Supporting information

Color tunable solid-state fluorescence of polycrystalline materials based on push-pull substituted 2,5-diphenyl-stilbene building block.

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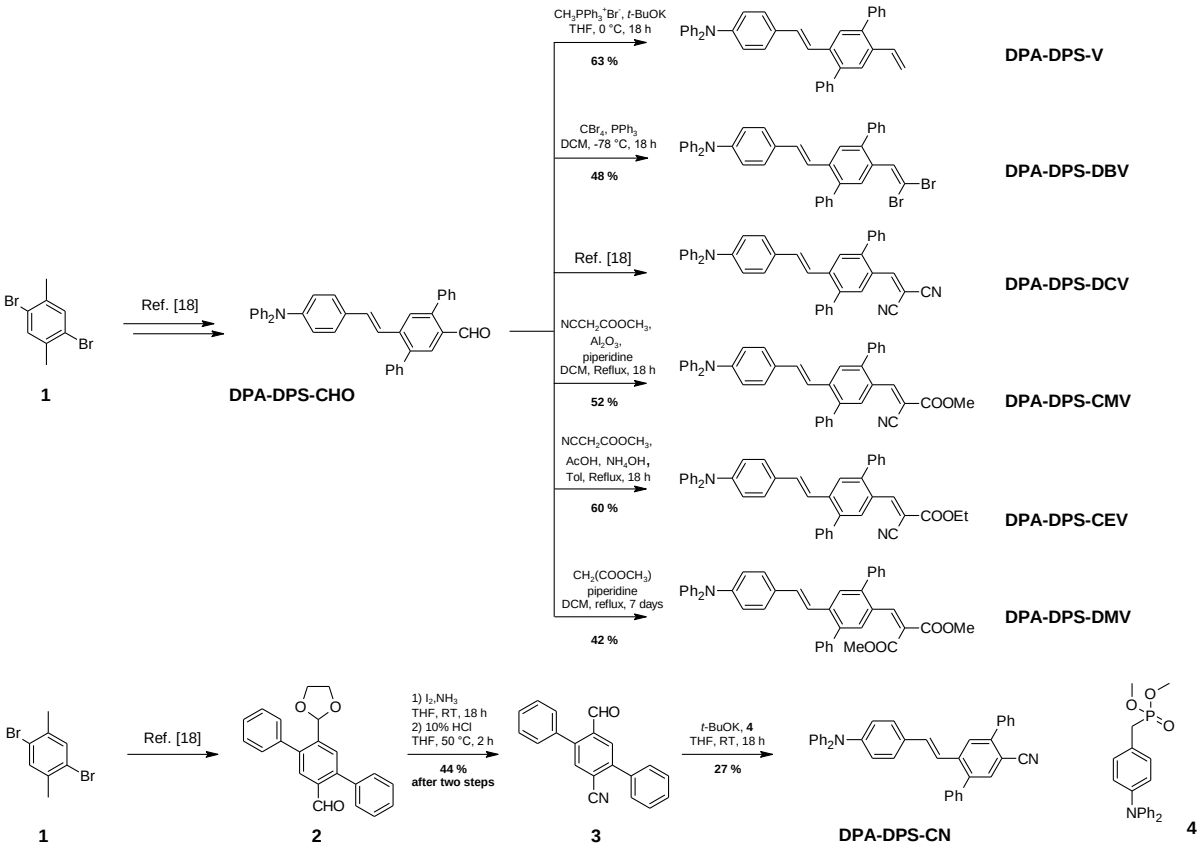
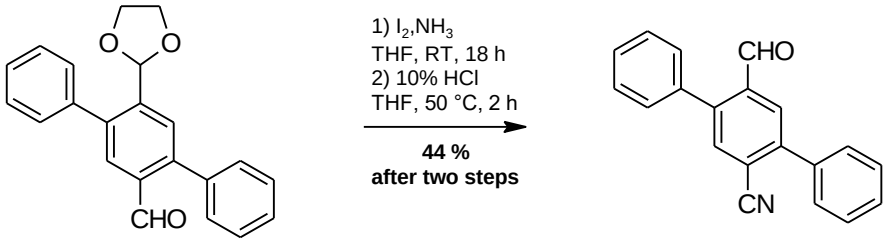
General experimental methods:

All reagents and solvents were purchased from commercial sources (Sigma–Aldrich, Fluorochem, Acros Organics, TCI Europe, Merck, and Lach-Ner). Commercial grade reagents were used without further purification. Reactions were monitored by using thin-layer chromatography (TLC) plates coated with 0.2 mm silica gel (60 F254, Merck). TLC plates were visualized by using UV irradiation (254 nm). All melting points were determined by using a Melting Point B-540 apparatus (Büchi, Switzerland) and are given in their uncorrected form. The IR spectra were recorded with a Nicolet iS50 using the ATR technique. The NMR spectra were measured in $CDCl_3$ and CD_2Cl_2-d_2 solutions at ambient temperature with a Bruker AvanceTM III 400 spectrometer at frequencies 400 MHz (1H) and 100.26 MHz (13C), or with a Bruker AscendTM 500 spectrometer at frequencies 500.13 MHz (1H) and 125.76 MHz (13C{1H}). The chemical shifts (d) reported in the Supporting Information are given in ppm and are related to the following residual solvent peaks: @4.79 (D_2O-d_2), @5.32 (CD_2Cl_2-d_2), @7.27 ($CDCl_3$). Tetramethylsilane (TMS) was used as an internal standard. The coupling constants (*J*) are reported in Hz. Elemental analyses (C, H, and N) were performed with an automatic microanalyzer (Flash 2000 Organic elemental analyzer). Mass spectrometry with high resolution was determined by the "dried droplet" method using a MALDI mass spectrometer LTQ Orbitrap XL (Thermo Fisher Scientific) equipped with a nitrogen UV laser (337 nm, 60 Hz). Spectra were measured in positive ion mode and in regular mass extent with a resolution of 100000 at a massto-charge ratio (m/z) of 400, with 2,5-dihydrobenzoic acid (DBH) used as the matrix. The FTIR spectra were recorded with a FTIR Nicolet iS50 using the ATR technique. The synthetic procedure for compounds **1, DPA-DPS-CHO** and **DPA-DPS-DCV** was described in K. Pauk, et. al., *Chem. Eur. J.,* 2021, **27**, 4341-4348.



Scheme S1: Synthesis of investigated DPA-DPSs and their intermediates.

5'-formyl-[1,1':4',1''-terphenyl]-2'-carbonitrile (3)

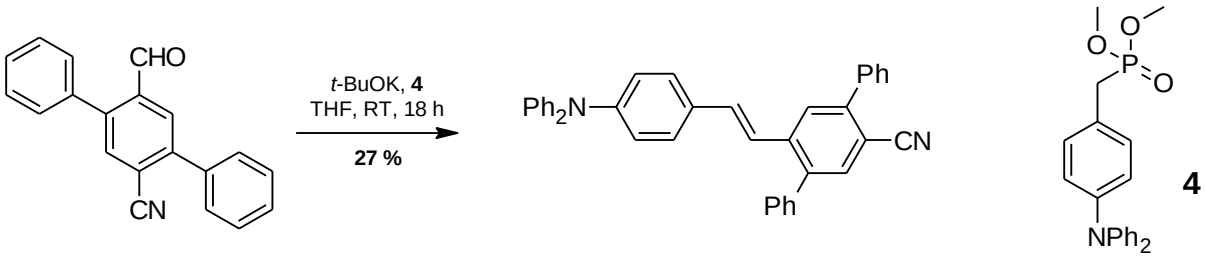


2 **3**

To a 250 mL one-necked flask was charged protected aldehyde **2** (1 g, 3.03 mmol), which was dissolved in THF (30 mL), then iodine (1.5365 g, 6.05 mmol) was added in one portion and cooled to cca 10 ° C. The solution of 28% ammonium hydroxide (40 ml) was slowly added dropwise. The mixture was allowed to stir at RT for 18 h. The reaction was then quenched by the addition of sodium thiosulfate solution (until the mixture was decolorized) and 25 mL of water. The mixture was extracted with EtOAc (3 x 50 mL), the organic phase was dried over Na_2SO_4, followed by column chromatography (applied to 5 g of silica gel, *n*-hexane / EtOAc phase = 7/1, v / v). It was obtained protected nitrile as 941 mg (95%) of white crystals. Rf: 0.38 (n-hexan/EtOAc = 3/1, v/v), **m.p.**: 139.5–140.5 °C. **IR (ATR, cm-1)**: 2891, 2223, 1479, 1446, 1390, 1177, 1073, 1020, 967, 901, 761, 695, 561, 539, 474. **^{1}H NMR** (400 MHz, CD_2Cl_2): δ = 7.90 (s, 1H), 7.75 (s, 1H), 7.67-7.65 (m, 2H), 7.59-7.53 (m, 3H), 7.52-7.48 (m, 5H), 5.72 (s, 1H), 4.16 (m, 2H), 3.96 (m, 2H). **^{13}C NMR** (400 MHz, CD_2Cl_2): δ= 144.3, 141.7, 140.1, 138.2, 137.7, 135.4, 129.7, 129.0, 128.9, 128.8, 128.7, 128.5, 128.3, 118.5, 111.8, 100.4, 65.9. **MALDI-TOF**: Calcd. for $C_{22}H_{17}NO_2$ [M+Na]+ m/z 350.114602; found 350.11572. **Elemental analysis** $C_{22}H_{17}NO_2$ calcd.: C, 80.71; H, 5.23; N, 4.28; found: C, 80.94; H, 5.25; N, 4.02.

