 (w), 1514 (w), 1456 (s), 1441 (m). 2953 (w), 2920 (m), 2850 (m), 1574 (w), 1558 (w), 1464 (m), 1456 (m), 1423 (m). MS (EI, 70 eV): *m/z* (%) = 536 (100), 531 (M^+, 75), 429 (12), 376 (7), 351 (10), 297 (7), 267 (21), 185 (40), 155 (27), 112 (8). HRMS (EI, 70 eV): [$C_{16}H_8OBr_4$] 531.73032, found 531.73071.

5,6-Di-*p*-tolyl-5,6-dihydrofuro[3,2-*b*,4,5-*b'*]diindole (3a)



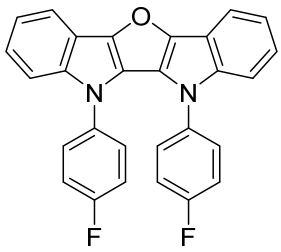
Green solid, 65 %, M.p. 221 – 223 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.87 (d, ^{3}J = 7.6 Hz, 2H, CH_{Ar}), 7.43 (d, ^{3}J = 8.5 Hz, 2H, CH_{Ar}), 7.29 – 7.15 (m, 4H, CH_{Ar}), 7.13 – 7.07 (m, 4H, CH_{Ar}), 6.88 (d, ^{3}J = 8.1 Hz, 4H, CH_{Ar}), 2.35 (s, 6H, $2CH_3$). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 145.7, 138.9, 136.4, 136.1 ($2C_{Ar}$), 129.5, 125.6 ($4CH_{Ar}$), 122.0 ($2CH_{Ar}$), 121.6 ($2C_{Ar}$), 120.7, 116.4 ($2CH_{Ar}$), 115.5, 111.2 ($2CH_{Ar}$), 21.2 ($2CH_3$). IR (ATR, cm^{-1}): ṽ = 1519 (m), 1454 (m), 1398 (m), 1363 (m), 1213 (m), 1193 (m), 1135 (m), 1110 (m), 1051 (m), 1012 (m), 819 (m), 802 (m), 725 (s), 713 (m), 597 (m). MS (EI, 70 eV): *m/z* (%) = 426 (M^+, 100), 411 (13, CH_3), 305 (3), 213 (10), 190 (3), 152 (1). HRMS (EI, 70 eV): [$C_{30}H_{22}ON_2$] 426.17266, found 426.17206.

5,6-Diphenyl-5,6-dihydrofuro[3,2-*b*,4,5-*b'*]diindole (3b)



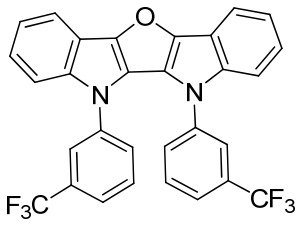
Green solid, 51 %, M.p. 220 – 222 °C. ^{1}H NMR (500 MHz, C_6D_6) δ = 8.01 – 7.95 (m, 2H, CH_{Ar}), 7.39 (m, 2H, CH_{Ar}), 7.24 – 7.18 (m, 2H, CH_{Ar}), 7.13 – 7.08 (m, 2H, CH_{Ar}), 6.90 – 6.84 (m, 4H, CH_{Ar}), 6.78 – 6.66 (m, 6H, CH_{Ar}). ^{13}C NMR (126 MHz, C_6D_6) δ = 146.5, 139.5, 139.1 ($2C_{Ar}$), 128.9 ($4CH_{Ar}$), 126.4 ($2CH_{Ar}$), 125.8 ($4CH_{Ar}$), 122.6 ($2CH_{Ar}$), 121.8 ($2C_{Ar}$), 121.4, 116.8 ($2CH_{Ar}$), 116.4 ($2C_{Ar}$), 111.4 ($2CH_{Ar}$). IR (ATR, cm^{-1}): ṽ = 3052 (w), 2917 (w), 2848 (w), 1594 (m), 1494 (m), 1456 (m), 1446 (m), 1313 (m), 1297 (m), 1230 (m), 1162 (m), 1120 (m), 1064 (m), 1016 (m), 904 (m), 879 (m), 860 (m), 754 (m), 742 (m), 730 (s), 702 (s), 684 (m), 653 (m). MS (EI, 70 eV): *m/z* (%) = 399 (29), 398 (M^+, 100), 397 (38), 369 (11), 292 (6), 264 (3), 199 (9). HRMS (EI, 70 eV): [$C_{28}H_{18}ON_2$] 398.14136, found 398.14080.

5,6-Bis(4-fluorophenyl)-5,6-dihydrofuro[3,2-*b*,4,5-*b'*]diindole (3c)



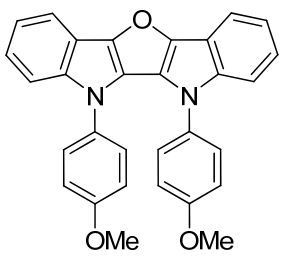
Green solid, 59 %, M.p. 224 – 225 °C. ^{1}H NMR (300 MHz, C_6D_6) δ = 8.17 – 7.97 (m, 2H, CH_{Ar}), 7.37 – 7.30 (m, 4H, CH_{Ar}), 7.27 – 7.21 (m, 2H, CH_{Ar}), 6.75 – 6.59 (m, 4H, CH_{Ar}), 6.59 – 6.30 (m, 4H, CH_{Ar}). ^{19}F NMR (282 MHz, C_6D_6) δ = -115.22. ^{13}C NMR (63 MHz, C_6D_6) δ = 161.5 (d, ^{1}J = 246.7 Hz, 2CF), 146.2, 139.5 ($2C_{Ar}$), 134.8 (d, ^{4}J = 2.9 Hz, $2C_{Ar}$), 127.6 (d, ^{3}J = 8.5 Hz, $4CH_{Ar}$), 122.7 ($2CH_{Ar}$), 121.7 ($2C_{Ar}$), 121.5, 116.8 ($2CH_{Ar}$), 116.2 ($2C_{Ar}$), 115.7 (d, ^{2}J = 22.9 Hz, $4CH_{Ar}$), 111.1 ($2CH_{Ar}$). IR (ATR, cm^{-1}): ṽ = 3052 (w), 2915 (w), 2848 (w), 1504 (m), 1461 (m), 1429 (m), 1319 (m), 1224 (m), 1149 (m), 1091 (m), 1066 (m), 1010 (m), 827 (m), 740 (m), 730 (s), 719 (m). MS (EI, 70 eV): *m/z* (%) = 434 (M^+, 100), 405 (11), 385 (3), 338 (2, F-C_6H_4), 310 (3), 283 (2), 217 (8). HRMS (EI, 70 eV): [$C_{28}H_{16}ON_2F_2$] 434.12252, found 434.12178.

5,6-Bis(3-(trifluoromethyl)phenyl)-5,6-dihydrofuro[3,2-*b*,4,5-*b'*]diindole (3d)



Green solid, 66 %, M.p. 205 – 207 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.87 (d, ^{3}J = 7.7 Hz, 2H, CH_{Ar}), 7.53 (s, 2H, CH_{Ar}), 7.44 (m, 4H, CH_{Ar}), 7.37 – 7.27 (m, 4H, CH_{Ar}), 7.26 – 7.15 (m, 4H, CH_{Ar}). ^{19}F NMR (282 MHz, $CDCl_3$) δ = -62.63. ^{13}C NMR (75 MHz, $CDCl_3$) δ = 146.5, 139.3, 139.0 ($2C_{Ar}$), 131.9 (q, ^{2}J = 33.1 Hz, $2CCF_3$), 129.7 ($2CH_{Ar}$), 128.6 (q, ^{3}J = 3.8 Hz, $2CH_{Ar}$), 123.4 (q, ^{4}J = 1.5 Hz, $2CH_{Ar}$), 123.3 (q, ^{1}J = 272.5 Hz, $2CF_3$), 122.9 ($2CH_{Ar}$), 122.2 (q, ^{3}J = 3.8 Hz, $2CH_{Ar}$), 121.6 ($2CH_{Ar}$), 120.6 ($2C_{Ar}$), 116.8 ($2CH_{Ar}$), 116.0 ($2C_{Ar}$), 110.7 ($2CH_{Ar}$). IR (ATR, cm^{-1}): ṽ = 3077 (w), 1494 (m), 1463 (m), 1456 (m), 1427 (m), 1365 (m), 1315 (m), 1305 (m), 1268 (m), 1232 (m), 1166 (m), 1118 (m), 1095 (m), 1066 (m), 798 (m), 730 (m), 698 (s), 676 (m). MS (EI, 70 eV): *m/z* (%) = 534 (M^+, 100), 505 (7), 437 (3), 388 (2, F_3C-C_6H_4), 290 (3), 267 (12), 232 (2), 145 (8). HRMS (EI, 70 eV): [$C_{30}H_{16}ON_2F_6$] 534.11613, found 534.11547

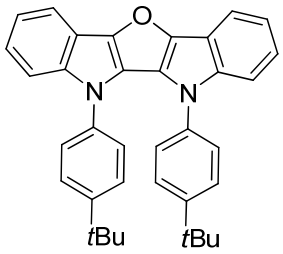
5,6-Bis(4-methoxyphenyl)-5,6-dihydrofuro[3,2-*b*,4,5-*b'*]diindole (3e)



Green solid, 53 %, M.p. 250 – 252 °C. ^{1}H NMR (500 MHz, C_6D_6) δ = 8.03 – 7.97 (m, 2H, CH_{Ar}), 7.41 – 7.36 (m, 2H, CH_{Ar}), 7.25 – 7.21 (m, 2H, CH_{Ar}), 7.15 – 7.12 (m, 2H, CH_{Ar}), 6.81 – 6.75 (m, 4H, CH_{Ar}), 6.35 – 6.26 (m, 4H, CH_{Ar}), 3.31 (s, 6H, OCH_3). ^{13}C NMR (126 MHz, C_6D_6) δ = 158.4, 146.1, 139.8, 131.8 ($2C_{Ar}$), 127.4 ($4CH_{Ar}$), 122.4 ($2C_{Ar}$), 122.4, 121.1, 116.8 ($2CH_{Ar}$), 116.1 ($2C_{Ar}$), 114.3 ($4CH_{Ar}$), 111.3 ($2CH_{Ar}$), 54.8 ($2OCH_3$). IR (ATR, cm^{-1}): ṽ = 3063 (w), 2955 (m), 2921 (m), 2850 (m), 2836 (m), 1581 (m), 1568 (m), 1504 (m), 1454 (m), 1427 (m), 1297 (m), 1247 (m), 1232 (m), 1178 (m), 1164 (m), 1101 (m), 1058 (m), 1029 (m), 821 (m), 800 (m), 732 (s).

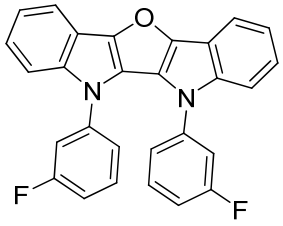
MS (EI, 70 eV): *m/z* (%) = 458 (M^+, 100), 443 (5, Me), 371 (5), 229 (13), 207 (1), 151 (3). HRMS (EI, 70 eV): [$C_{30}H_{22}O_3N_2$] 458.16249, found 458.16239.

5,6-Bis(4-(*tert*-butyl)phenyl)-5,6-dihydrofuro[3,2-*b*,4,5-*b*´]diindole (3f)



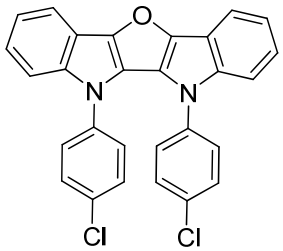
Green solid, 86 %, M.p. 230 – 232 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.85 (d, ^3J = 7.7 Hz, 2H, CH_{Ar}), 7.40 (d, ^3J = 8.2 Hz, 2H, CH_{Ar}), 7.25 – 7.10 (m, 12H, CH_{Ar}), 1.29 (s, 18H, $6CH_3$). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 149.6, 146.0, 140.0, 136.2 ($2C_{Ar}$), 125.8, 125.3 ($4CH_{Ar}$), 122.1 ($2CH_{Ar}$), 121.5 ($2C_{Ar}$), 120.9, 116.3 ($2CH_{Ar}$), 115.7 ($2C_{Ar}$), 111.7 ($2CH_{Ar}$), 34.6 ($2C_{Ar}$), 31.6 ($6CH_3$). IR (ATR, cm^{-1}): ṽ = 3057 (w), 3041 (w), 2962 (m), 1608 (w), 1576 (w), 1513 (m), 1487 (m), 1461 (m), 1446 (m), 1427 (m), 1361 (m), 1232 (m), 1313 (m), 1232 (m), 1112 (m), 1068 (m), 1014 (m), 819 (m), 734 (s), 557 (m). MS (EI, 70 eV): *m/z* (%) = 510 (M^+, 100), 437 (7), 409 (2), 320 (4), 292 (1), 248 (4), 213 (5). HRMS (EI, 70 eV): [$C_{36}H_{34}ON_2$] 510.26657, found 510.26635.

5,6-Bis(3-fluorophenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3g)



Green solid, 50 %, M.p. 198 – 200 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ = 7.90 – 7.84 (m, 2H, CH_{Ar}), 7.52 – 7.46 (m, 2H, CH_{Ar}), 7.37 – 7.16 (m, 4H, CH_{Ar}), 7.16 – 7.09 (m, 4H, CH_{Ar}), 7.04 – 6.96 (m, 2H, CH_{Ar}), 6.90 – 6.81 (m, 2H, CH_{Ar}). ^{19}F NMR (235 MHz, CDCl3) δ = -110.85. ^{13}C NMR (63 MHz, $CDCl_3$) δ = 162.9 (d, ^1J = 248.5 Hz, 2CF), 146.2 ($2C_{Ar}$), 140.3 (d, $^3J_{CF}$ = 9.9 Hz, $2C_{Ar}$), 138.9 ($2C_{Ar}$), 130.3 (d, ^3J = 9.3 Hz, $2CH_{Ar}$), 122.7 ($2CH_{Ar}$), 121.4 ($2CH_{Ar}$), 121.4 (d, ^4J = 2.2 Hz, $2CH_{Ar}$), 121.0 ($2C_{Ar}$), 116.7 ($2CH_{Ar}$), 115.9 ($2C_{Ar}$), 114.0 (d, ^2J = 21.1 Hz, $2CH_{Ar}$), 113.1 (d, ^{2}J = 23.4 Hz, $2CH_{Ar}$), 111.1 ($2CH_{Ar}$). IR (ATR, cm^{-1}): ṽ = 3064 (w), 3035 (w), 2961 (w), 1611 (m), 1591 (m), 1488 (m), 1459 (m), 1445 (m), 1426 (m), 1318 (m), 1295 (m), 1242 (m), 1216 (m), 1154 (m), 1129 (m), 1118 (m), 1066 (m), 866 (m), 824 (m), 800 (m), 777 (m), 741 (m), 731 (s), 710 (m), 677 (m). MS (EI, 70 eV): *m/z* (%) = 436 (4), 435 (28), 434 (M^+, 100), 433 (33), 415 (5), 405 (11), 385 (4), 338 (4, F-C_6H_4), 310 (5, F+F-C_6H_4), 309 (4), 208 (4), 95 (16), 76 (8), 75 (14). HRMS (EI, 70 eV): [$C_{28}H_{16}O_1N_2F_2$] 434.12252 found 434.12163.

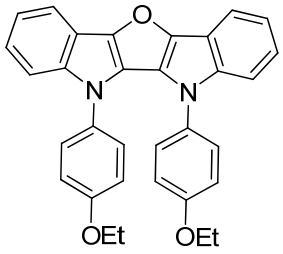
5,6-Bis(4-chlorophenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3h)



Green solid, 51 %, M.p. 249 – 251 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.89 – 7.83 (m, 2H, CH_{Ar}), 7.41 (d, ^3J = 8.2 Hz, 2H, CH_{Ar}), 7.28 (ddd, ^3J = 8.0 Hz, ^3J = 7.2 Hz, ^4J = 1.0 Hz, 2H, CH_{Ar}), 7.22 (ddd, ^3J = 8.4 Hz, ^3J = 7.1 Hz, ^4J = 1.3 Hz, 2H, CH_{Ar}), 7.17 – 7.11 (m, 8H, CH_{Ar}). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 146.1 ($2C_{Ar}$), 138.9 ($2C_{Ar}$), 137.2 ($2C_{Ar}$), 133.1 ($2C_{Ar}$), 129.3 ($4CH_{Ar}$), 127.0 ($4CH_{Ar}$), 122.6

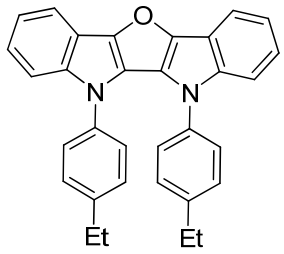
($2CH_{Ar}$), 121.3 ($2CH_{Ar}$), 121.1 ($2C_{Ar}$), 116.7 ($2CH_{Ar}$), 115.8 ($2C_{Ar}$), 110.9 ($2CH_{Ar}$). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 1490 (m), 1463 (m), 1430 (m), 1317 (m), 1304 (m), 1234 (m), 1088 (m), 1067 (m), 1012 (m), 818 (m), 735 (s), 723 (m). MS (EI, 70 eV): *m/z* (%) = 470 (14), 469 (23), 468 (M^+, 68), 467 (37), 466 (M^+, 100), 465 (16), 431 (6), 403 (6), 401 (7), 367 (8), 292 (8), 291 (8), 290 (7), 264 (6), 234 (6), 233 (7), 215 (7), 188 (7), 184 (7), 163 (8), 152 (8), 113 (14), 111 (41), 104 (10), 77 (10), 76 (37), 75 (48), 74 (7), 73 (7), 50 (10). HRMS (EI, 70 eV): [$C_{28}H_{16}O_1N_2Cl_2$] 466.06342 found 466.06303, [$C_{28}H_{16}O_1N_2Cl_1{}^{37}Cl_1$] 468.06047 found 468.06151.

5,6-Bis(4-ethoxyphenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b´*]diindole (3i)



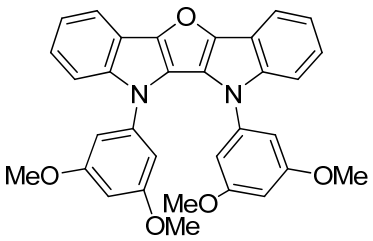
Green solid, 56 %, M.p. 188 – 190 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.89 (d, ^3J = 7.8 Hz, 2H, CH_{Ar}), 7.38 (d, ^3J = 8.3 Hz, 2H, CH_{Ar}), 7.26 (pt, ^3J = 7.1 Hz, 2H, CH_{Ar}), 7.20 (pt, ^3J = 7.6 Hz, 2H, CH_{Ar}), 7.10 – 7.02 (m, 4H, CH_{Ar}), 6.63 – 6.52 (m, 4H, CH_{Ar}), 3.96 (q, ^3J = 7.0 Hz, 4H, $2CH_2$), 1.49 (t, ^3J = 7.0 Hz, 6H, $2CH_3$). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 157.9 ($2C_{Ar}$), 145.6 ($2C_{Ar}$), 139.4 ($2C_{Ar}$), 131.5 ($2C_{Ar}$), 127.3 ($4CH_{Ar}$), 122.2 ($2CH_{Ar}$), 122.1 ($2C_{Ar}$), 120.8 ($2CH_{Ar}$), 116.5 ($2CH_{Ar}$), 115.5 ($2C_{Ar}$), 114.9 ($4CH_{Ar}$), 110.9 ($2CH_{Ar}$), 63.8 ($2CH_2$), 15.3 ($2CH_3$). IR (ATR, cm-1): $\tilde{\nu}$ = 2974 (w), 2930 (w), 2895 (w), 1512 (m), 1463 (m), 1432 (m), 1391 (m), 1313 (m), 1246 (m), 1238 (m), 1171 (m), 1151 (m), 1112 (m), 1043 (m), 826 (m), 733 (s). MS (EI, 70 eV): *m/z* (%) = 488 (6), 487 (32), 486 (M^+, 100), 457 (4), 442 (6, OEt), 429 (4), 401 (4), 385 (3), 372 (3), 371 (5), 342 (3), 279 (3), 215 (3). HRMS (EI, 70 eV): [$C_{32}H_{26}O_3N_2$] 486.19379 found 486.19277.

5,6-Bis(4-ethylphenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b´*]diindole (3j)



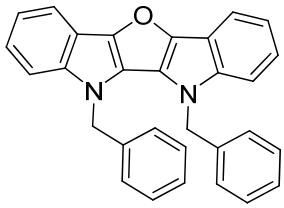
Green solid, 73 %, M.p. 167 – 169 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ = 7.92 (dd, ^3J = 7.8 Hz, ^4J = 1.5 Hz, 2H, CH_{Ar}), 7.48 (dd, ^3J = 8.0 Hz, ^4J = 1.3 Hz, CH_{Ar}), 7.33 – 7.18 (m, 4H, CH_{Ar}), 7.17 – 7.10 (m, 4H, CH_{Ar}), 6.94 – 6.87 (m, 4H, CH_{Ar}), 2.63 (q, ^3J = 7.6 Hz, 4H, $2CH_2$), 1.28 (t, ^3J = 7.6 Hz, 6H, $2CH_3$). ^{13}C NMR (63 MHz, $CDCl_3$) δ = 145.7 ($2C_{Ar}$), 142.4 ($2C_{Ar}$), 139.1 ($2C_{Ar}$), 136.2 ($2C_{Ar}$), 128.2 ($4CH_{Ar}$), 125.6 ($4CH_{Ar}$), 122.0 ($2CH_{Ar}$), 121.5 ($2C_{Ar}$), 120.7 ($2CH_{Ar}$), 116.3 ($2CH_{Ar}$), 115.4 ($2C_{Ar}$), 111.3 ($2CH_{Ar}$), 28.4 ($2CH_2$), 15.4 ($2CH_3$). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2966 (w), 2931 (w), 2874 (w), 1512 (m), 1457 (m), 1426 (m), 1318 (m), 1310 (m), 1231 (m), 1064 (m), 1010 (m), 818 (m), 731 (s). MS (EI, 70 eV): *m/z* (%) = 456 (6), 455 (34), 454 (M^+, 100), 453 (12), 438 (3), 426 (4), 425 (13), 410 (3), 320 (3 Et-C_6H_4), 305 (3), 292 (3), 105 (4), 104 (5), 91 (3), 89 (3), 77 (6), 76 (3). HRMS (EI, 70 eV): [$C_{32}H_{26}O_1N_2$] 454.20396 found 454.20303.

5,6-Bis(3,5-dimethoxyphenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b´*]diindole (3k)



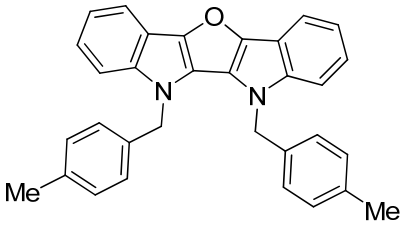
Green solid, 53 %, M.p. 213 – 215 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.93 – 7.86 (m, 2H, CH_{Ar}), 7.60 – 7.55 (m, 2H, CH_{Ar}), 7.35 – 7.17 (m, 4H, CH_{Ar}), 6.50 (d, ^{4}J = 2.2 Hz, 4H, CH_{Ar}), 6.28 (pt, ^{4}J = 2.3 Hz, 2H, CH_{Ar}), 3.71 (s, 12H, $2OCH_3$). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 161.0 ($4C_{Ar}$), 145.8 ($2C_{Ar}$), 140.4 ($2C_{Ar}$), 138.7 ($2C_{Ar}$), 122.3 ($2CH_{Ar}$), 121.3 ($2C_{Ar}$), 120.9 ($2CH_{Ar}$), 116.5 ($2CH_{Ar}$), 115.6 ($2C_{Ar}$), 111.3 ($2CH_{Ar}$), 104.0 ($4CH_{Ar}$), 99.3 ($2CH_{Ar}$), 55.2 ($4OCH_3$). IR (ATR, cm^{-1}): ṽ = 2962 (w), 2923 (w), 2842 (w), 1596 (m), 1456 (m), 1425 (m), 1286 (m), 1256 (m), 1204 (m), 1155 (m), 1051 (m), 826 (m), 785 (m), 742 (s), 678 (m). MS (EI, 70 eV): *m/z* (%) = 520 (6), 519 (33), 518 (M^+, 100), 487 (4, OMe), 444 (2), 443 (2), 279 (2), 264 (2), 259 (2), 79 (2), 77 (2), 69 (2), 63 (2). HRMS (EI, 70 eV): [$C_{32}H_{26}O_5N_2$] 518.18362 found 518.18261.

5,6-Dibenzyl-5,6-dihydrofuro[3,2-*b*,4,5-*b*']diindole (3l)



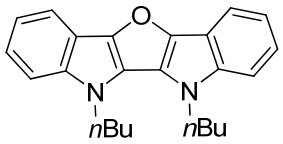
Green solid, 53 %, M.p. 230 – 232 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ = 7.82 – 7.74 (m, 2H, CH_{Ar}), 7.24 – 7.05 (m, 12H, CH_{Ar}), 6.92 – 6.82 (m, 4H, CH_{Ar}), 5.21 (s, 4H, CH_2). ^{13}C NMR (63 MHz, $CDCl_3$) δ = 144.7, 138.8, 137.2 ($2C_{Ar}$), 128.9 ($4CH_{Ar}$), 127.5 ($2CH_{Ar}$), 125.6 ($4CH_{Ar}$), 121.6 ($2CH_{Ar}$), 121.4 ($2C_{Ar}$), 119.9, 116.3 ($2CH_{Ar}$), 114.9 ($2C_{Ar}$), 110.0 ($2CH_{Ar}$), 48.8 ($2CH_2$). IR (ATR, cm^{-1}): ṽ = 3027 (w), 2919 (w), 1732 (w), 1699 (w), 1576 (m), 1556 (w), 1495 (m), 1464 (m), 1452 (m), 1427 (m), 1344 (m), 1315 (m), 1295 (m), 1257 (m), 1197 (m), 1128 (m), 1093 (m), 1074 (m), 1043 (m), 1029 (m), 1014 (m), 1002 (m), 732 (s), 711 (m), 692 (m). MS (EI, 70 eV): *m/z* (%) = 426 (M^+, 100), 335 (39, Bn), 306 (12), 91 (24), 73 (5), 60 (7), 43 (8). HRMS (EI, 70 eV): [$C_{30}H_{22}ON_2$] 426.17266, found 426.17337.

5,6-Bis(4-methylbenzyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3m)



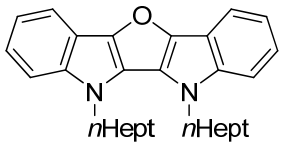
Green solid, 51 %, M.p. 210 – 212 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.30 – 7.20 (m, 2H, CH_{Ar}), 6.69 – 6.52 (m, 6H, CH_{Ar}), 6.42 – 6.35 (m, 4H, CH_{Ar}), 6.25 – 6.19 (m, 4H, CH_{Ar}), 4.67 (s, 4H, CH_2), 1.67 (s, 6H, CH_3). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 144.8 ($2C_{Ar}$), 138.8 ($2C_{Ar}$), 137.2 ($2C_{Ar}$), 134.3 ($2C_{Ar}$), 129.6 ($4CH_{Ar}$), 125.6 ($4CH_{Ar}$), 121.6 ($2CH_{Ar}$), 121.6 ($2C_{Ar}$), 119.9 ($2CH_{Ar}$), 116.3 ($2CH_{Ar}$), 115.0 ($2C_{Ar}$), 110.2 ($2CH_{Ar}$), 48.7 ($2CH_2$), 21.1 ($2CH_3$). IR (ATR, cm^{-1}): ṽ = 3050 (w), 2920 (w), 2854 (w), 1514 (m), 1461 (m), 1446 (m), 1428 (m), 1341 (m), 1315 (m), 1258 (m), 1180 (m), 1118 (m), 1091 (m), 1042 (m), 1016 (m), 791 (m), 733 (s), 725 (s), 469 (m). MS (EI, 70 eV): *m/z* (%) = 456 (5), 455 (35), 454 (M^+, 100), 350 (9), 349 (31, Me-Bn), 348 (10), 334 (8), 321 (5), 320 (6), 305 (5), 245 (6), 105 (54), 79 (9), 77 (8). HRMS (EI, 70 eV): [$C_{32}H_{26}O_1N_2$] 454.20396 found 454.20349.

5,6-Di-*n*-butyl-5,6-dihydrofuro[3,2-*b*:4,5-*b´*]diindole (3n)



Green soild, 48 %, M.p. 150 – 152 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.87 – 7.76 (m, 2H, CH_{Ar}), 7.48 – 7.38 (m, 2H, CH_{Ar}), 7.30 – 7.14 (m, 4H, CH_{Ar}), 4.46 – 4.34 (m, 4H, $2CH_2$), 2.00 – 1.84 (m, 4H, $2CH_2$), 1.51 – 1.36 (m, 4H, $2CH_2$), 0.97 (t, ^{3}J = 7.3 Hz, 6H, CH_3). ^{13}C NMR (63 MHz, $CDCl_3$) δ = 144.6 ($2C_{Ar}$), 138.4 ($2C_{Ar}$), 121.4 ($2C_{Ar}$), 121.3 ($2CH_{Ar}$), 119.6 ($2CH_{Ar}$), 116.4 ($2CH_{Ar}$), 115.0 ($2C_{Ar}$), 110.2 ($2CH_{Ar}$), 46.6 ($2CH_2$), 33.0 ($2CH_2$), 20.7 ($2CH_2$), 14.1 ($2CH_3$). IR (ATR, cm^{-1}): ṽ = 3062 (w), 2953 (m), 2921 (m), 2862 (m), 1463 (m), 1428 (m), 1343 (m), 1317 (m), 1293 (m), 1201 (m), 1155 (m), 1122 (m), 1115 (m), 1044 (m), 1012 (m), 723 (s), 706 (m), 427 (m). MS (EI, 70 eV): *m/z* (%) = 360 (5), 359 (25), 358 (M^+, 100), 315 (7), 273 (6), 272 (4), 271 (5), 260 (4), 259 (16), 258 (10), 245 (5), 231 (4), 229 (9), 216 (4), 190 (4), 76 (5), 57 (5), 41 (17). HRMS (EI, 70 eV): [$C_{24}H_{26}O_1N_2$] 358.20396 found 358.20364.

5,6-Diheptyl-5,6-dihydrofuro[3,2-*b*,4,5-*b'*]diindole (3o)



Green solid, 46 %, M.p. 109 – 111 °C. ^{1}H NMR (300 MHz, Acetone) δ = 7.85 – 7.68 (m, 2H, CH_{Ar}), 7.65 – 7.52 (m, 2H, CH_{Ar}), 7.30 – 7.10 (m, 4H, CH_{Ar}), 4.69 – 4.39 (m, 4H, $2CH_2$), 2.02 – 1.88 (m, 4H, $2CH_2$), 1.50 – 1.25 (m, 16H, $8CH_2$), 0.84 (t, ^{3}J = 6.8 Hz, 6H, $2CH_3$). ^{13}C NMR (75 MHz, Acetone) δ = 145.0, 139.4 ($2C_{Ar}$), 122.2 ($2CH_{Ar}$), 122.1 ($2C_{Ar}$), 120.4, 116.6 ($2CH_{Ar}$), 115.5 ($2C_{Ar}$), 111.5 ($2CH_{Ar}$), 47.2, 32.5, 31.5, 29.9, 27.8, 23.2 ($2CH_2$), 14.3 ($2CH_3$). IR (ATR, cm^{-1}): ṽ = 2950 (m), 2923 (m), 2854 (m), 1645 (w), 1620 (w), 1577 (m), 1463 (m), 1429 (m), 1346 (m), 1319 (m), 1226 (m), 1157 (m), 1126 (m), 1047 (m), 1012 (m), 723 (s), 707 (m). MS (EI, 70 eV): *m/z* (%) = 442 (M^+, 100), 357 (3), 314 (1), 259 (8), 137 (3), 96 (1), 76 (1), 43 (4). HRMS (EI, 70 eV): [$C_{30}H_{38}ON_2$] 442.29787, found 442.29764.

DFT Calculations

Figure 1: Calculated electron distribution of HOMO (left) and LUMO (right) of compound **3c**.

Figure 2: Calculated electron distribution of HOMO (left) and LUMO (right) of compound **3e**.

Figure 3: Calculated electron distribution of HOMO (left) and LUMO (right) of compound **3l**.

Geometry optimisation

Geometry optimization for **3a**
1\1\GINC-NODE194\Freq\RB3LYP\6-311G(d,p)\C30H22N2O1\ \#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-311G(d,p) Freq\\3a\\0,1\O, -1.5137083859, 0.9900571049, -0.0236098544\C, -1.3751762958, -0.3727096678, -0.0177927864\C, -0.2202235878, 1.4408304387, -0.0183881975\C, -0.0522144686, -0.7858874132, 0.0039547363\C, 0.7138303856, 0.4166606638, -0.0227813382\C, 0.433437527, 2.6967774804, 0.0492327978\N, 1.9900399257, 0.9706571148, 0.0412515819\C, 1.8269442781, 2.3678409249, 0.0637147128\C, -2.2360283293, -1.4967275885, -0.0866304739\C, -1.3484545864, -2.6203549362, -0.0832610383\N, -0.0137087521, -2.1770174597, -0.0495551086\C, -3.621859302, -1.705428875, -0.1262256501\C, -1.8459481777, -3.9228554397, -0.0731938802\C, -3.2247760411, -4.1006487743, -0.1066086464\C, -4.1035000365, -3.0051890964, -0.1413532664\H, -1.1795378403, -4.7750064371, -0.036050833\H, -3.6268293588, -5.1072414837, -0.1039956766\H, -5.1726310613, -3.180810094, -0.1727453024\H, -4.2990804315, -0.8597302322, -0.1372059584\C, 2.7971027935, 3.369274085, 0.0579199849\C, 0.0361554256, 4.0410760616, 0.0754058024\C, 1.0102199816, 5.0271944136, 0.0949477768\C, 2.3748425031, 4.694092912, 0.0778253175\H, 0.7169976282, 6.0704882631, 0.1161106831\H, -1.0165872987, 4.2973296365, 0.0728580259\H, 3.1169000386, 5.4841714064, 0.0783421524\H, 3.8513469287, 3.1251490595, 0.0342688263\C, 3.2245311597, 0.2915609074, -0.1555228358\C, 4.2798526454, 0.4771183079, 0.7385011606\C, 5.4956141391, -0.1659219385, 0.5229281758\C, 5.6839813217, -1.0180456488, -0.5688162664\C, 4.6079896898, -1.2096639562, -1.44248366\C, 3.3955940135, -0.5585076517, -1.2500340581\H, 4.1413953951, 1.1137382464, 1.603952069\H, 6.3079022466, -0.0097774828, 1.2253944138\H, 4.7219475734, -1.8719962605, -2.2942923104\C, 7.0120309452, -1.6919525738, -0.8150103237\H, 6.8795441971, -2.7127557348, -1.1820153802\H, 7.6129297466, -1.7341367781, 0.0959852512\H, 7.5945975277, -1.1492334569, -1.5674232482\H, 2.5787051172, -0.7030492189, -1.9469539751\C, 1.1221921759, -3.0062857617, 0.1643595234\C, 1.954155601, -2.7926776229, 1.2660771124\C, 1.4086551518, -4.0484042131, -0.7174107792\C, 3.0545902629, -3.6136404513, 1.47610729\C, 2.5042029427, -4.8761955514, -0.4841749023\C, 3.3460633203, -4.6761079624, 0.612494878\H, 0.7808555689, -4.2009549748, -1.5869039568\H, 2.7122994472, -5.6850080669, -1.1769771501\H, 3.6935164225, -3.4307426881, 2.3338961388\H,

1.7315817427, -1.9864812618, 1.9548478673\C, 4.5274068347, -5.5794689048, 0.8713217734\H, 4.7053765522, -6.2531350781, 0.0307803222\H, 4.3652334078, -6.1959798698, 1.7615790759\H, 5.4402313893, -5.0012664207, 1.0400794066 \\Version=ES64L-G09RevE.01 \State=1-A \HF=-1341.4717613 \RMSD=4.289e-09 \RMSF=2.430e-06 \ZeroPoint=0.4364439 \Thermal=0.4626765 \Dipole=1.6985656, -1.0673865, 0.0, \DipoleDeriv=-0.7869492, 0.1656882, 0.0, \Polar=458.4168076, 15.8775336, 472.8010882, 17.2689245, 23.8783279, 188.1208707 \PG=C01 [X(C30H22N2O1)] \NImag=0\\0.0, 0.0, 0.0, \\@

Geometry optimization for **3c**

1\1\GINC-NODE064\Freq\RB3LYP\6-311G(d,p)\C28H16F2N2O1\ \#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-311G(d, p) Freq\\3c\\0, 1\O, -1.5110586123, 0.9950084722, -0.038995807\C, -1.3871699439, -0.3679438732, 0.0156299015\C, -0.2134212673, 1.4321107082, -0.0713044359\C, -0.0682886084, -0.7937446335, 0.0304736419\C, 0.7091943731, 0.3980269276, -0.0510002881\C, 0.4553754031, 2.6824358222, -0.0632720047\N, 1.9919780486, 0.9398683447, -0.028111541\C, 1.8451190591, 2.3388735404, -0.0566020563\C, -2.2601288482, -1.4852955602, 0.0044413059\C, -1.3842538753, -2.6173193063, 0.0333608559\N, -0.0449746535, -2.186250869, 0.0282108424\C, -3.6482585665, -1.6818105143, -0.0030732872\C, -1.8922556972, -3.9139952025, 0.0966666188\C, -3.2730200359, -4.0791955229, 0.0933212483\C, -4.1416284728, -2.9766765542, 0.036144029\H, -1.2332799188, -4.7711652185, 0.1519950807\H, -3.6844890969, -5.080872951, 0.1379852653\H, -5.2126381933, -3.1427728805, 0.0301727486\H, -4.3180557037, -0.8307373561, -0.0321337355\C, 2.8269987093, 3.3269231118, -0.1123422563\C, 0.0740081686, 4.0314083437, -0.0832853252\C, 1.0596189492, 5.0056890735, -0.1146477802\C, 2.4200649527, 4.6564431654, -0.1368990817\H, 0.7786048049, 6.052345208, -0.1297190409\H, -0.9755513819, 4.3001434559, -0.0811707964\H, 3.1707804174, 5.4371762844, -0.1761541617\H, 3.8783399847, 3.0701865474, -0.1408518527\C, 3.2166732003, 0.2356667296, -0.183835448\C, 4.2582858994, 0.4332267661, 0.7267022436\C, 5.4675021041, -0.2365345924, 0.5656885331\C, 5.6092023826, -1.1153488382, -0.4976649027\C, 4.5857303924, -1.3389186791, -1.4064867291\C, 3.3880473291, -0.649777683, -1.2511691463\H, 4.1156430512, 1.1052353921, 1.5637020471\H, 6.2887257883, -0.0960547319, 1.2571834143\H, 4.7377549825, -2.0319206388, -2.2240468408\H, 2.5827224238, -0.792910978, -1.9610018329\C, 1.0905007256, -3.0192413286, 0.2200707722\C, 1.9465378604, -2.8028601277, 1.3031043423\C, 1.3502773661, -4.0644614865, -0.67049479\C, 3.0573834257, -3.6172058249, 1.493785601\C, 2.4479466751, -4.8970933938, -0.4741561865\C, 3.286018059, -4.6562952006, 0.6041591179\H, 0.6960583018, -4.2175727452, -1.5196540842\H, 2.6662040358, -5.7146050702, -1.1496889475\H, 3.7349876736, -3.4644825359, 2.3240220152\H, 1.7367390206, -1.9985601184, 1.9973564062\F, 6.7780775663, -1.7725648704, -0.652322232\F, 4.3560617417, -5.4572486075, 0.7930985596 \\Version=ES64L-G09RevE.01 \State=1-A \HF=-1461.3432374 \RMSD=7.511e-09 \RMSF=4.786e-06 \ZeroPoint=0.3656242 \Thermal=0.389743 \Dipole=0.3816189, -0.24852, 0.0059619 \DipoleDeriv=-0.7579092, 0.1585875, 0.0, \Polar=417.0094543, 30.6836826, 444.7032838, 13.6511238, 15.5162661, 168.7050579 \PG=C01 [X(C28H16F2N2O1)] \NImag=0\\0.0, 0.0, 0.0, \\@

Geometry optimization for **3e**

1\1\GINC-NODE066\Freq\RB3LYP\6-311G(d,p)\C30H22N2O3\ \#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-311G(d,p) Freq\\3e\\0,1\O, -1.5133554533, 0.9432922886, -0.0080075273\C, -1.346416422, -0.4155752257, 0.0632944677\C, -0.2290733276, 1.4182623344, -0.0747941348\C, -0.0145045656, -0.8010398692, 0.0529462084\C, 0.7244759341, 0.4117307006, -0.0574081261\C, 0.4044753056, 2.6859212448, -0.1116865919\N, 1.9901493852, 0.9880615842, -0.0819446591\C, 1.8037769482, 2.3786417412, -0.1342076066\C, -2.182239201, -1.5600316714, 0.0994229078\C, -1.2673035367, -2.6622895933, 0.1290493856\N,