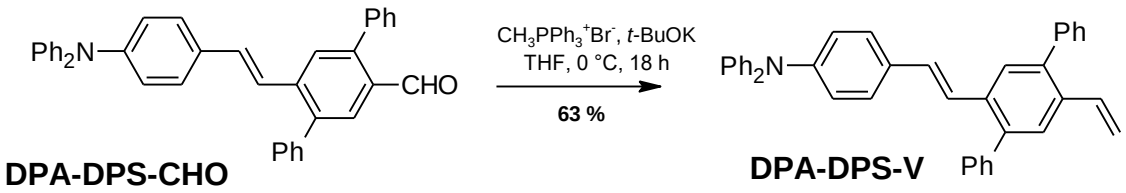
To a 250 mL three-necked flask equipped with a stirrer, reflux condenser, and thermometer was charged protected nitrile obtained above (0.914 g, 2.79 mmol), which was dissolved in 60 mL of THF and then added dropwise with cooling (10 ° C) 20 mL of 10% HCl. The mixture was allowed to stir at 50 °C. After two hours, the reaction was quenched by TLC by adding 150 mL of saturated $NaHCO_3$ solution (to neutral pH - indicated by pH paper). The mixture was extracted with EtOAc (3 x 50 mL), the organic phases were combined and washed with saturated $NaHCO_3$ solution (2 x 70 mL). The organic phases were dried over sodium sulfate, filtered and evaporated. Crude aldehyde was crystallized from EtOAc. It was obtained 785 mg (99%) of white-orange crystals. **R_f**: 0.45 (*n*-hexan/EtOAc = 3/1, v/v), **m.p.**: 194.9–195.9 °C**. IR (ATR, cm^{-1}):** 2959, 2925, 2860, 2331, 1729, 1689, 1605, 1473, 1446, 1384, 1263, 1145, 1078, 1017, 924, 808, 762, 698, 573, 480, 455. **^{1}H NMR** (500 MHz, CD_2Cl_2): δ = 10.04 (s, 1H), 8.13 (s, 1H), 7.92 (s, 1H), 7.67-7.65 (m, 2H), 7.58-7.52 (m, 6H), 7.46-7.45 (m, 2H). **^{13}C NMR** (400 MHz, CD_2Cl_2): δ = 191.1, 144.5, 137.3, 136.5, 136.4, 135.6, 130.2, 129.4, 129.2, 129.0, 128.9, 117.9, 115.6. **MALDI-TOF**: Calcd. for $C_{20}H_{13}NO$ $[M+Na]^+$ m/z 306.08894; found 306.08952. **Elemental analysis** $C_{20}H_{13}NO$ calcd.: C, 84.78; H, 4.62; N, 4.94; found: C, 85.13 ± 0.12; H, 4.62 ± 0.02; N, 4.65 ± 0.01.

(*E*)-5'-(4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-carbonitrile (DPA-DPS-CN)



To a 100 mL flame-dried three-necked flask equipped with a stirrer and thermometer was charged phosphonate **4** (1.173 g, 3.19 mmol), which was dissolved in anhydrous THF (35 mL) under nitrogen. The mixture was then cooled to -10 ° C and solution of *t*-BuOK in THF (1.44 M, 2.77 mL) was added dropwise over 15 minutes. The mixture was allowed to stir for 30 minutes and then aldehyde **3** (0.754 g, 2.66 mmol) dissolved in 10 mL of anhydrous THF was added dropwise at -5 °C over 15 minutes. The mixture was stirred for another 30 minutes at 0 °C and then the mixture was allowed to stir at RT for 18 h. The water (60 ml) was added and the mixture was extracted with ethyl acetate (3 x 50 ml). The organic phases were dried over sodium sulfate, filtered and evaporated. The material was recrystallized twice from EtOAc. It was obtained 384 mg (27%) of yellow crystals. **R_f**: 0.39 (*n*-hexan/EtOAc = 7/1, v/v), **m.p.**: 125.4–126.9 °C. **IR (ATR, cm^{-1})**: 3029, 2221, 1584, 1489, 1314, 1281, 1268, 1177, 1151, 1074, 1022, 961, 904, 817, 755, 695, 616, 492. **^{1}H NMR** (CD_2Cl_2, 500 MHz): δ = 7.92 (s, 1H), 7.75 (s, 1H), 7.72-7.70 (d, *J=7.65 Hz*, 2H), 7.61-7.58 (m, 2H), 7.56-7.52 (m, 3H), 7.49-7.45 (m, 3H), 7.32-7.27 (m, 6H), 7.23-7.20 (m, 1H), 7.12-7.08 (m, 6H), 7.06-7.03 (m, 1H), 7.00-6.99 (m, 2H). **^{13}C NMR** (CD_2Cl_2, 100 MHz): δ = 148.3, 147.4, 144.1, 140.4, 140.3, 138.8, 138.5, 135.6, 132.5, 130.6, 129.8, 129.5, 128.9, 128.8, 128.7, 128.1, 127.9, 127.1, 125.0, 123.9, 123.6, 122.9, 118.9, 109.3. **MALDI-TOF**: $[M]^+$ Calcd. for $C_{39}H_{28}N_2$ 524.2247; found 524.22489. **Elemental analysis:** Calc. for $C_{39}H_{28}N_2$: C, 89.28; H, 5.38; N, 5.34; found: C, 88.70 ± 0.31; H, 5.36 ± 0.06; N, 5.08 ± 0.02.