0.054033541, -2.1899873176, 0.0813208993\C, -3.5626772686, -1.8052664734, 0.1297947184\C, -1.7284853981, -3.974558865, 0.2235555169\C, -3.1021892403, -4.18717973, 0.2571793981\C, -4.0095783919, -3.1154776888, 0.2042571321\H, -1.0359288979, -4.8055686095, 0.2727156599\H, -3.4782285527, -5.2013945321, 0.3275251065\H, -5.0741816442, -3.3180719877, 0.2280503402\H, -4.2628204249, -0.9788024442, 0.101212417\C, 2.7586137457, 3.3902450865, -0.2270894019\C, -0.0108334984, 4.0249146202, -0.1474814989\C, 0.9486330174, 5.0229412842, -0.2202955588\C, 2.3174203164, 4.7082815755, -0.266209224\H, 0.6403128089, 6.0617631782, -0.2482205208\H, -1.0665207762, 4.2679060826, -0.1243087696\H, 3.0463633721, 5.507556274, -0.3354092233\H, 3.8149523238, 3.1560041028, -0.2708373355\C, 3.2336700588, 0.3135443532, -0.2476721171\C, 4.2565065173, 0.4828974739, 0.6808238747\C, 5.485563655, -0.1555233718, 0.512456746\C, 5.688416685, -0.989942953, -0.5897671451\C, 4.6564356888, -1.1658500349, -1.5208387489\C, 3.4462545362, -0.5148264541, -1.3556147089\H, 4.0905907397, 1.1129161213, 1.546476116\H, 6.2623125232, -0.004747631, 1.2496465327\H, 4.8335492768, -1.8127158461, -2.3709825846\O, 6.8399582745, -1.6697604291, -0.8481760575\H, 2.6564826803, -0.6413537093, -2.0864208105\C, 1.2230410354, -2.9849293057, 0.2554311829\C, 2.0513014307, -2.7900250373, 1.3666797733\C, 1.5461581146, -3.9746828968, -0.6681440405\C, 3.1840505098, -3.5662439457, 1.5400645084\C, 2.6763329048, -4.773426266, -0.491547032\C, 3.5055073239, -4.5671848773, 0.6140150296\H, 0.9144258736, -4.1191395063, -1.536384878\H, 2.9022449016, -5.5353222313, -1.225030664\H, 3.8359841511, -3.424002882, 2.3928818259\H, 1.7979822605, -2.0276406945, 2.0936049613\O, 4.6364705885, -5.2778116645, 0.8803645022\C, 7.9156148458, -1.5561130593, 0.0735696171\H, 7.6319507729, -1.922741787, 1.0661413697\H, 8.269624894, -0.5222224184, 0.1531655509\H, 8.7150649903, -2.1784411512, -0.3248663042\C, 5.033143356, -6.2891371876, -0.0358084403\H, 4.2770460939, -7.0780810939, -0.1162521796\H, 5.9508147246, -6.7127988002, 0.3686157318\H, 5.2337404936, -5.8725408043, -1.0289355907\ \Version=ES64L-G09RevE.01 \State=1-A \HF=-1491.9231932 \RMSD=7.412e-09 \RMSF=5.367e-06 \ZeroPoint=0.4465574 \Thermal=0.4743343 \Dipole=2.1765726, -1.3260735, 0.0075384 \DipoleDeriv=-0.7959176, 0.1582905, 0.0, \Polar=472.2593581, 9.4617715, 482.1432207, 5.91884, 8.2367439, 192.2590073\PG=C01 [X(C30H22N2O3)]\NImag=0\\0.0, 0.0, 0.0, \\@

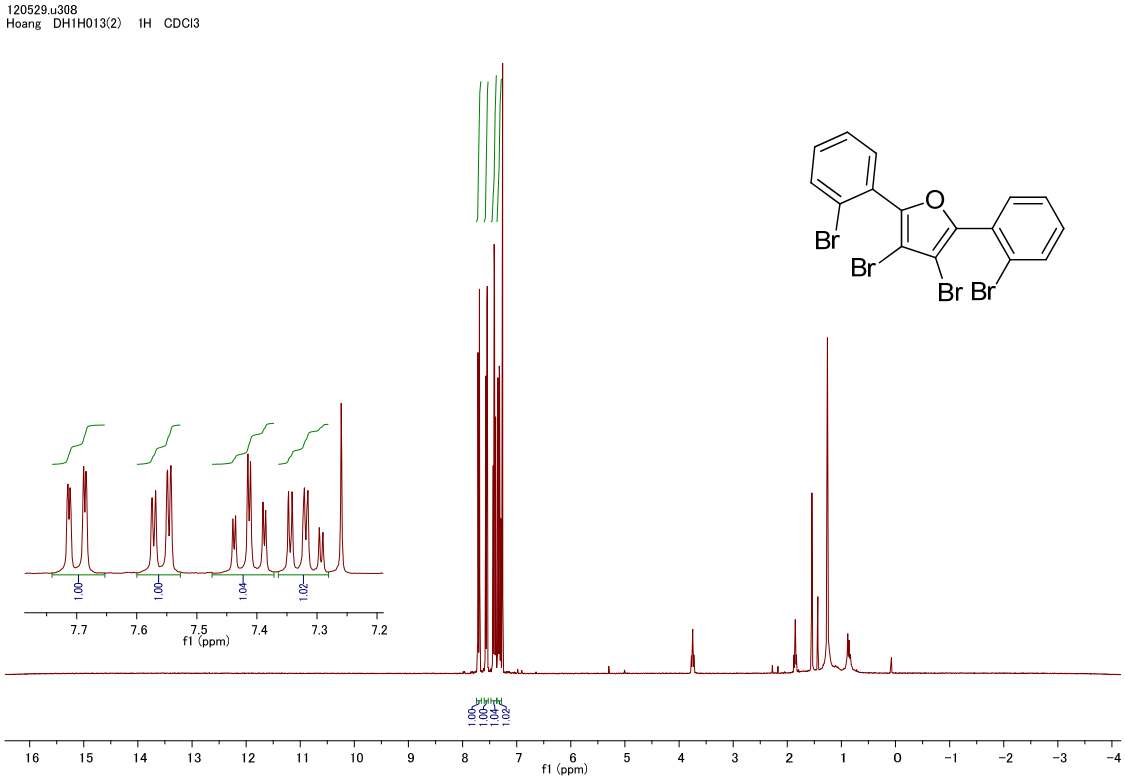
Geometry optimization for **3l**

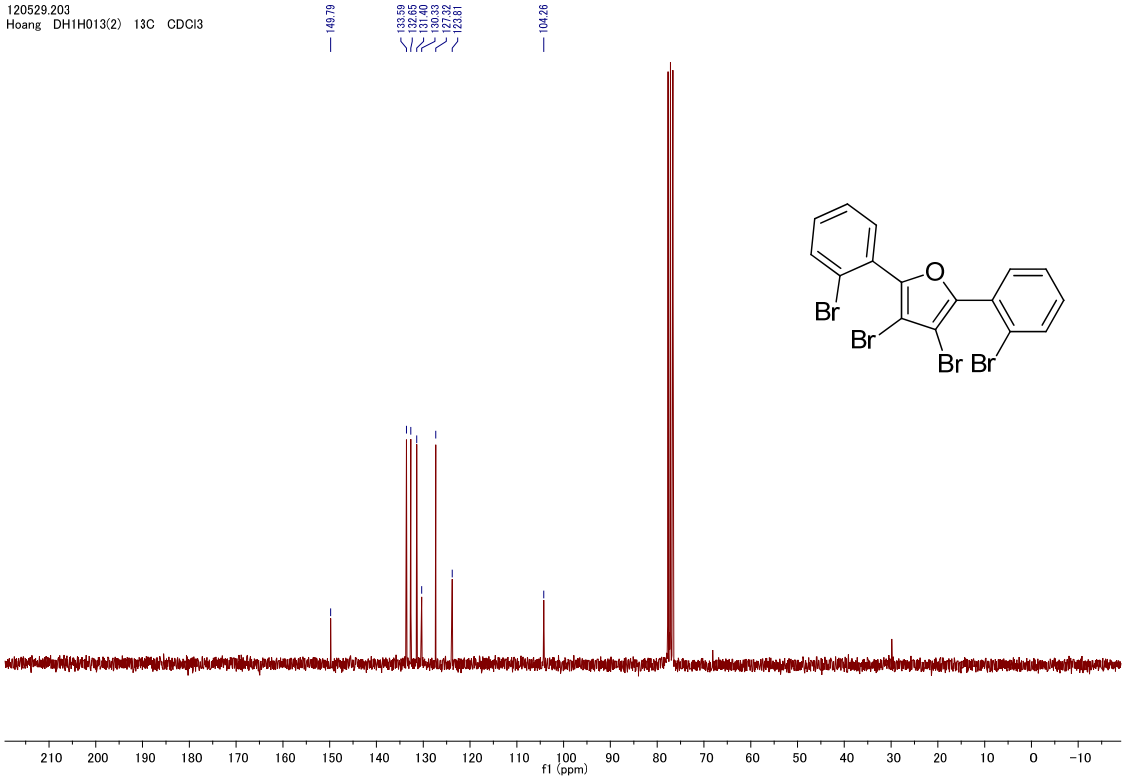
1\1\GINC-NODE069\Freq\RB3LYP\6-311G(d,p)\C30H22N2O1\ \#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-311G(d,p) Freq\\3l\\0, 1\C, 4.3059312706, -1.347562179, 0.0834370195\C, 4.1382646792, -2.7223528684, 0.1557877272\O, 5.3250625206, -3.4095408662, 0.1177887992\C, 6.265873526, -2.4157103996, 0.0213882791\C, 5.7111074898, -1.1447983217, 0.0018147339\C, 7.6789714823, -2.322578311, -0.0507676387\C, 7.9340264445, -0.911419119, -0.1177118848\N, 6.7286596968, -0.2064623156, -0.0774211906\N, 3.0617123444, -0.7365177741, 0.108965274\C, 2.1081281054, -1.7524489173, 0.2091815145\C, 2.7569726854, -3.0327769384, 0.2356686169\C, 8.7552985798, -3.2210349302, -0.0669311853\C, 10.0460914053, -2.7217972676, -0.1498228172\C, 10.2840675658, -1.3387839925, -0.2209361009\C, 9.2375313213, -0.4232427567, -0.2088386155\C, 0.7186121632, -1.6526586262, 0.2799806688\C, -0.0222561699, -2.8263472704, 0.3647141605\C, 0.6022005552, -4.0849332957, 0.3853019681\C, 1.9826257287, -4.1983799191, 0.3235661677\C, 2.7940020897, 0.6826506919, -0.0139867873\C, 6.577983009, 1.2349085601, -0.053616585\C, 6.2879280944, 1.8867604651, -1.3999495163\C, 2.8720639727, 1.4798507808, 1.282197752\C, 2.9463994509, 0.8634769296, 2.5313915215\C, 2.9972504974, 1.6309540111, 3.6951452348\C, 2.9725777988, 3.0206438621, 3.6232905085\C, 2.8981172941, 3.6437209863, 2.3777924551\C, 2.8502566319, 2.8778524491, 1.216825705\C, 5.9079951608, 3.2335725022, -1.4295977386\C, 5.6545318481, 3.873289764, -2.6392392416\C, 5.7739895412, 3.1721645681, -3.8388869454\C, 6.1488706674, 1.8320181231, -3.8162414834\C,

6.4056418428, 1.1918198893, -2.6037615444\H, 8.5739289595, -4.288035386, -0.0154557973\H, 10.885852942, -3.4069495477, -0.1633636518\H, 11.3028505906, -0.9756750172, -0.2916639998\H, 9.4372624088, 0.6394061489, -0.2804590968\H, 0.2224468021, -0.6892976239, 0.2812441869\H, -1.1029868632, -2.7659992194, 0.4208196675\H, -0.0064850036, -4.9791550764, 0.4537588356\H, 2.4622276156, -5.1697936318, 0.342854771\H, 5.7824057054, 1.4864003602, 0.6541639081\H, 7.495698191, 1.6564295412, 0.3660438294\H, 2.9658278508, -0.2177692891, 2.5958014752\H, 3.0556290909, 1.1378541409, 4.6590151635\H, 3.0118857518, 3.6152953242, 4.5288262694\H, 2.8784159718, 4.725935504, 2.3113048256\H, 2.7964534824, 3.3687110907, 0.249629388\H, 5.8093743626, 3.7835826883, -0.4984319114\H, 5.3629705403, 4.9177692758, -2.6463729311\H, 5.5751574661, 3.6679529633, -4.7821847443\H, 6.2437282617, 1.2788068204, -4.7439049727\H, 6.69718887, 0.1484899535, -2.5945851335\H, 1.7982891493, 0.7946334914, -0.4521593985\H, 3.4914585605, 1.1026099747, -0.7449595143 \\Version=ES64L-G09RevE.01 \State=1-A \HF=-1341.4633902 \RMSD=7.260e-09 \RMSF=4.390e-06 \ZeroPoint=0.4397711 \Thermal=0.4647891 \Dipole=-0.2399792, 1.6406347, -0.0568827 \DipoleDeriv=0.5296259, -0.5947826, -0.0, \Polar=454.3956353, 9.6426826, 384.2048895, -22.7877491, -7.8913622, 251.8921341 \PG=C01 [X(C30H22N2O1)] \NImag=0\\0.0, 0.0, 0.0, \\@

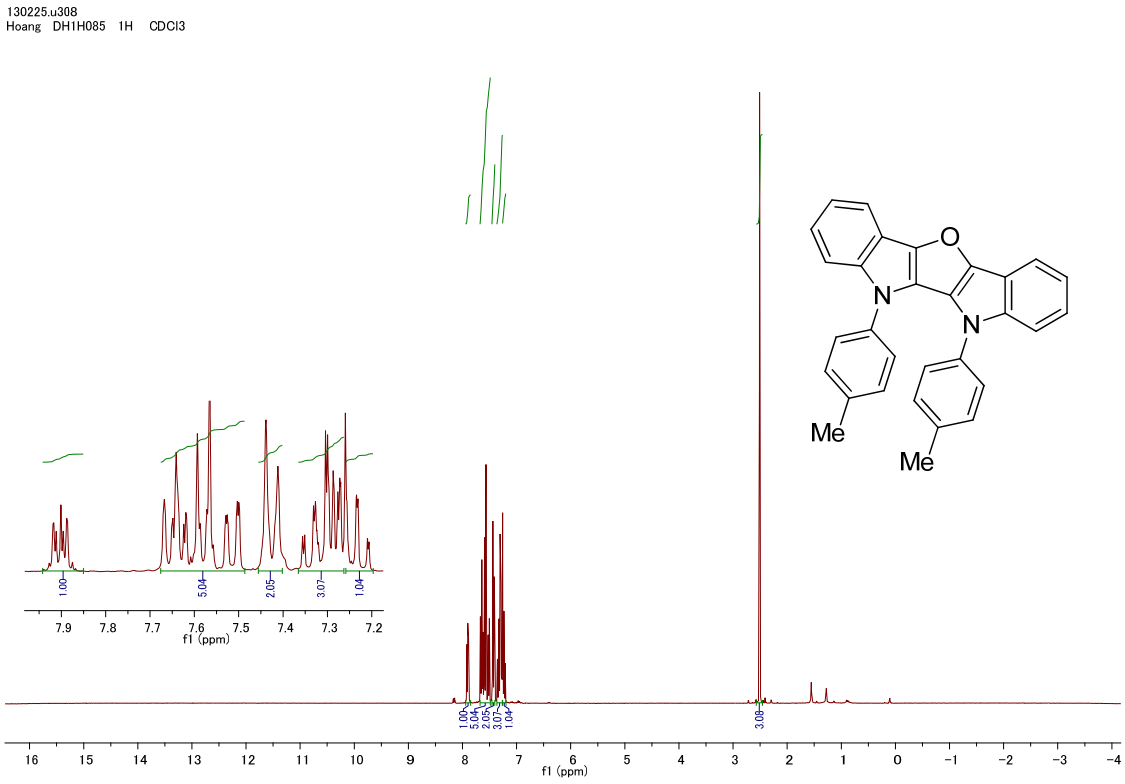
NMR-Spectra

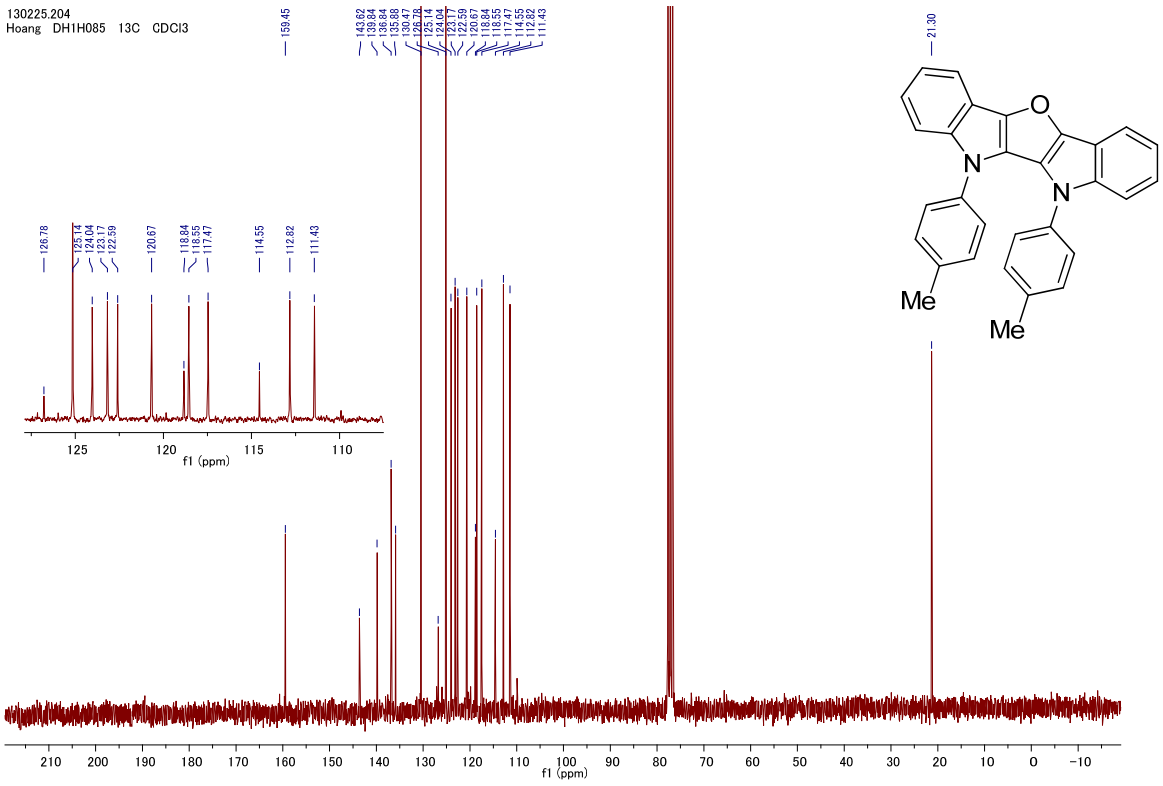
3,4-Dibromo-2,5-bis(2-bromophenyl)furan (2)



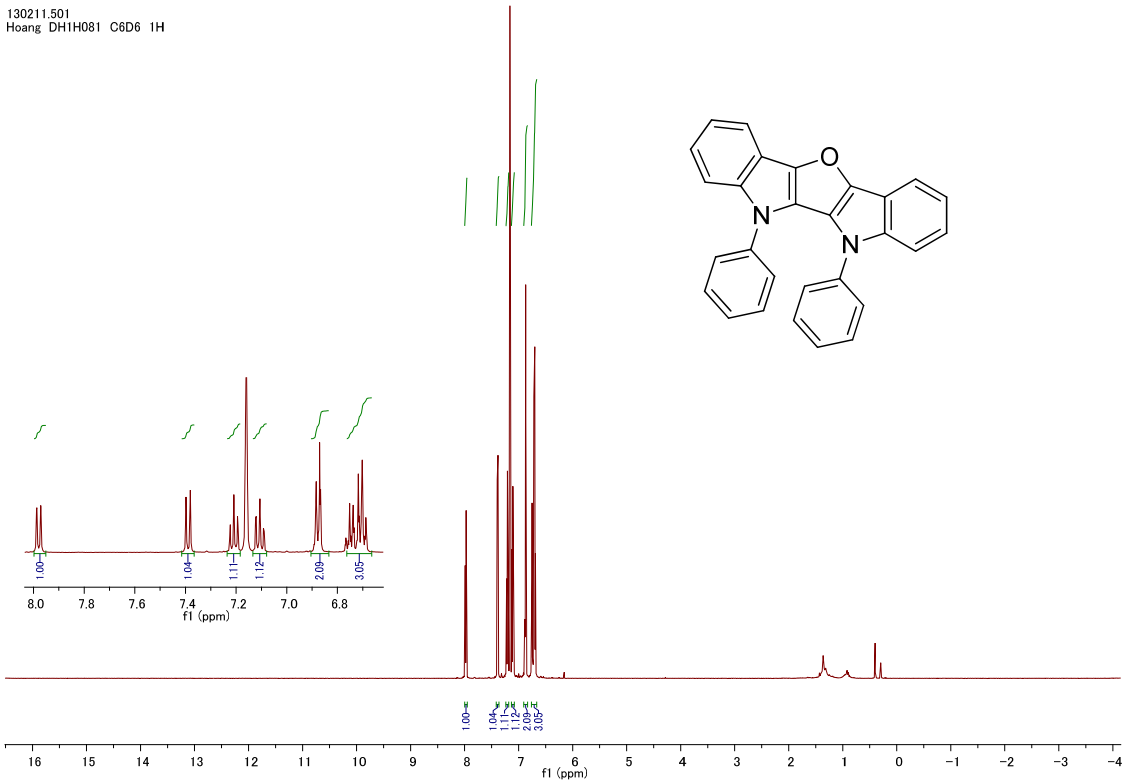


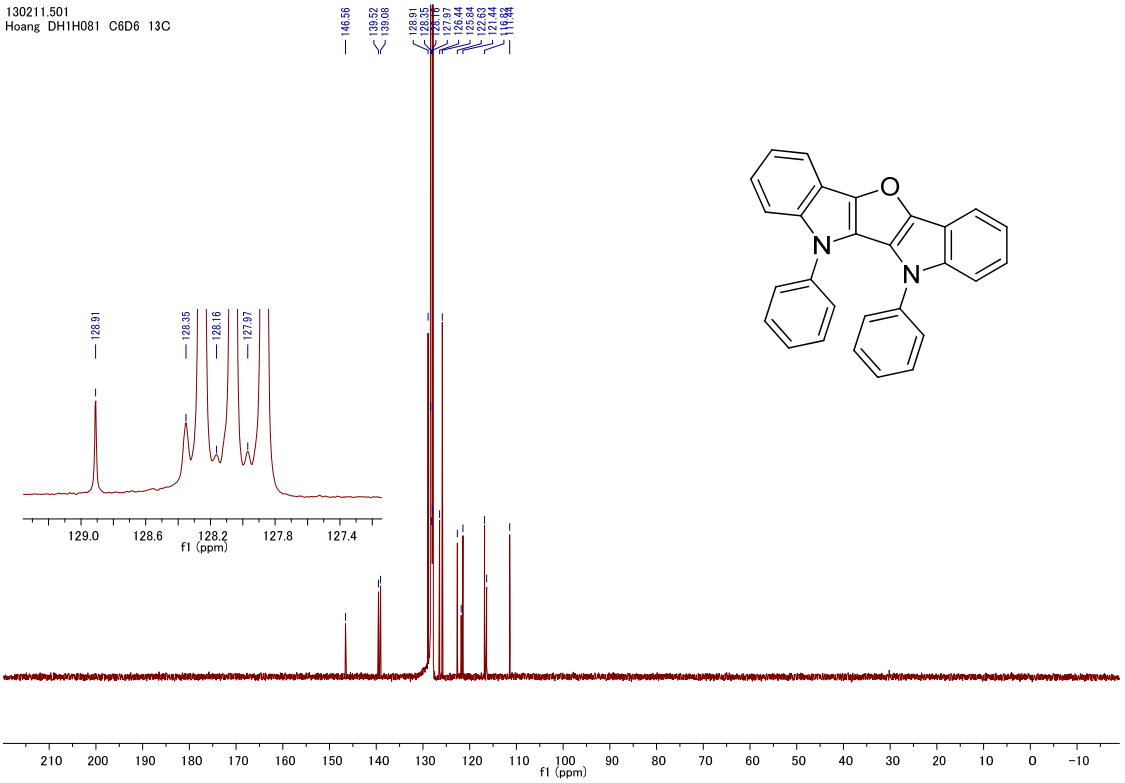
5,6-Di-*p*-tolyl-5,6-dihydrofuro[3,2-*b*:4,5-*b*′]diindole (3a)



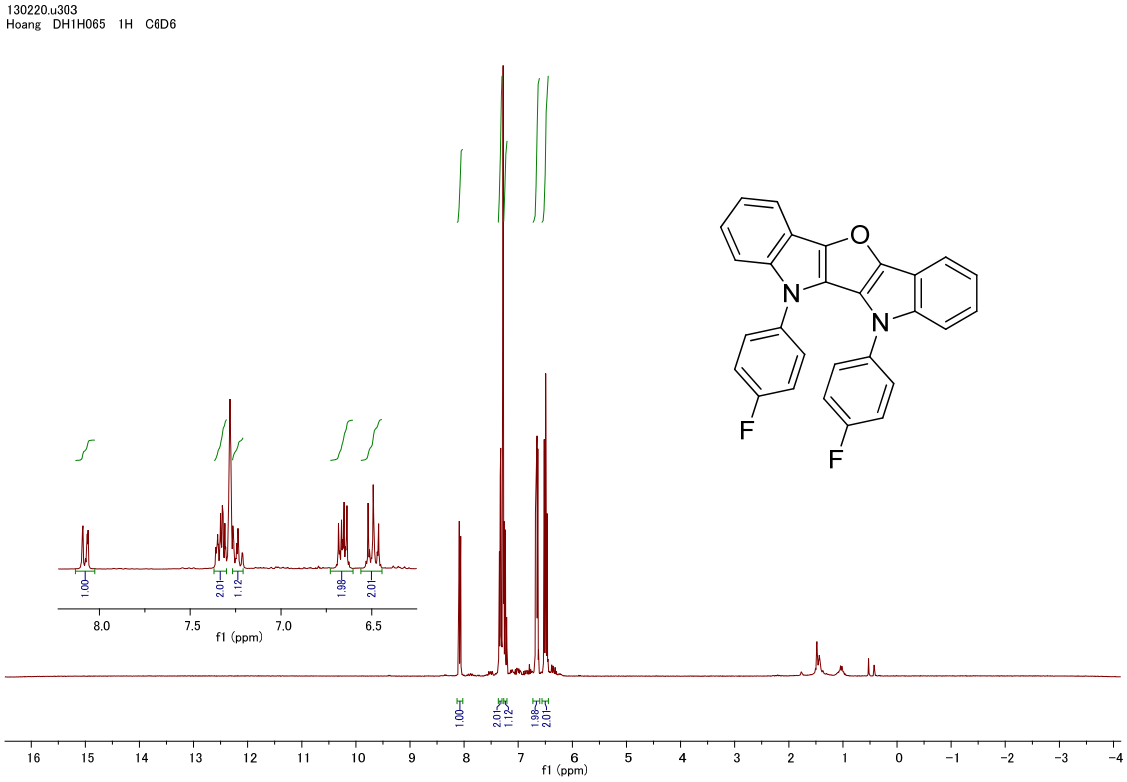


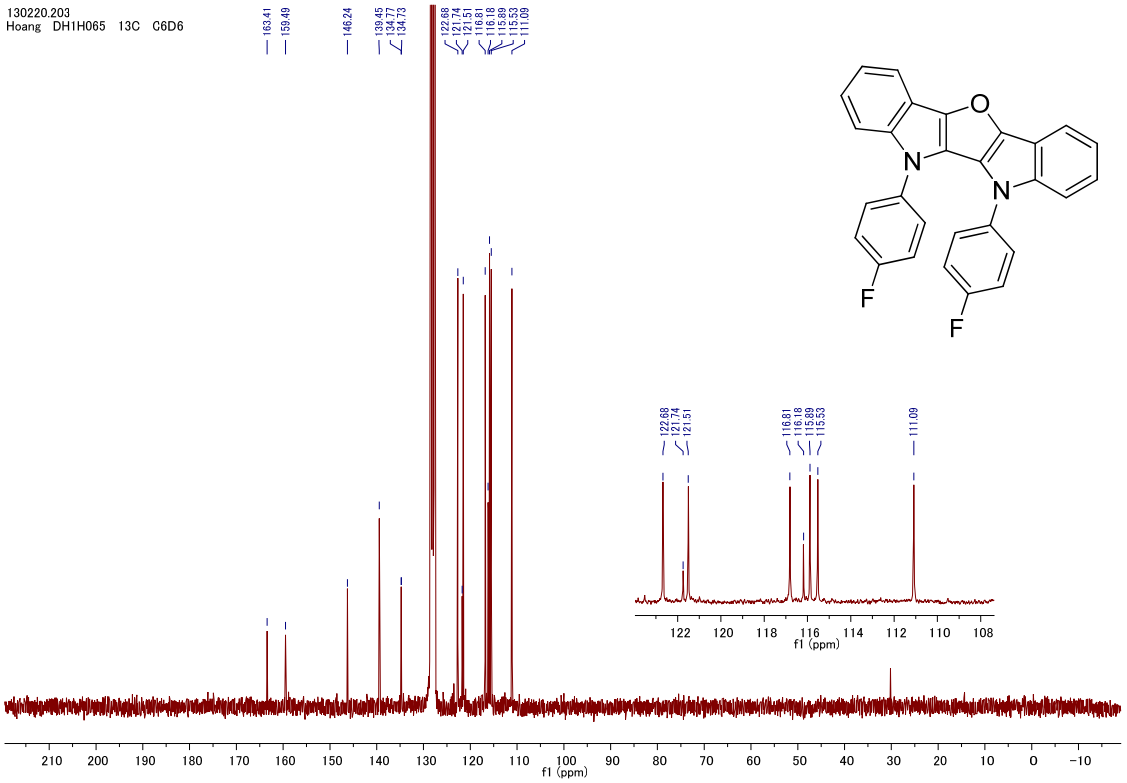
5,6-Diphenyl-5,6-dihydrofuro[3,2-*b*:4,5-*b*']diindole (3b)



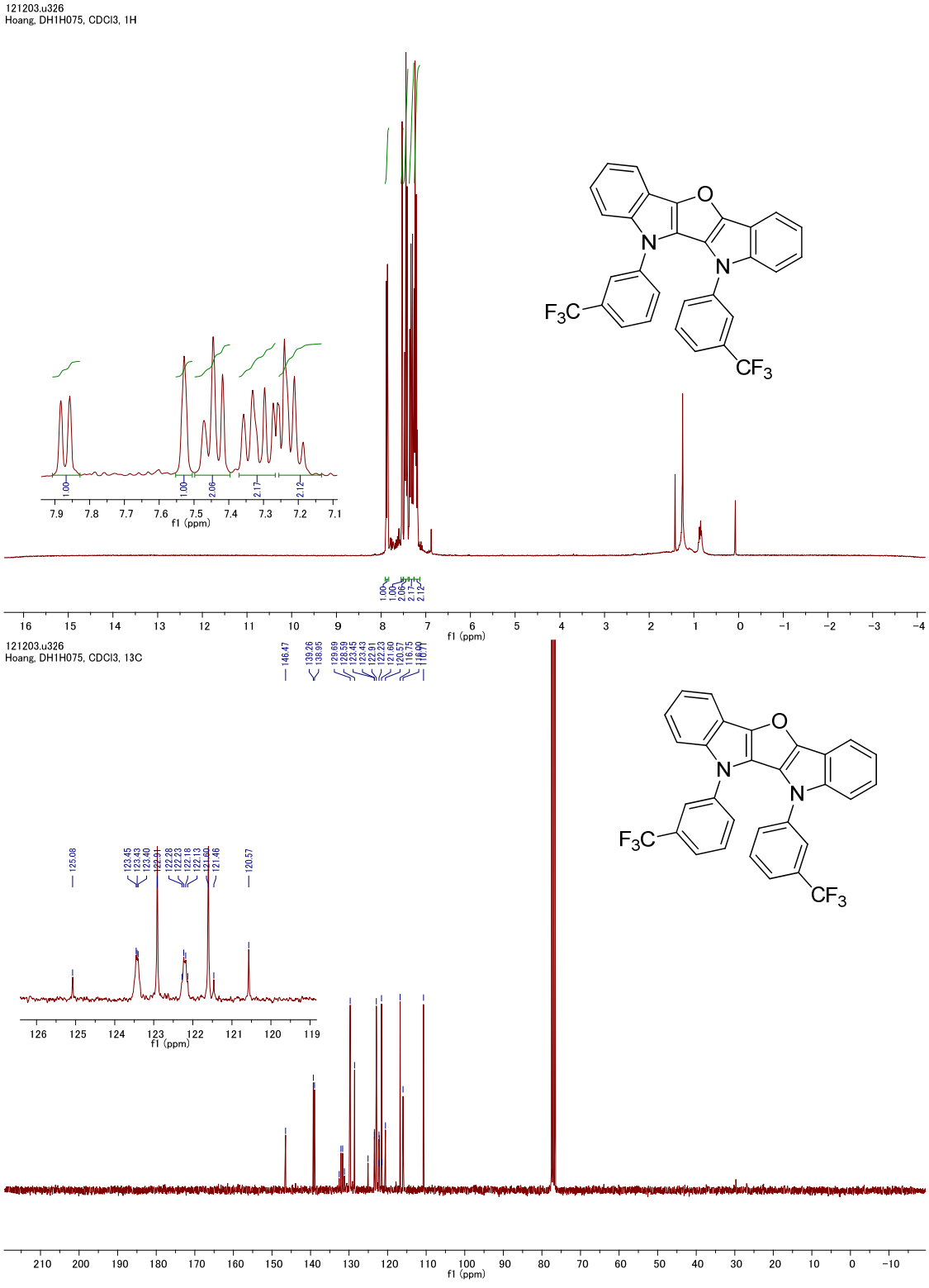


5,6-Bis(4-fluorophenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*′]diindole (3c)

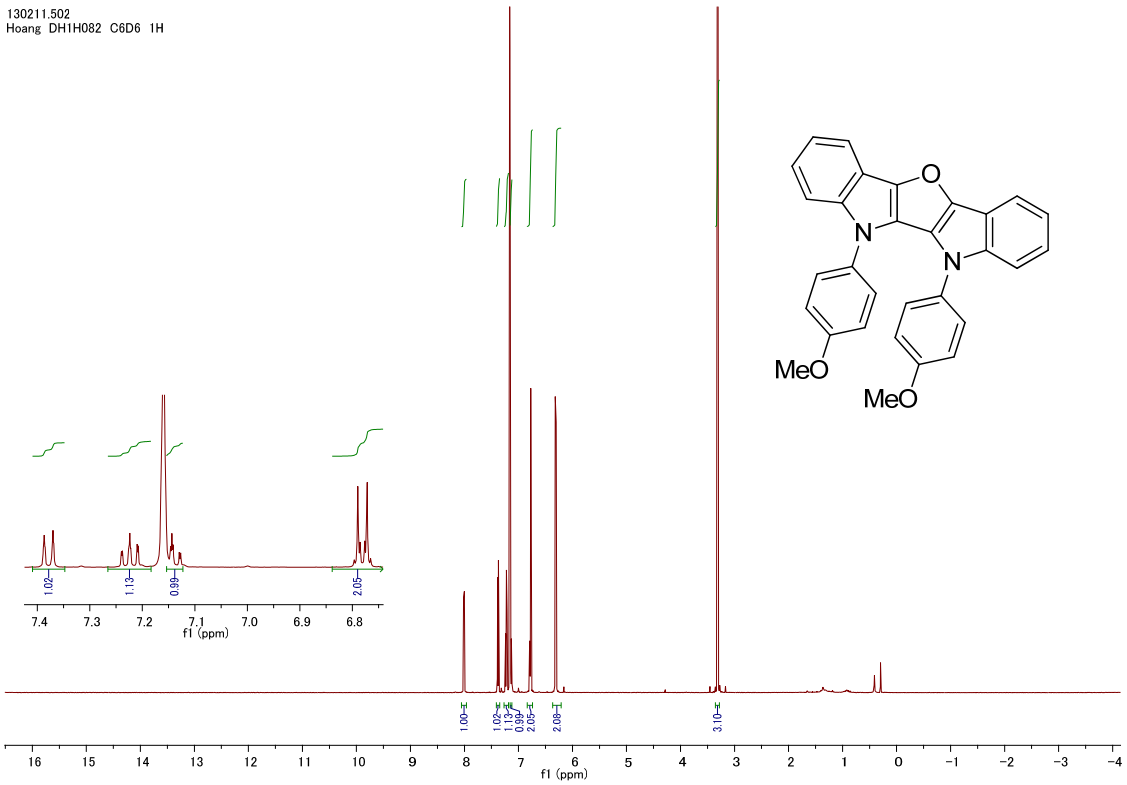


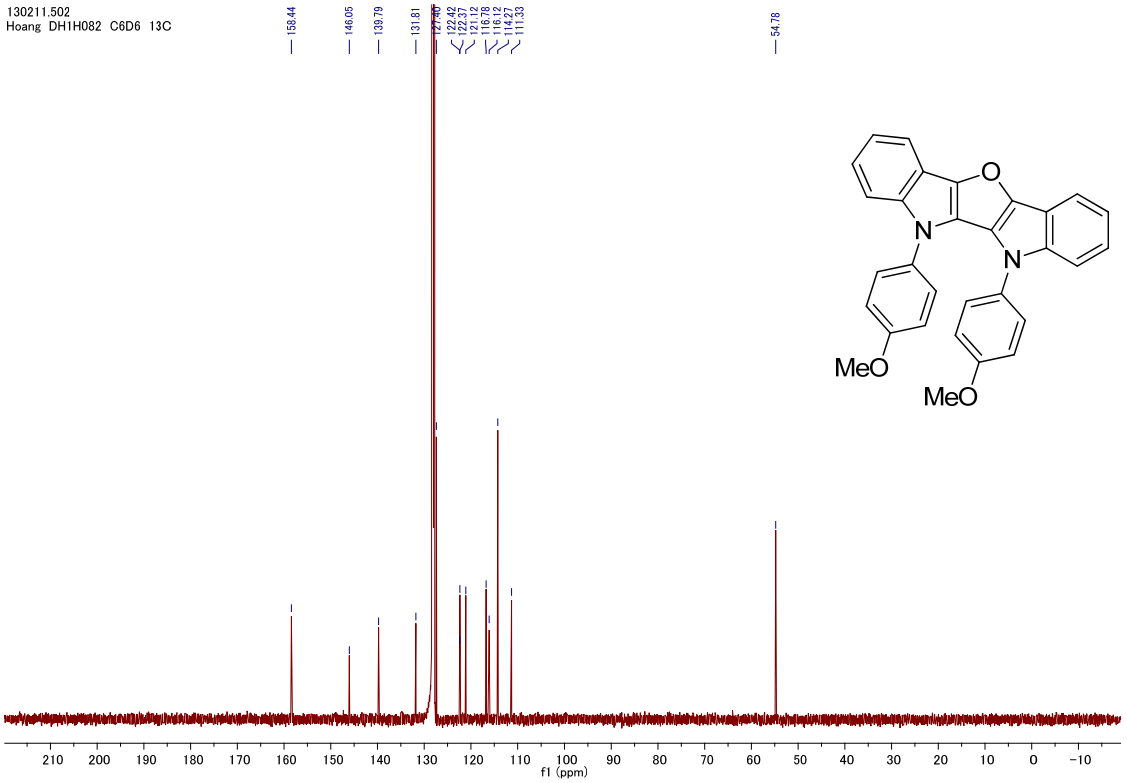


5,6-Bis(3-(trifluoromethyl)phenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*']diindole (3d)