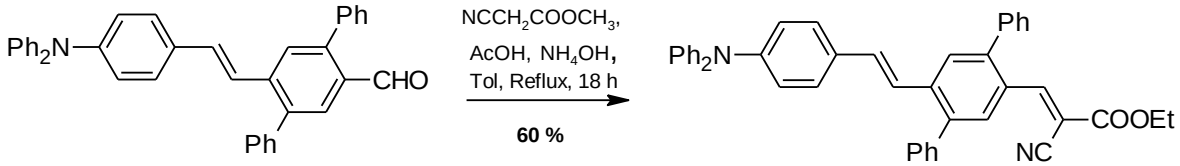
(*E*)-*N*,*N*-diphenyl-4-(2-(5'-vinyl-[1,1':4',1''-terphenyl]-2'-yl)vinyl)aniline (DPA-DPS-V)



A 3-necked 250 mL round bottom flask equipped with a stirrer and thermometer was charged with $CH_3Ph_3P^+Br^-$ (2.25 g, 6.28 mmol), which was then dissolved in anhydrous THF (130 mL). The mixture was cooled to 0 °C and solution of *t*-BuOK in THF (1.47 M, 3.83 mL, 5.63 mmol) was added dropwise via syringe pump over 15 minutes, the mixture was stirred for another 30 minutes at the same temperature. Subsequently, aldehyde (2.71 g, 5.13 mmol) dissolved in 30 mL of anhydrous THF was added dropwise via syringe pump over 15 minutes, and the mixture was stirred at 0 °C for another 10 minutes and then allowed to stir at RT for 18 hours. The reaction was quenched by the addition of saturated NH_4Cl solution (100 mL) and the mixture was extracted with EtOAc (3 x 75 mL). The organic phases were dried over sodium sulphate, evaporated, followed by column chromatography (*n*-hexane/EtOAc phase = 100/1, v/v, applied to 12 g of silica gel). Chromatography gave 2.3 g of the product, followed the crystallization from EtOAc to give 1.7 g (63%) of slightly greenish crystals. **Rf**: 0.7

(*n*-hexan/EtOAc = 7/1, v/v), **m.p.**: 163.1–163.7 °C. **IR (ATR, cm^{-1})**: 3020, 1584, 1486, 1326, 1274, 1174, 1075, 1016, 993, 960, 891, 821, 748, 694, 621, 535, 497. **^{1}H NMR** (CD_2Cl_2, 500 MHz): 7.72-7.66 (d, 2H), 7.52-7.42 (m, 10H), 7.31-7.25 (m, 7H), 7.10-7.04 (m, 7H), 6.99-6.98 (m, 2H), 6.81-6.75 (dd, 1H), 5.80-5.76 (d, *J=17.5 Hz,* 1H), 5.24-5.22 (d, *J=11.1 Hz* ,1H). **^{13}C NMR** (CD_2Cl_2, 125 MHz,): 147.6, 147.5, 147.4, 147.3, 146.9, 141.0, 140.8, 140.6, 140.5, 140.4, 140.2,139.4, 137.4, 135.2, 134.9, 134.5, 131.6, 129.8, 129.7, 129.3, 129.0, 128.2, 128.1, 127.4, 127.3, 127.2, 127.2, 127.1, 127.0, 126.5, 125.1, 124.5, 124.3, 123.3, 123.1, 114.5. **MALDI-TOF**: $[M]^+$ Calcd. for $C_{40}H_{31}N$ 525.2451; found 525.24604. **Elemental analysis:** Calc. for $C_{40}H_{31}N$: C, 91.39; H, 5.94; N, 2.66; found: C, 91.75 ± 0.37; H, 5.98 ± 0.01; N, 2.52 ± 0.01.