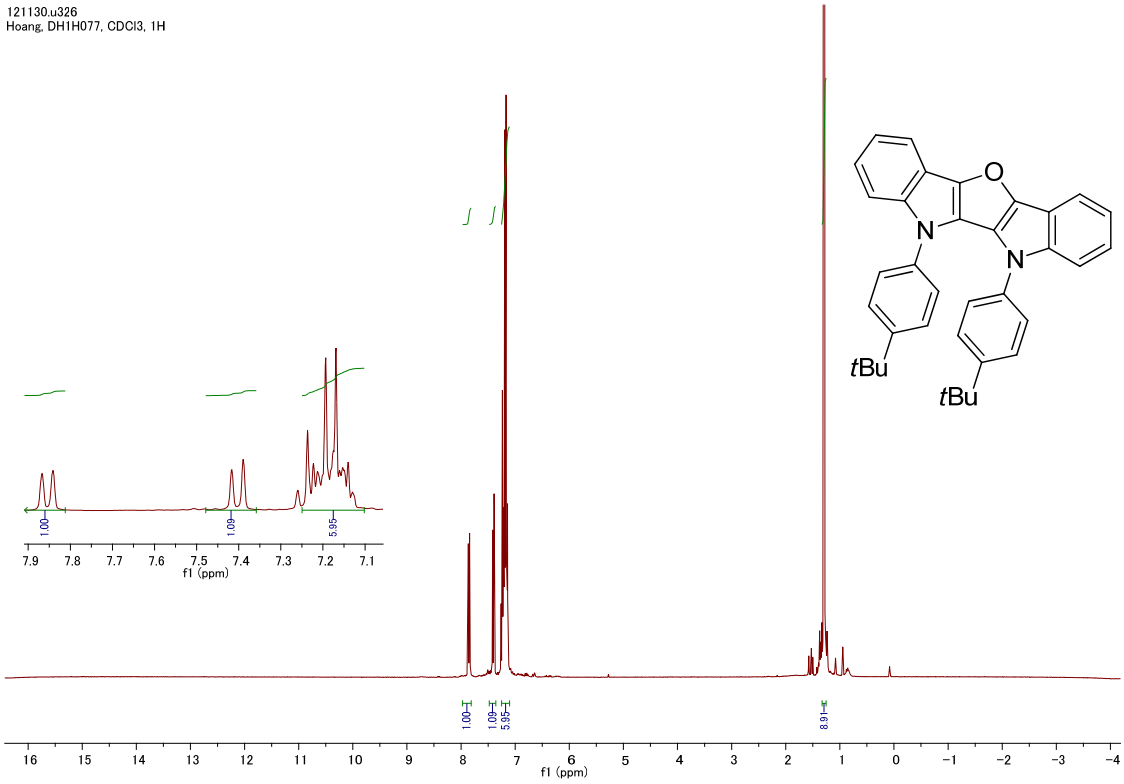


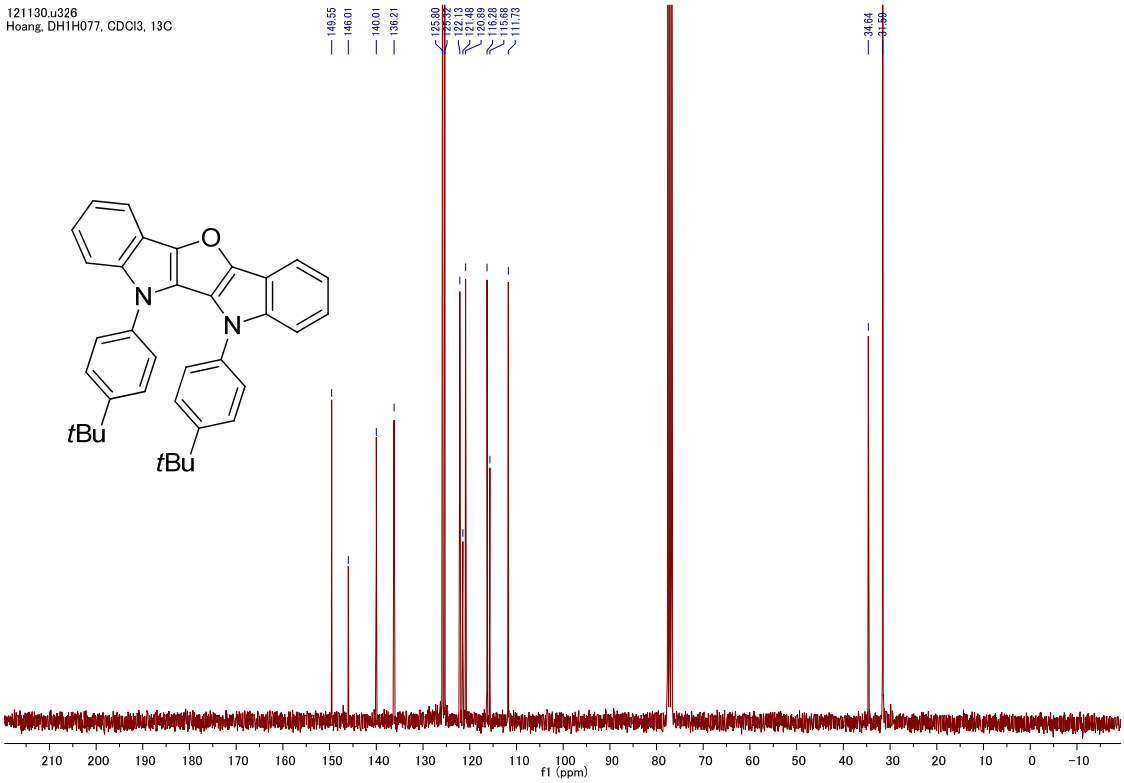
5,6-Bis(4-methoxyphenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*']diindole (3e)



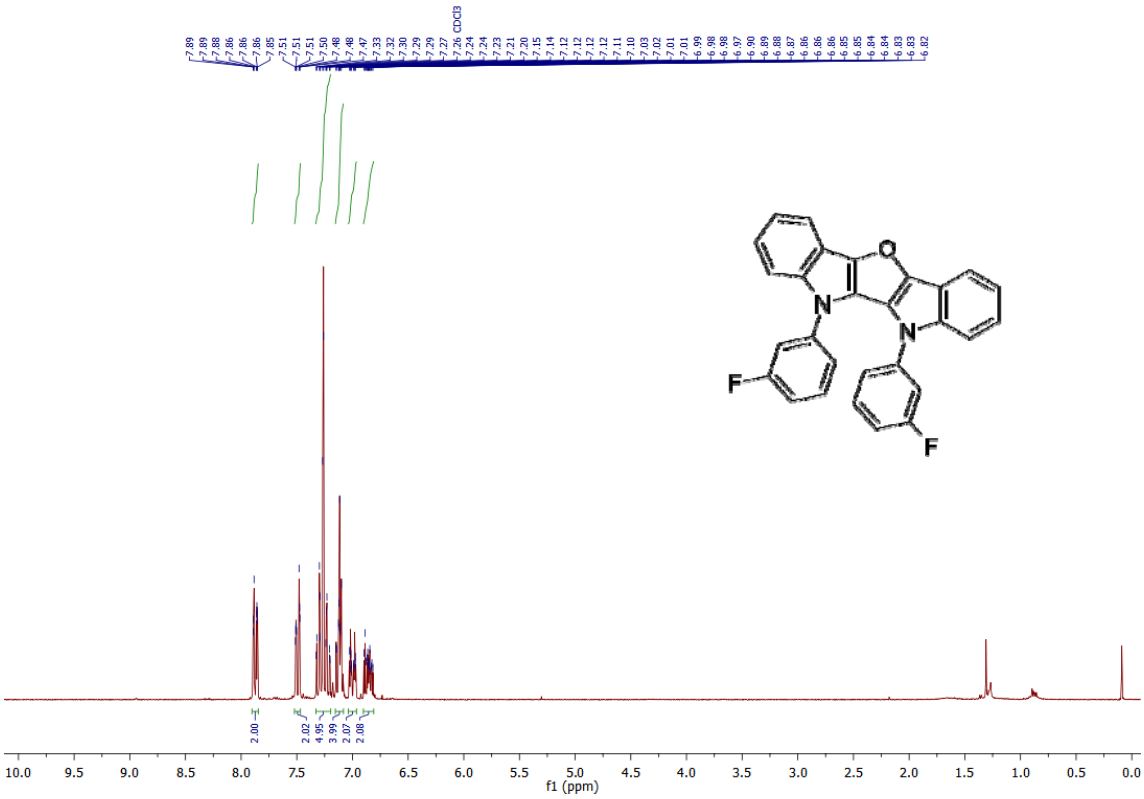


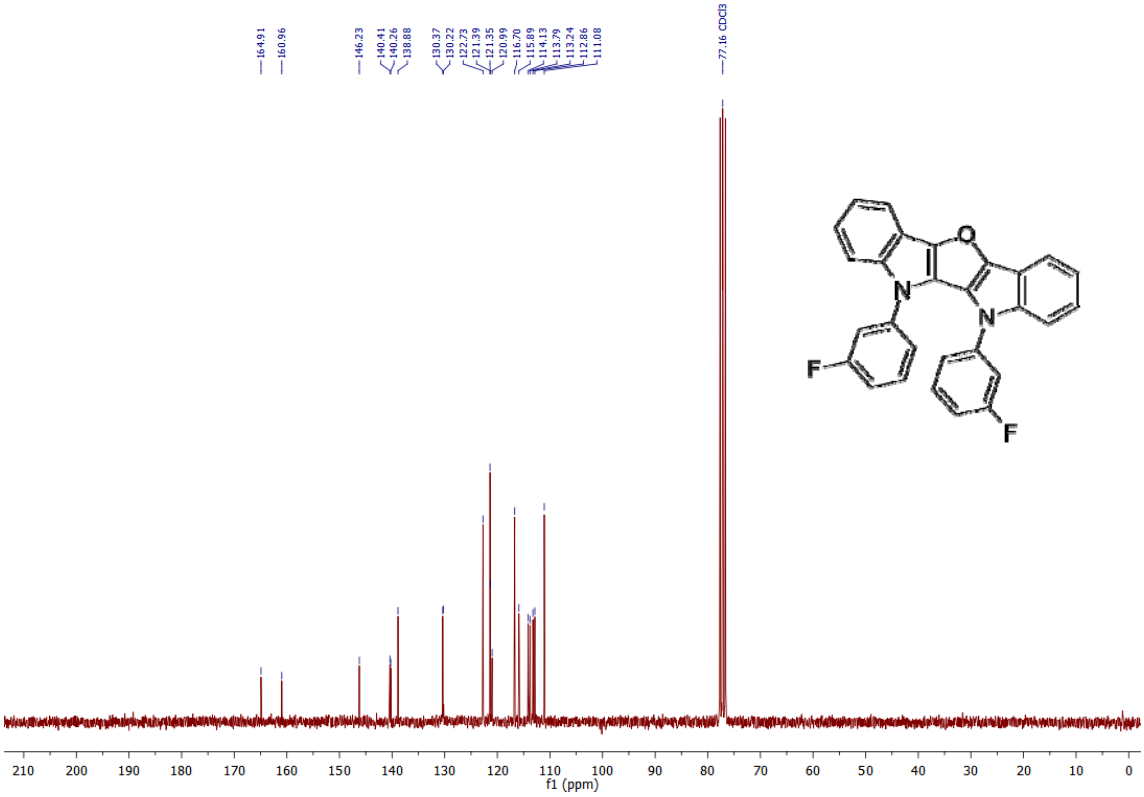
5,6-Bis(4-(*tert*-butyl)phenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*']diindole (3f)



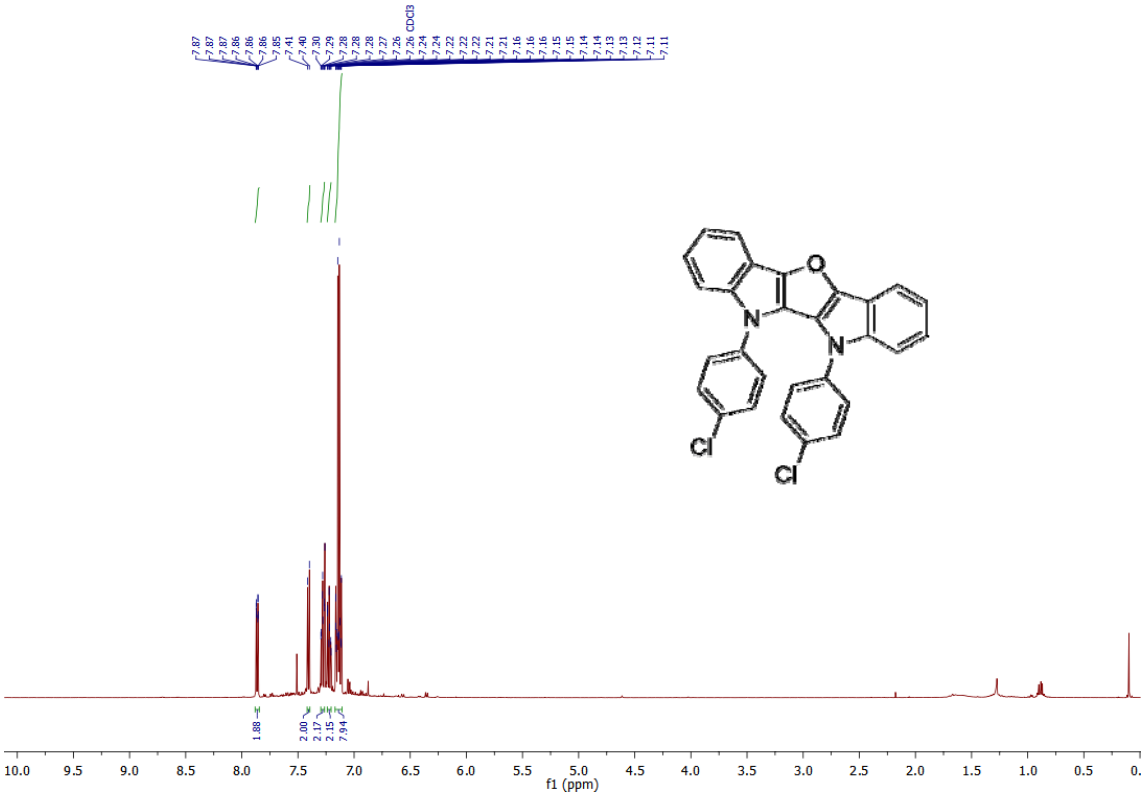


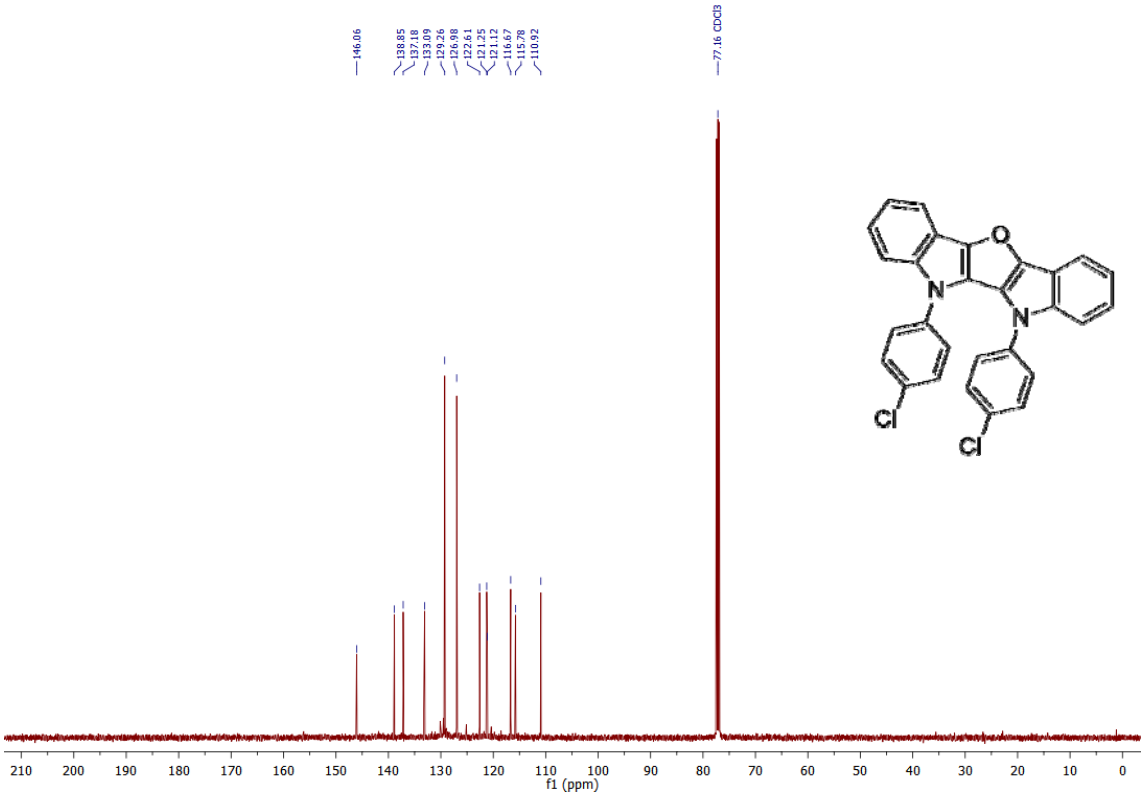
5,6-Bis(3-fluorophenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3g)



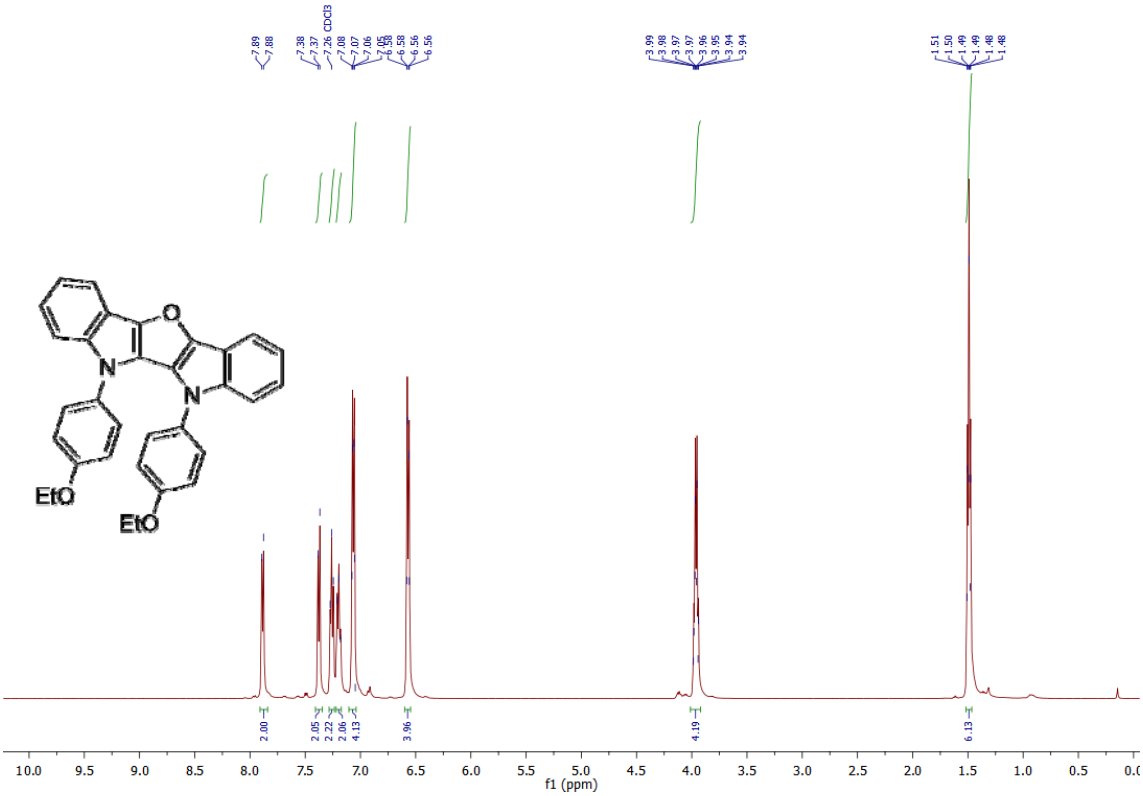


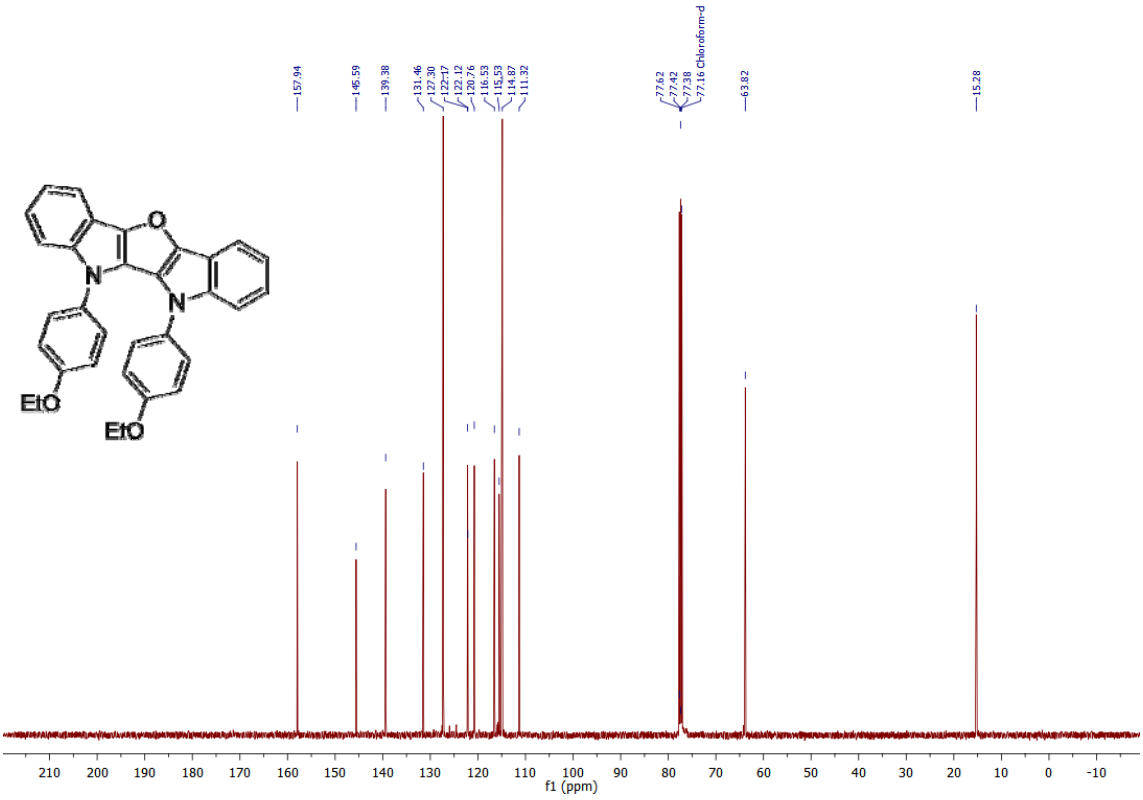
5,6-Bis(4-chlorophenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3h)



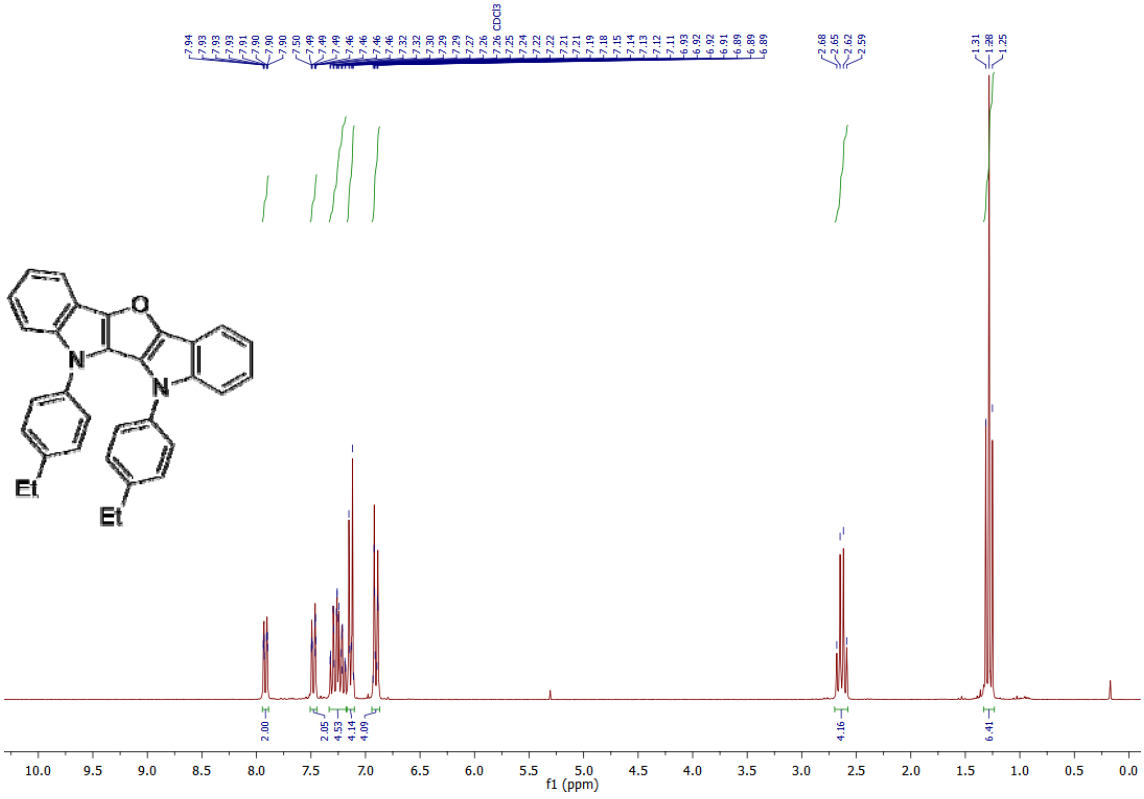


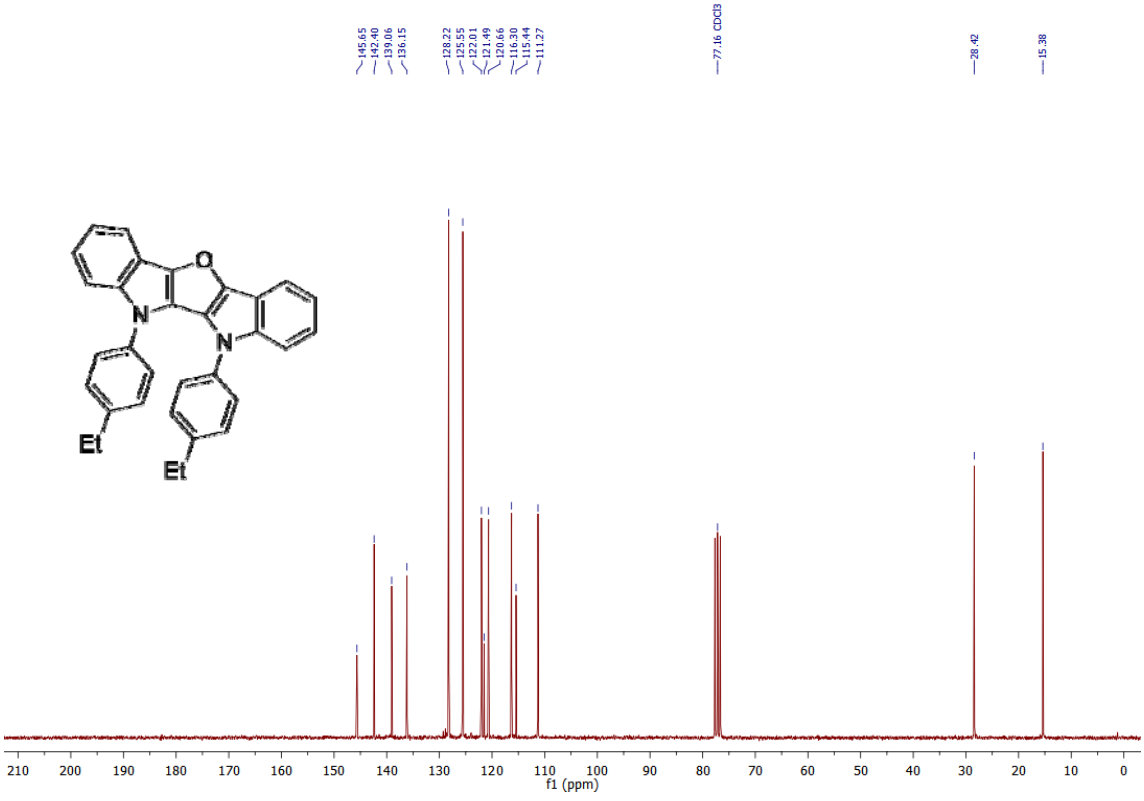
5,6-Bis(4-ethoxyphenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3i)



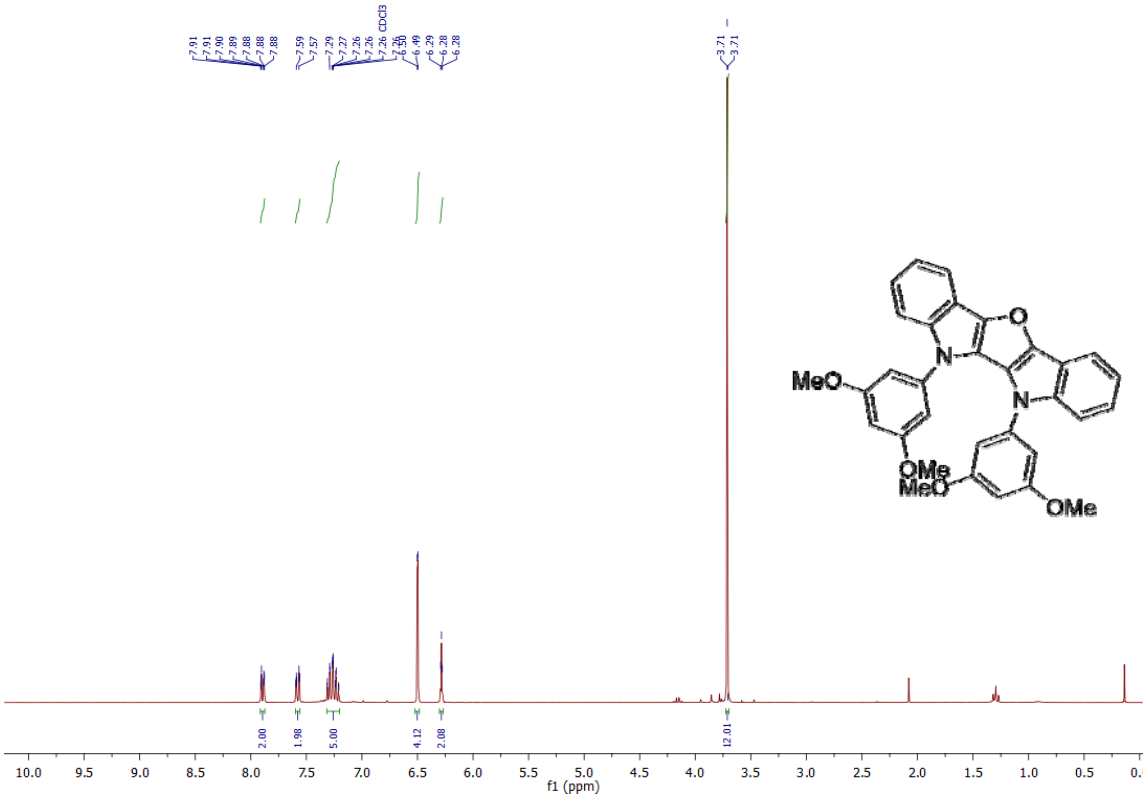


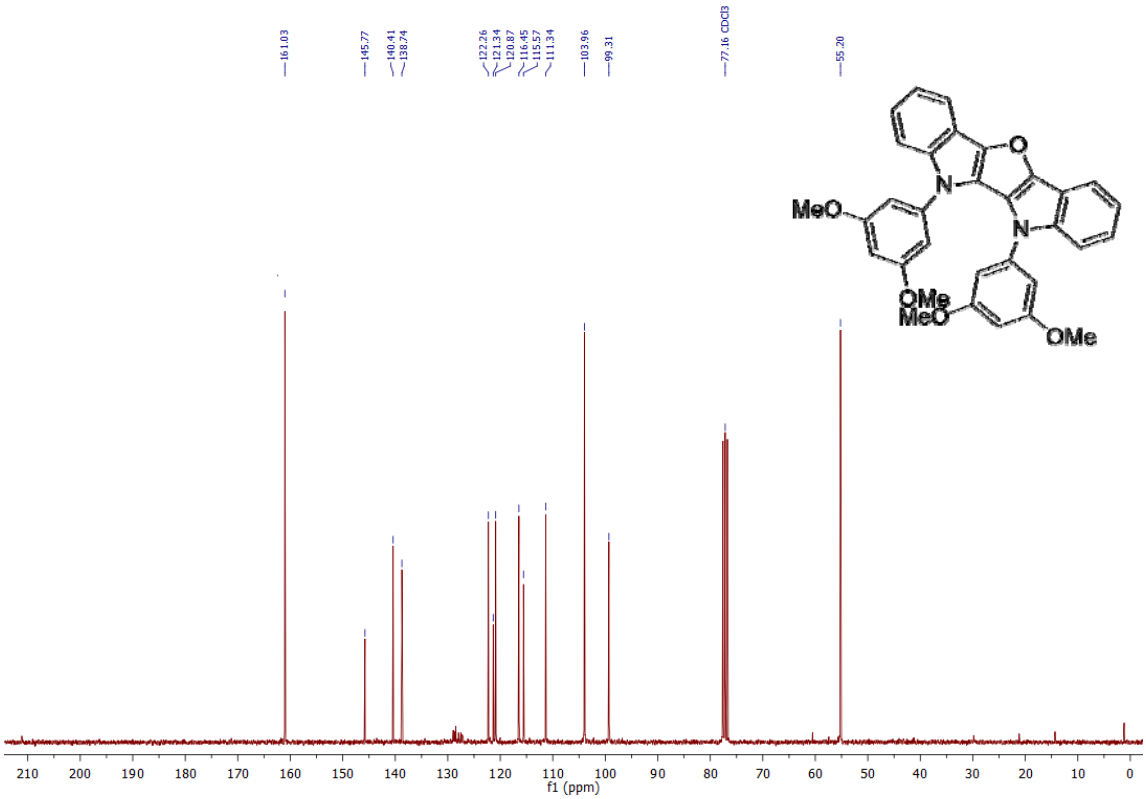
5,6-Bis(4-ethylphenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3j)



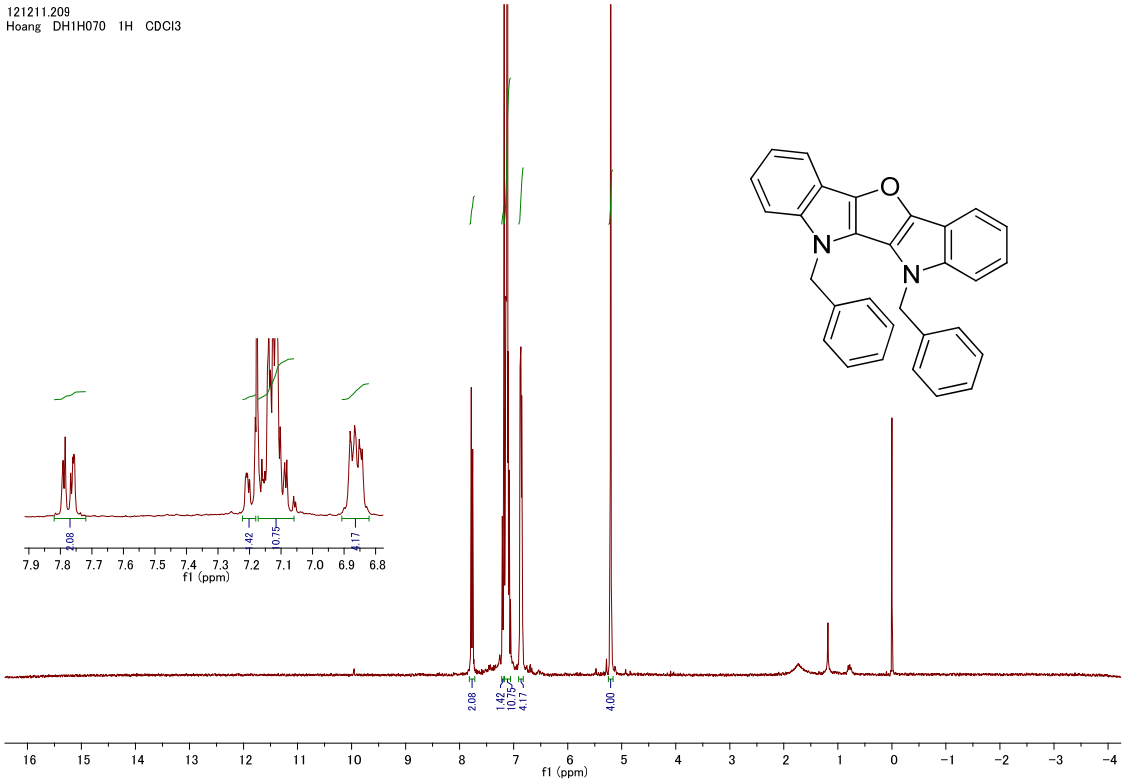


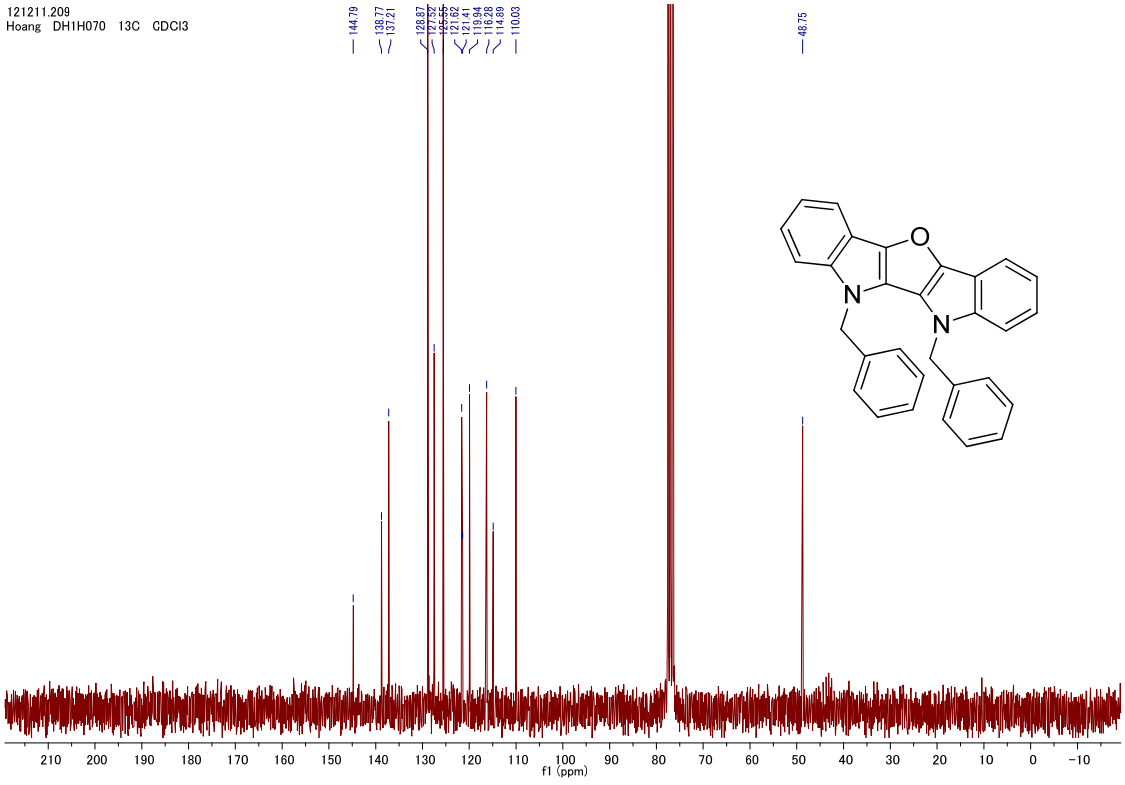
5,6-Bis(3,5-dimethoxyphenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3k)



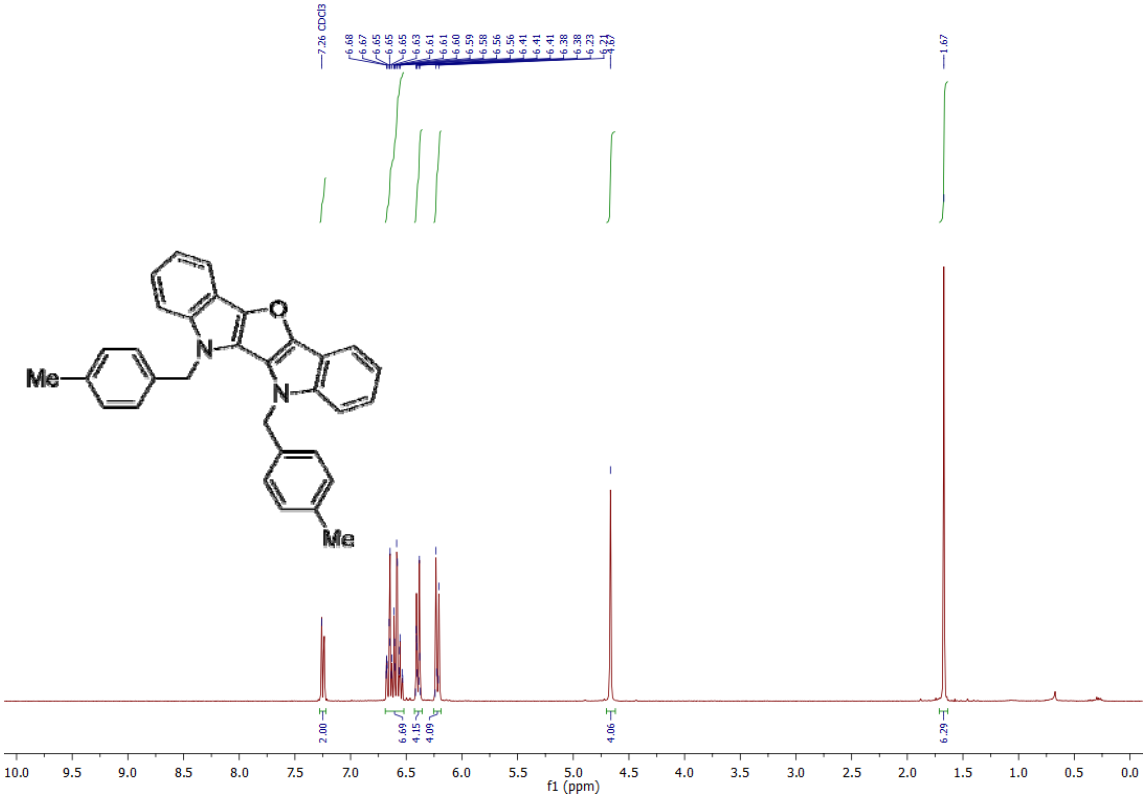


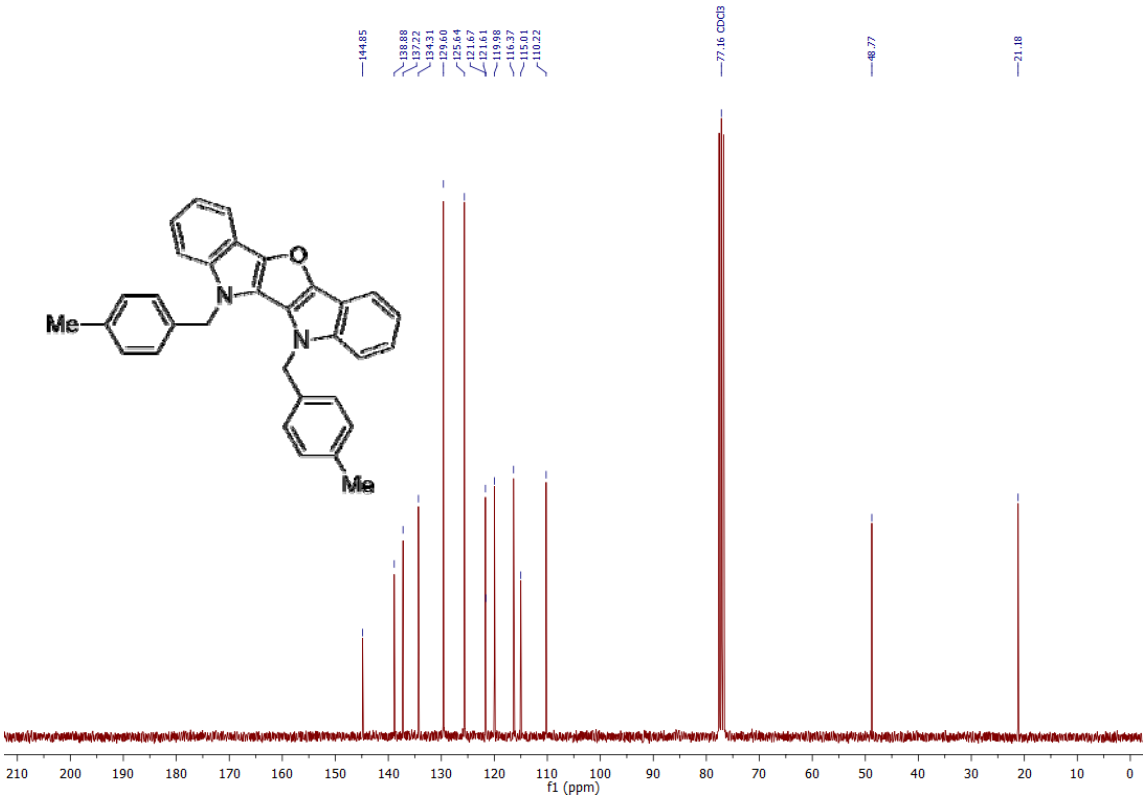
5,6-Dibenzyl-5,6-dihydrofuro[3,2-*b*:4,5-*b*']diindole (3l)