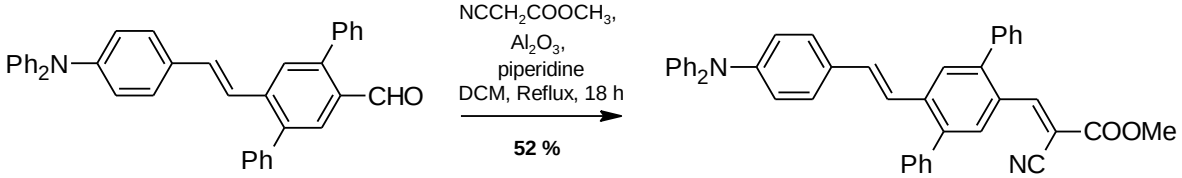
Ethyl (*E*)-2-cyano-3-(5'-((*E*)-4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)acrylate (DPA-DPS-CEV)



DPA-DPS-CHO **DPA-DPS-CEV**

To a 100 mL three-necked flask equipped with a stirrer and thermometer was charged 0.5 g of aldehyde (9.48 mmol), which was dissolved in 40 mL of toluene. Then 0.3 mL of ethyl cyanoacetate (2.84 mmol), 0.44 mL of 25% NH_4OH (2.84 mmol) and 4.6 mL of acetic acid were added. The mixture was brought to reflux for 18 hours. After that time, the reaction was quenched and extracted with DCM (3 x 50 mL), the organic phases were combined, washed with water (3 x 50 mL) and dried over sodium sulphate. After filtration and evaporation, 731 mg of a crude mixture was crystallized from a mixture of EtOAc/MeOH/*n*-hexane/DCM to give red crystals (354 mg, 60%). **R_f**: 0.26 (*n*-hexan/EtOAc = 7/1, v/v). **m.p.**: 218.5–219.5 °C. **IR (ATR, cm^{-1})**: 3032, 2220, 1720, 1580, 1487, 1323, 1244, 1162, 1090, 1019, 967, 899, 820, 753, 696, 619, 566, 500. **^{1}H NMR** (CD_2Cl_2, 500 MHz): 8.31 (s, 1H), 8.26 (s, 1H), 7.92 (s, 1H), 7.57-7.53 (m, 7H), 7.49-7.44 (m, 3H), 7.31-7.23 (m, 7H), 7.13-7.07 (m, 7H), 7.00-6.98 (d, 2H), 4.35-4.31 (q, 2H), 1.37-1.34 (t, 3H). **^{13}C NMR** (CD_2Cl_2, 125 MHz): 162.4, 154.0, 148.0, 147.3, 143.9, 140.2, 139.8, 139.4, 139.0, 131.7, 130.7, 130.6, 130.0, 129.8, 129.3, 128.5, 128.4, 128.3, 127.7, 127.3, 124.8, 124.5, 124.2, 123.4, 122.8, 115.8, 103.4, 62.5, 13.9. **MALDI-TOF**: $[M]^+$ Calcd. for $C_{44}H_{34}N_2O_2$ 622.26148; found 622.26173.

Methyl (*E*)-2-cyano-3-(5'-((*E*)-4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)acrylate (DPA-DPS-CMV)

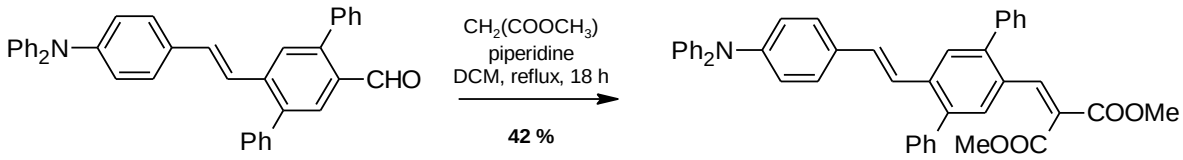


DPA-DPS-CHO **DPA-DPS-CMV**

To a 50 mL flask equipped with a stirrer and thermometer was charged 0.5 g of aldehyde (9.48 mmol), which was dissolved in 12 mL of DCM. Then half a teaspoon of basic alumina and 0.25 mL of methyl

cyanoacetate (2.84 mmol) were added. The mixture was allowed to stir at RT for 2 hours after refluxed for 18 hours. After 18 hours, the mixture was filtered, evaporated. It was obtained 750 mg of crude mixture, which was crystallized, from DCM. After crystallization was obtained 303 mg (52%) of a red powder. (R_f: 0.18 (*n*-hexan/EtOAc = 7/1, v/v). **m.p.**: 233.3–234.5 °C. **IR (ATR, cm^{-1})**: 3037, 2223, 1729, 1569, 1485, 1432, 1334, 1252, 1166, 1089, 1024, 965, 943, 906, 819, 758, 698, 621, 562, 520, 498. **^{1}H NMR** (CD_2Cl_2, 500 MHz): 8.31 (s, 1H), 8.27 (s, 1H), 7.92 (s, 1H), 7.56-7.53 (m, 7H), 7.45-4.44 (m, 3H), 7.31-7.23 (m, 7H), 7.13-7.07 (m, 7H), 7.00-6.98 (d, 2H), 3.88 (s, 3H). **^{13}C NMR** (CD_2Cl_2, 125 MHz): 162.9, 154.3, 148.1, 147.3, 143.9, 140.2, 139.9, 139.4, 138.9, 131.8, 130.7, 130.6, 130.0, 129.8, 129.3, 129.1, 128.5, 128.4, 128.3, 128.2, 127.8, 127.4, 124.9, 124.8, 124.5, 124.2, 123.4, 122.7, 115.8, 102.9, 53.2. **MALDI-TOF**: $[M]^+$ Calcd. For $C_{43}H_{32}N_2O_2$ 608.24583; found 608.24819.

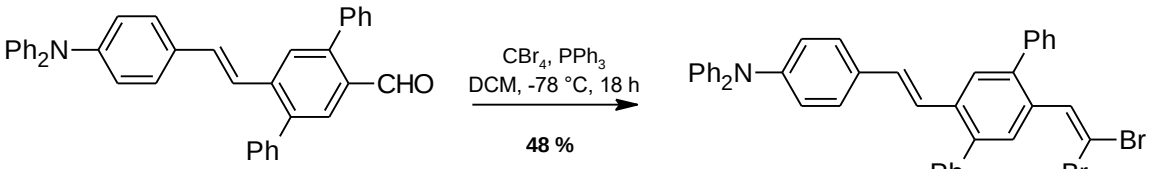
Dimethyl (*E*)-2-((5'-(4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)methylene)malonate (DPA-DPS-DMV)



DPA-DPS-CHO **DPA-DPS-DMV**

To a 100 mL round bottom flask was charged 0.5 g of aldehyde (9.48 mmol), which was dissolved in 12 mL of DCM, then 0.32 mL of dimethyl malonate was added, and few drops of piperidine were added dropwise. The mixture was allowed to stir at reflux for 18 h, then water was added. The mixture was extracted with DCM (3 x 50 mL), the organics were combined, dried over sodium sulphate and evaporated. The material was crystallized from a mixture of DCM/*n*-hexane/EtOAc/MeOH to give 270 mg (45%) as fine red crystals. R_f: 0.16 (*n*-hexan/EtOAc = 7/1, v/v). **m.p.**: 211.0–211.6 °C. **IR (ATR, cm^{-1})**: 3032, 2946, 1723, 1625, 1583, 1488, 1439, 1378, 1332, 1273, 1240, 1220, 1159, 1067, 1022, 989, 967, 905, 818, 751, 696, 620, 535, 499, 445. **^{1}H NMR** (CD_2Cl_2, 500 MHz): 7.85 (s, 1H), 7.71 (s, 1H), 7.54-7.49 (m, 7H), 7.46-7.42 (m, 4H), 7.31-7.27 (m, 6H), 7.19-7.16 (d, 1H), 7.11-7.03 (m, 7H), 6.99-6.98 (d, 2H), 3.79 (s, 3H), 3.78 (s, 3H). **^{13}C NMR** (CD_2Cl_2, 125 MHz): 169.9, 164.3, 147.7, 147.4, 142.8, 142.0, 140.1, 139.9, 139.5, 137.6, 131.0, 130.6, 130.3, 130.2, 129.8, 129.6, 129.3, 128.4, 128.3, 127.9, 127.6, 127.5, 127.1, 126.2, 124.6, 124.5, 123.3, 122.9, 52.5. **MALDI-TOF**: $[M]^+$ Calcd. For $C_{44}H_{35}NO_4$: 641.25606; found 641.25797. **Elemental analysis:** Calc. for $C_{44}H_{35}NO_4$: C, 82.35; H, 5.50; N, 2.18; found: C, 82.16 ± 0.28; H, 5.62 ± 0.02; N, 2.09 ± 0.03.

(*E*)-4-(2-(5'-(2,2-dibromovinyl)-[1,1':4',1''-terphenyl]-2'-yl)vinyl)-*N,N*-diphenylaniline (DPA-DPS-DBV)