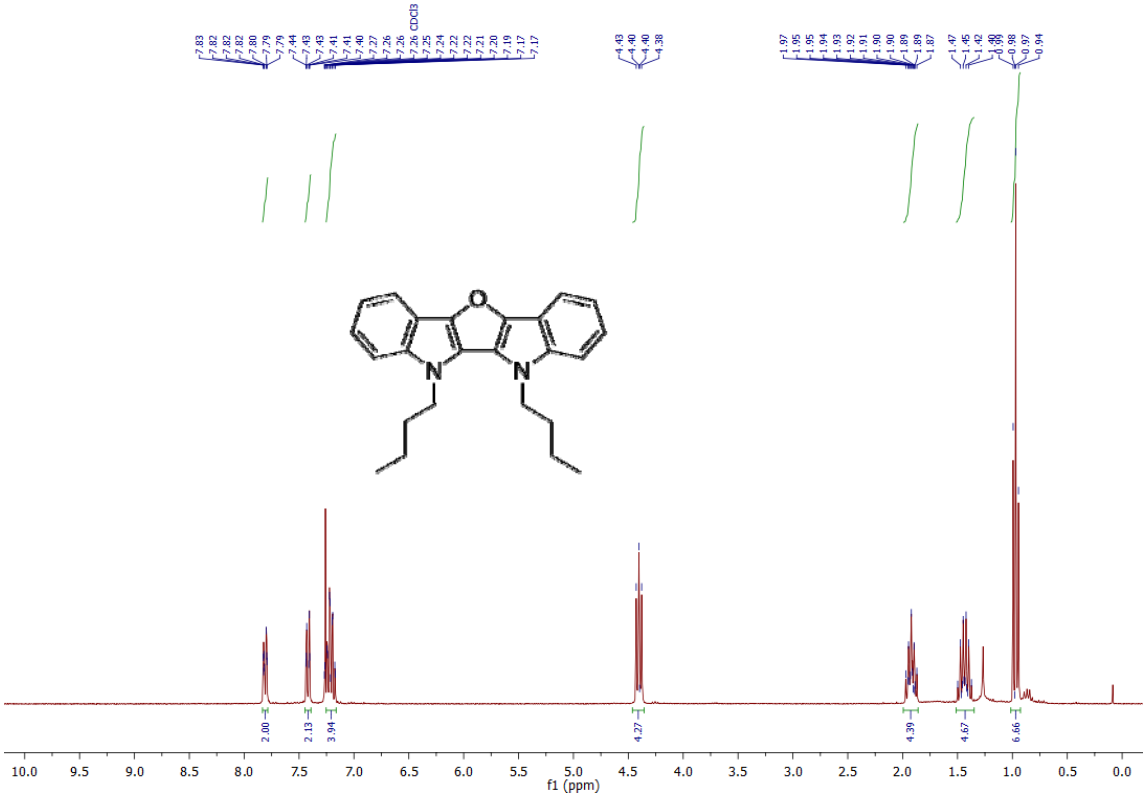


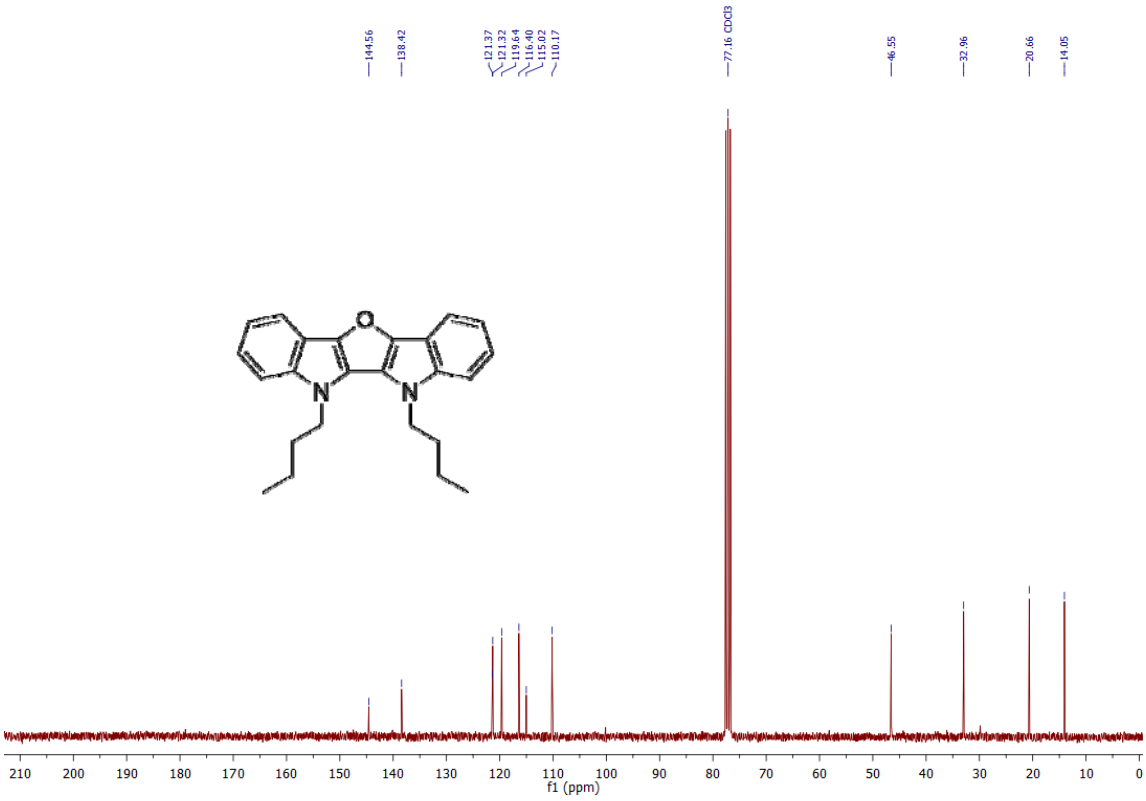
5,6-Bis(4-methylbenzyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3m)



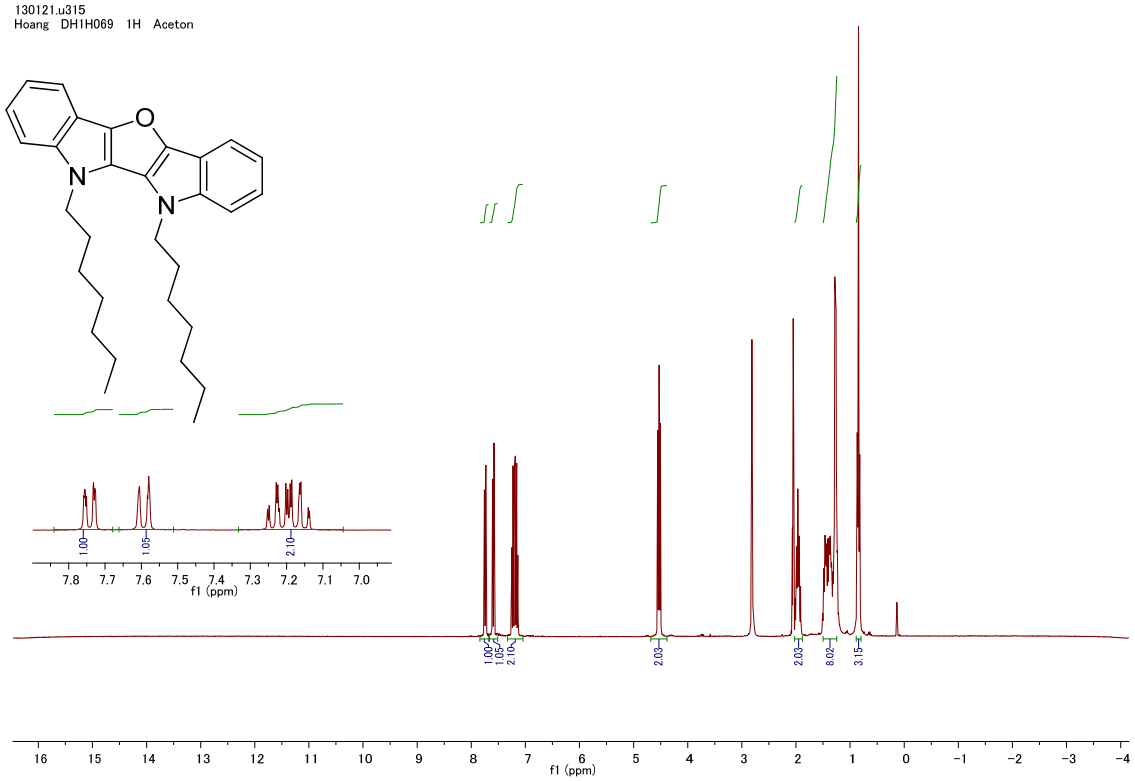


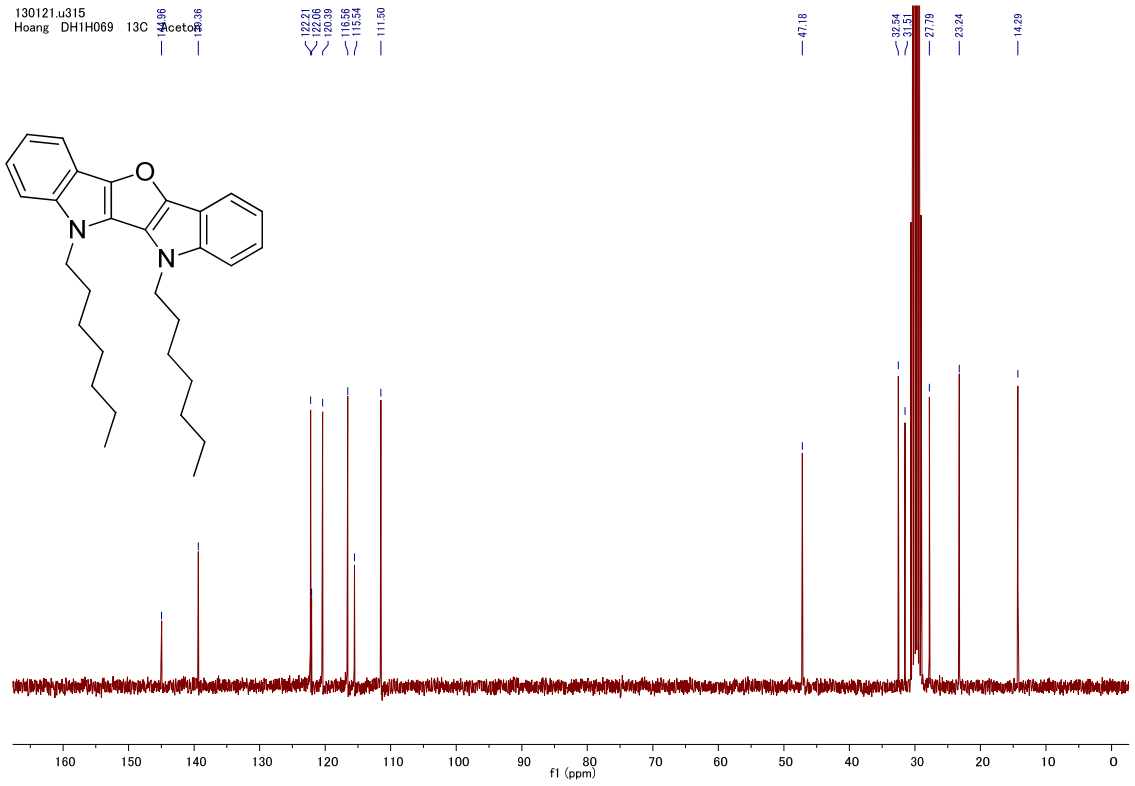
5,6-Di-*n*-butyl-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3n)





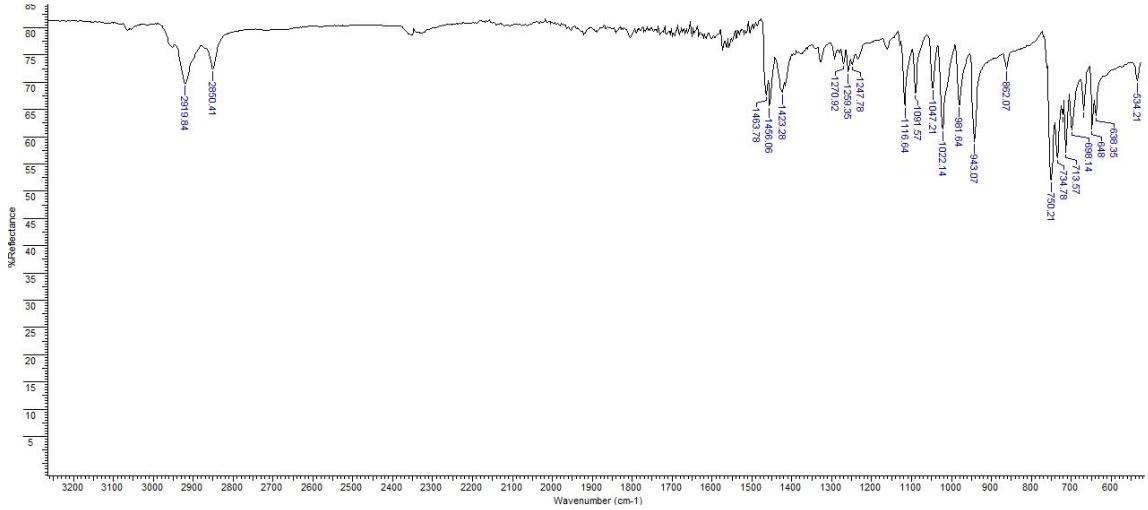
5,6-Diheptyl-5,6-dihydrofuro[3,2-*b*:4,5-*b*′]diindole (3o)



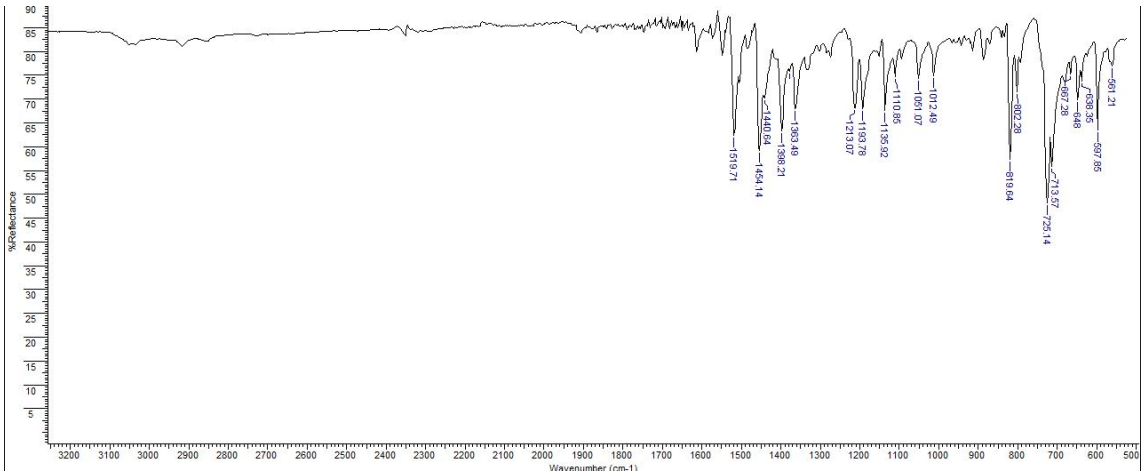


IR-Spectra

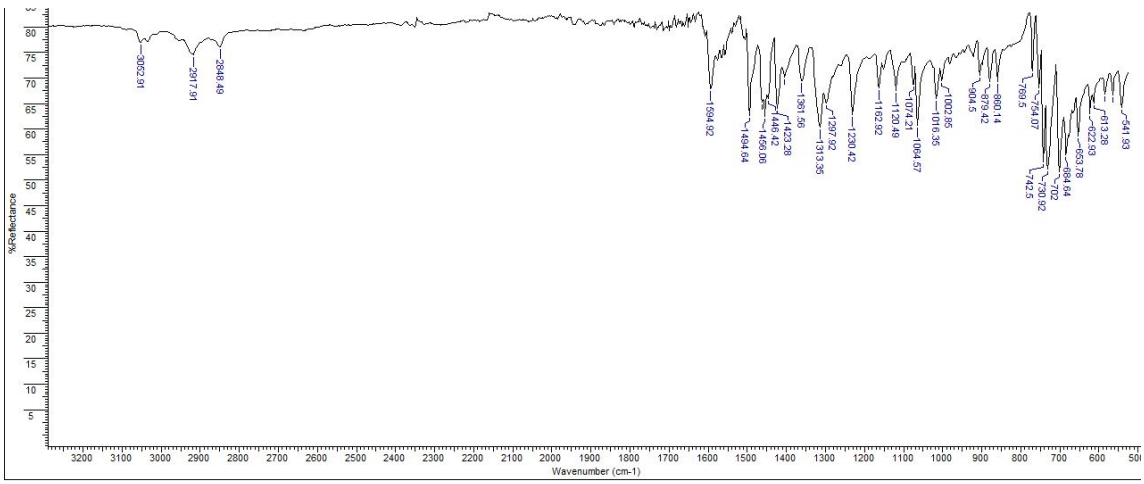
3,4-Dibromo-2,5-bis(2-bromophenyl)furan (2)



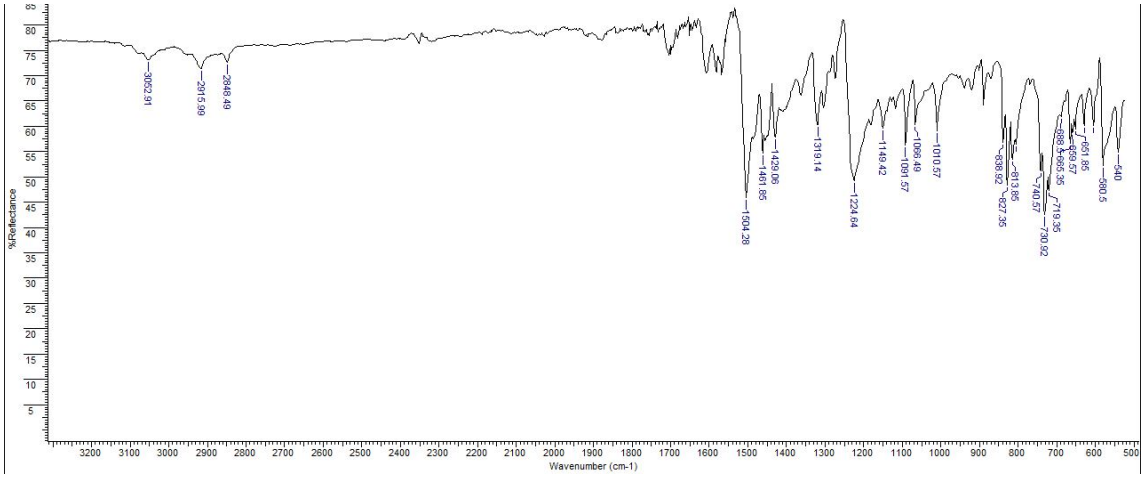
5,6-Di-*p*-tolyl-5,6-dihydrofuro[3,2-*b*:4,5-*b'*]diindole (3a)