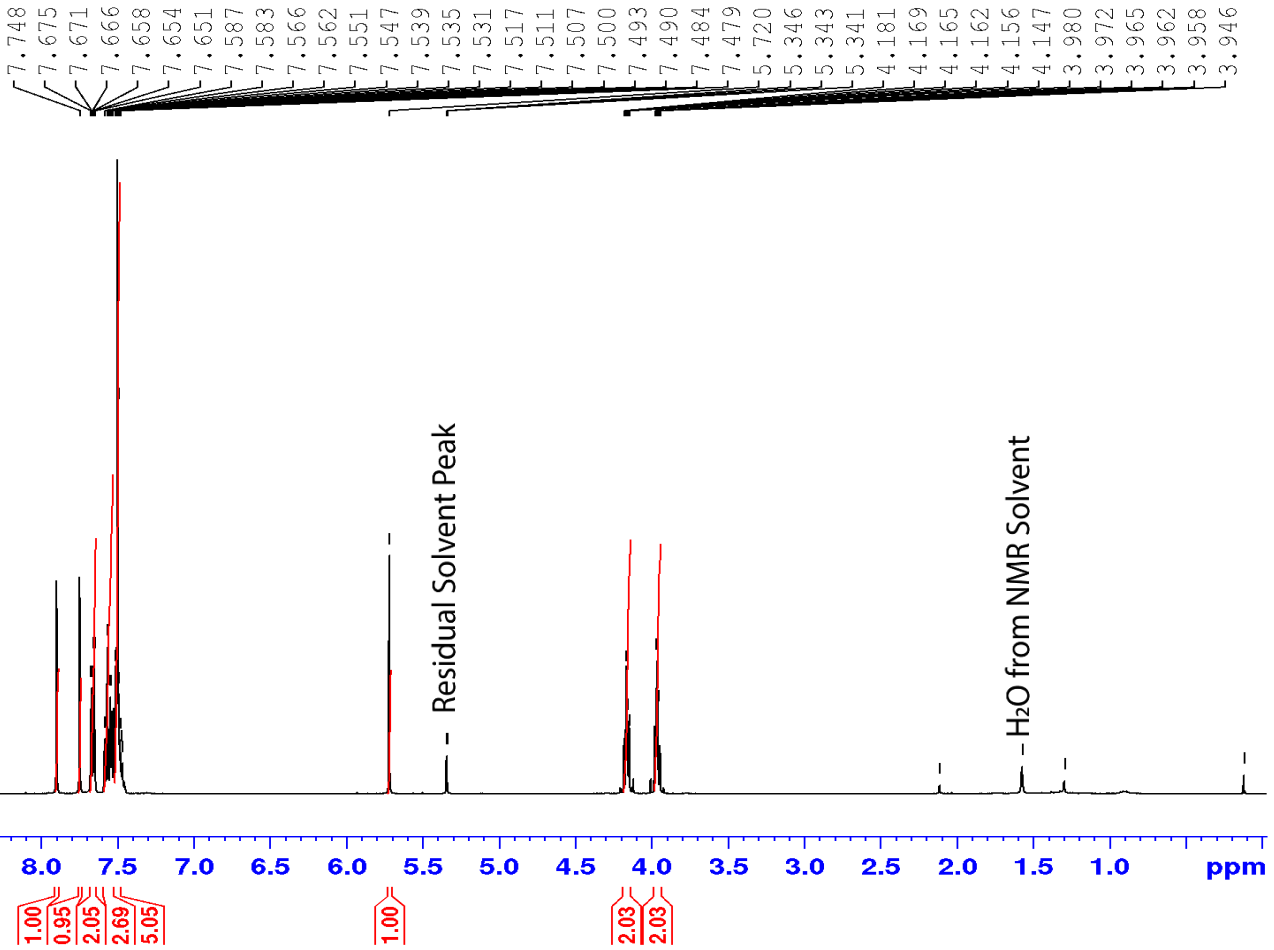


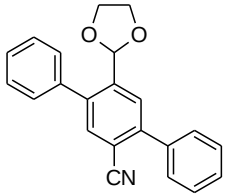
DPA-DPS-CHO **DPA-DPS-DBV**

To the 100 ml flame-dried three-necked flask equipped with a stirrer and a thermometer was added CBr_4 (0.556 g, 1.7 mmol), which was dissolved in 40 ml of anhydrous DCM. The solution was cooled to

-5 °C and a solution of PPh_3 (0.895 g, 3.4 mmol) in 5 mL of anhydrous DCM was added dropwise. The mixture was cooled to -78 °C and a solution of aldehyde (0.5 g, 9.48 mmol) in 5 mL of dry DCM was added dropwise. The mixture was allowed to stir for 2 hours at -78 °C and then for 18 hours at RT. Then, the reaction was quenched by the addition of 50 mL of saturated NH_4Cl solution, followed by extraction with DCM (3 x 50 mL) and drying over sodium sulphate. For purification, column chromatography was performed (n-hexane/EtOAc phase = 39/1, v / v, substance applied to 6 g of silica gel). 441 mg of product was isolated and crystallized from EtOAc to give 310 mg (48%) of yellow crystals. **R_f**: 0.45 (n-hexan/EtOAc = 19/1, v/v). **m.p.**: 198–199 °C. **IR (ATR, cm^{-1})**: 3029, 1587, 1491, 1314, 1282, 1175, 1155, 1072, 1023, 958, 904, 858, 819, 797, 749, 692, 622, 521, 499. **^{1}H NMR** ($CDCl_3$, 500 MHz): δ = 7.75-7.74 (m, 2H), 7.53-7.41 (m, 11H), 7.28 (m, 3H), 7.25-7.24 (m, 2H), 7.11-7.10 (m, 4H), 7.07-6.99 (m, 6H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ= 147.7, 147.6, 140.5, 140.3, 140.1, 139.9, 137.1, 136.0, 132.7, 131.6, 131.2, 130.1, 130.0, 129.7, 129.5, 128.6, 128.5, 127.9, 127.7, 127.6, 127.2, 125.3, 124.8, 123.5, 123.3, 90.9. **MALDI-TOF**: $[M]^+$ Calcd. For $C_{40}H_{29}Br_2N_2$: 695.0692; found 681.06693. **Elemental analysis:** Calc. for $C_{40}H_{29}Br_2N_2$: C, 70.29; H, 4.28; N, 2.05; found: C, 70.51 ± 0.02; H, 4.58 ± 0.04; N, 1.88 ± 0.02.