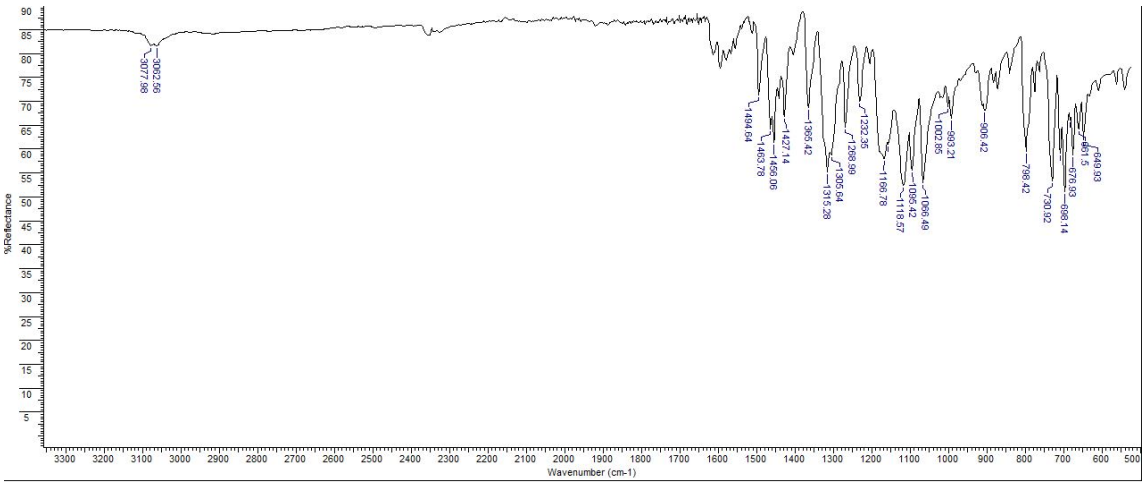
5,6-Diphenyl-5,6-dihydrofuro[3,2-*b*:4,5-*b*']diindole (3b)



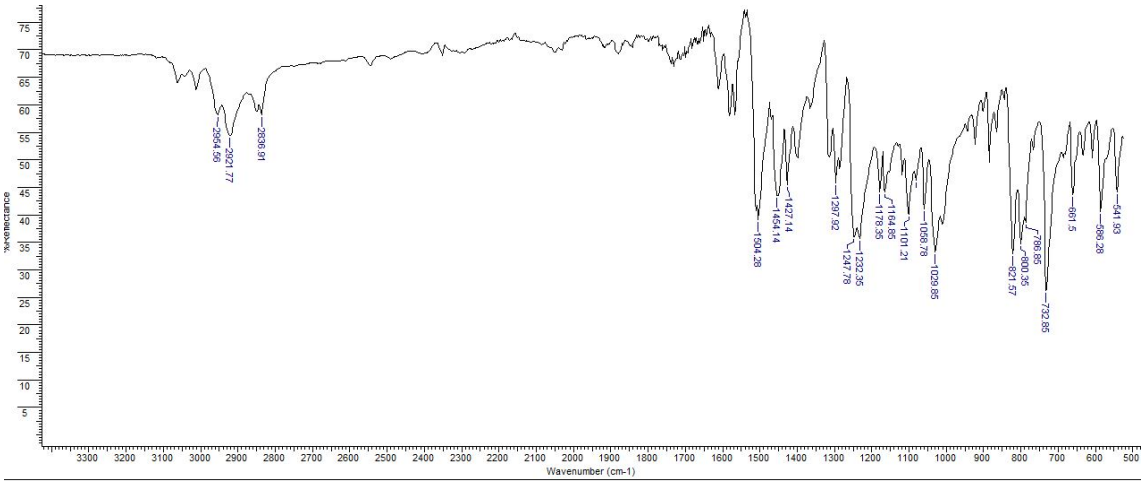
5,6-Bis(4-fluorophenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b'*]diindole (3c)



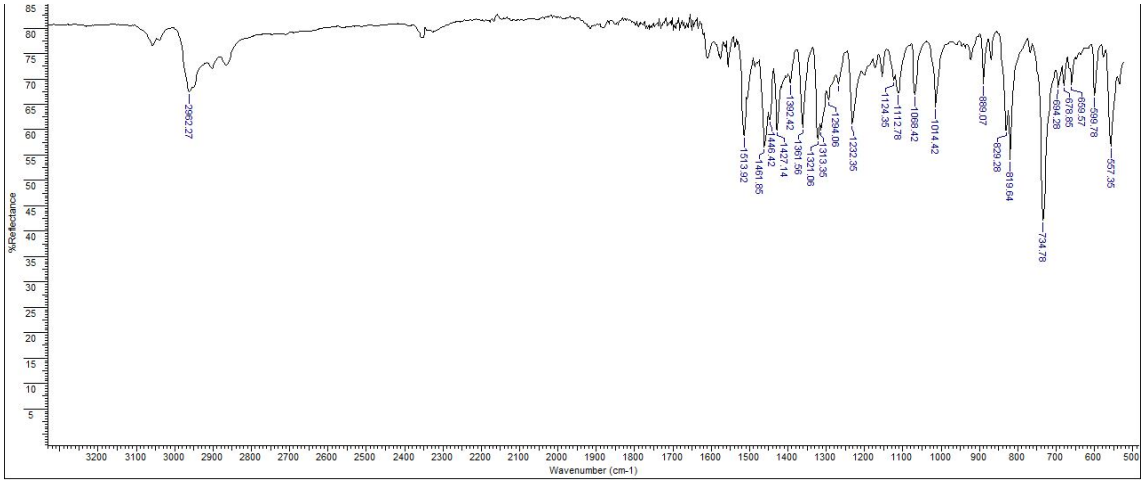
5,6-Bis(3-(trifluoromethyl)phenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*']diindole (3d)



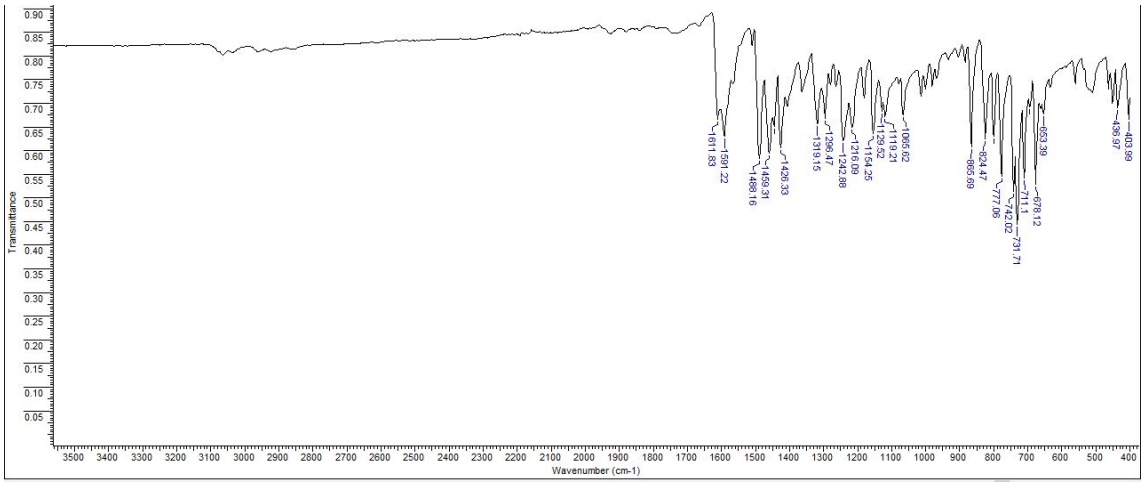
5,6-Bis(4-methoxyphenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b'*]diindole (3e)



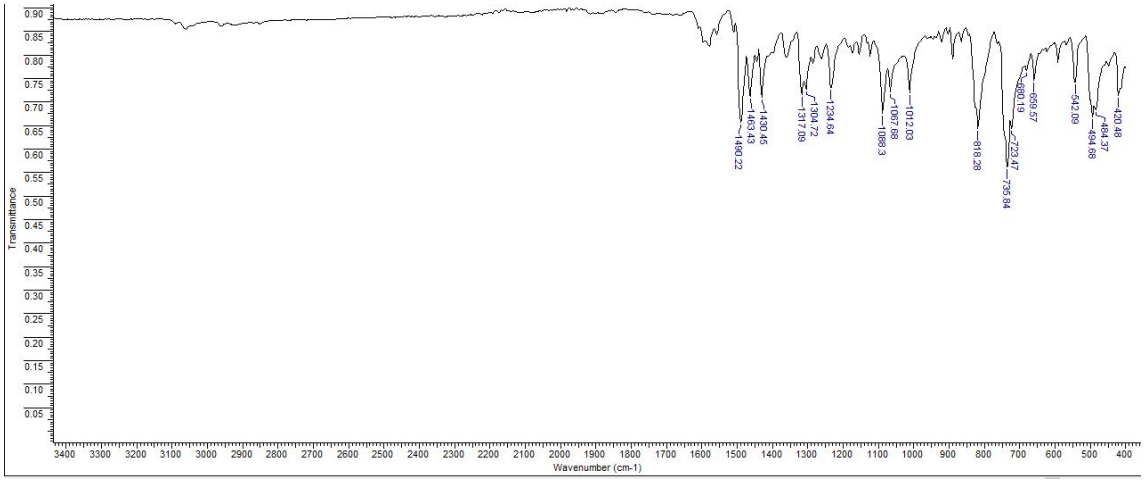
5,6-Bis(4-(*tert*-butyl)phenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b'*]diindole (3f)



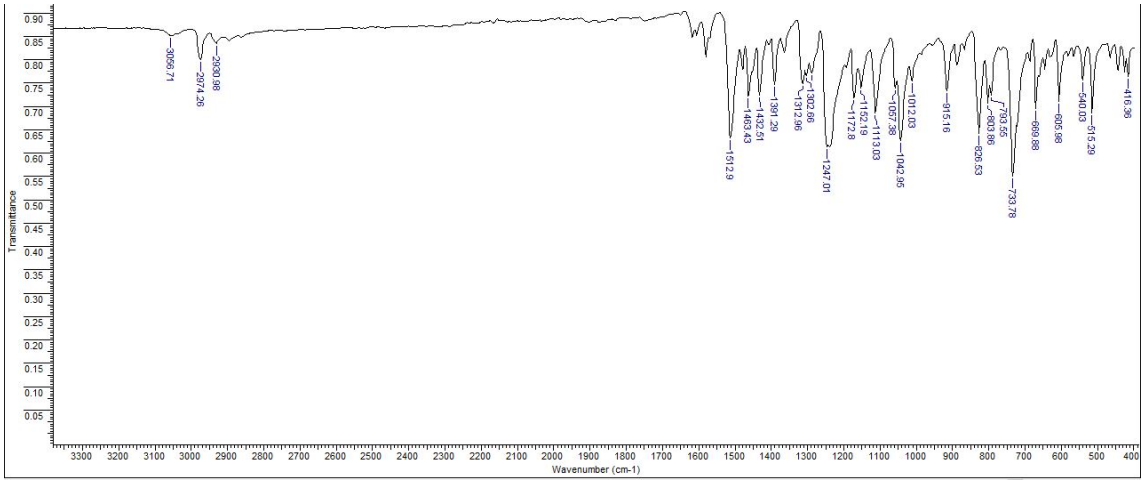
5,6-Bis(3-fluorophenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b´*]diindole (3g)



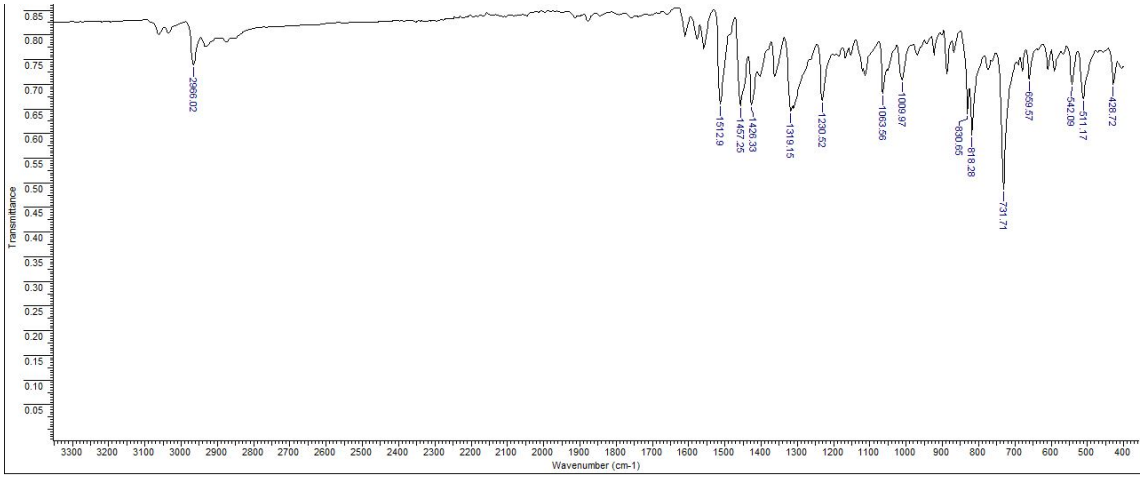
5,6-Bis(4-chlorophenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b´*]diindole (3h)



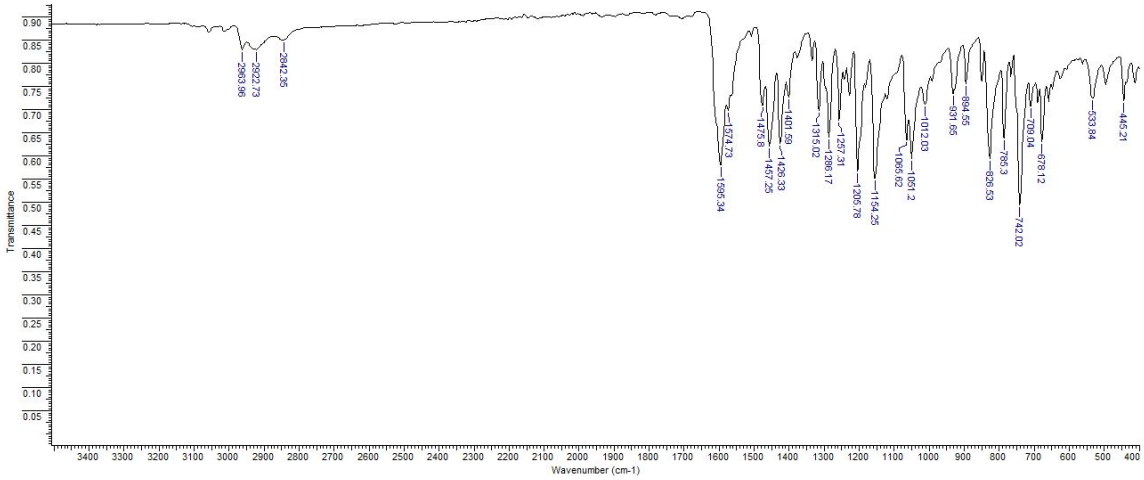
5,6-Bis(4-ethoxyphenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3i)



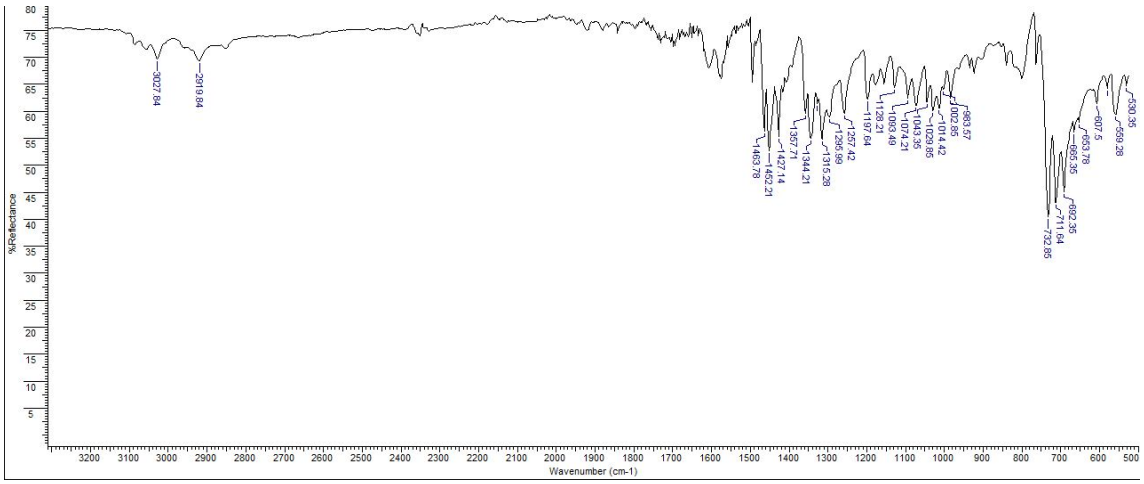
5,6-Bis(4-ethylphenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3j)



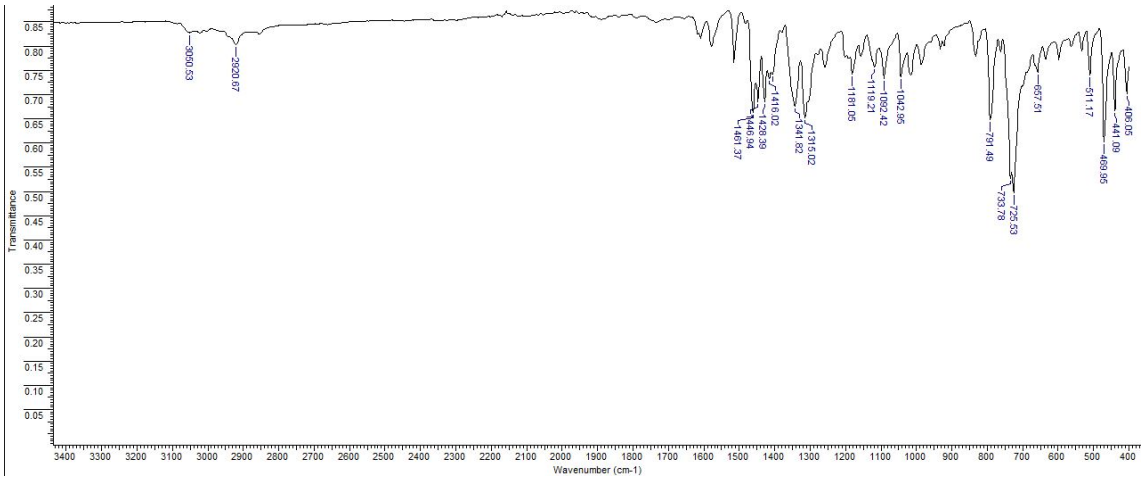
5,6-Bis(3,5-dimethoxyphenyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3k)



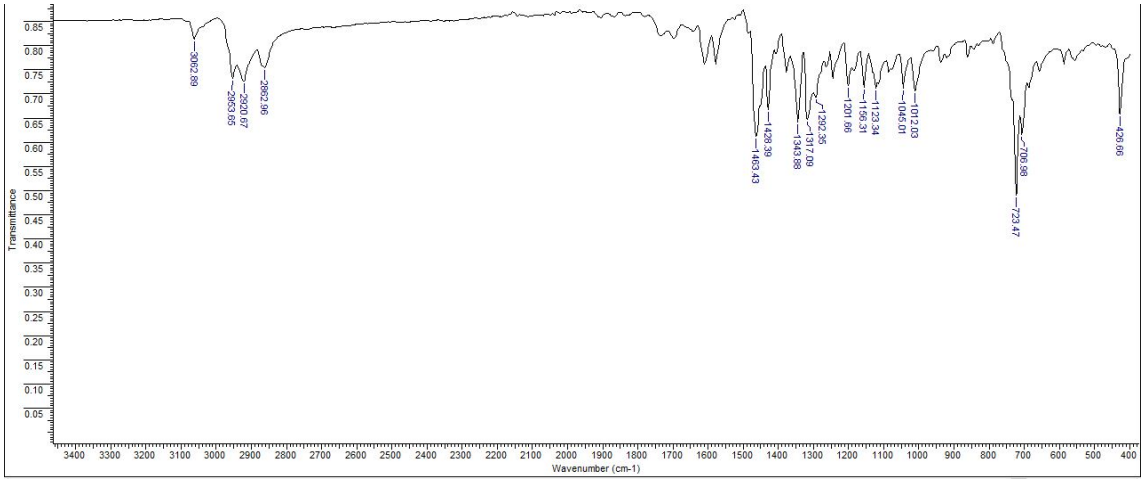
5,6-Dibenzyl-5,6-dihydrofuro[3,2-*b*:4,5-*b*']diindole (3l)



5,6-Bis(4-methylbenzyl)-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3m)



5,6-Di-*n*-butyl-5,6-dihydrofuro[3,2-*b*:4,5-*b*´]diindole (3n)



5,6-Diheptyl-5,6-dihydrofuro[3,2-*b*:4,5-*b*′]diindole (3o)