^{1}H NMR spectrum of 5'-(1,3-dioxolan-2-yl)-[1,1':4',1''-terphenyl]-2'-carbonitrile



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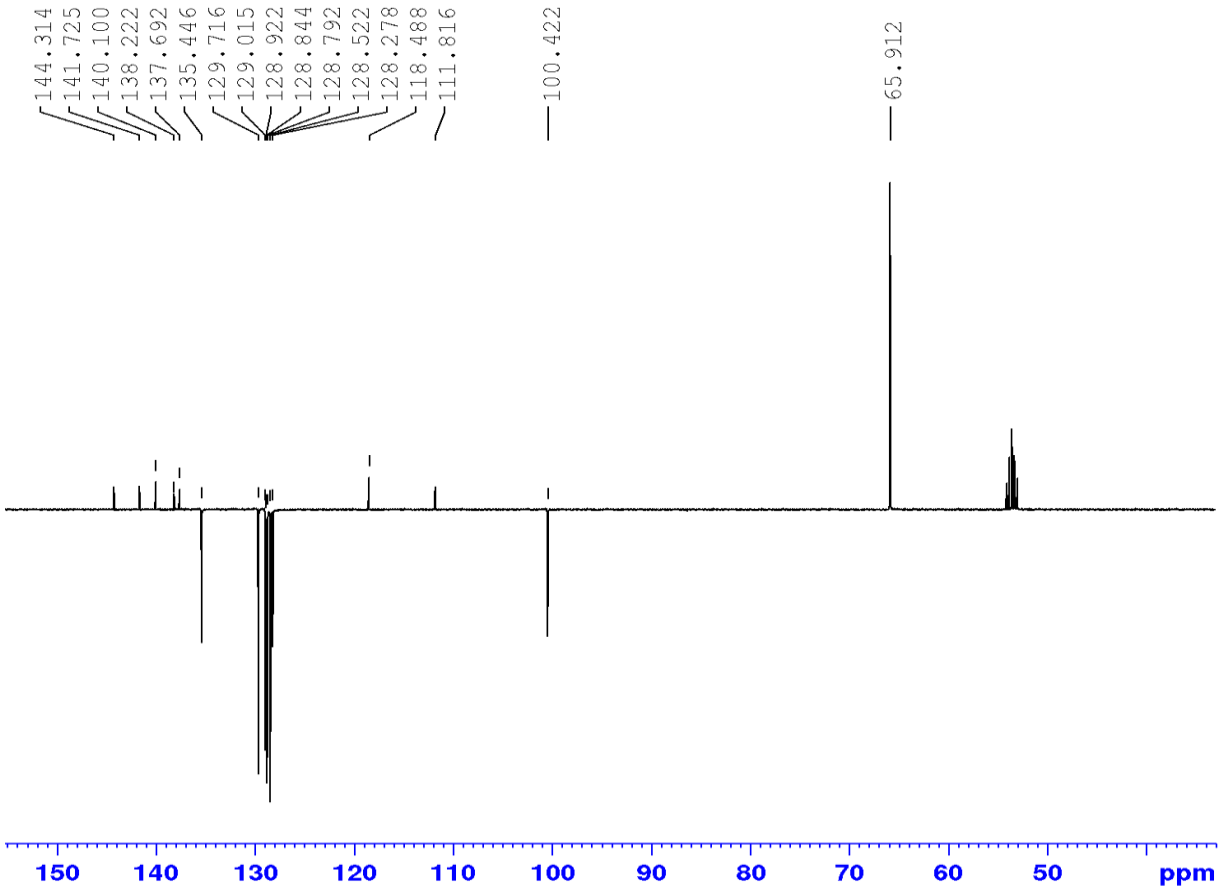
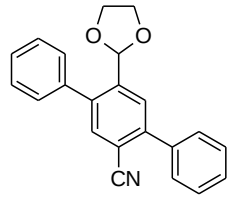
^{13}C NMR spectrum of 5'-(1,3-dioxolan-2-yl)-[1,1':4',1''-terphenyl]-2'-carbonitrile



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Current Data Parameters
NAME                   DPP
EXPNO                  292
PROCNO                   1

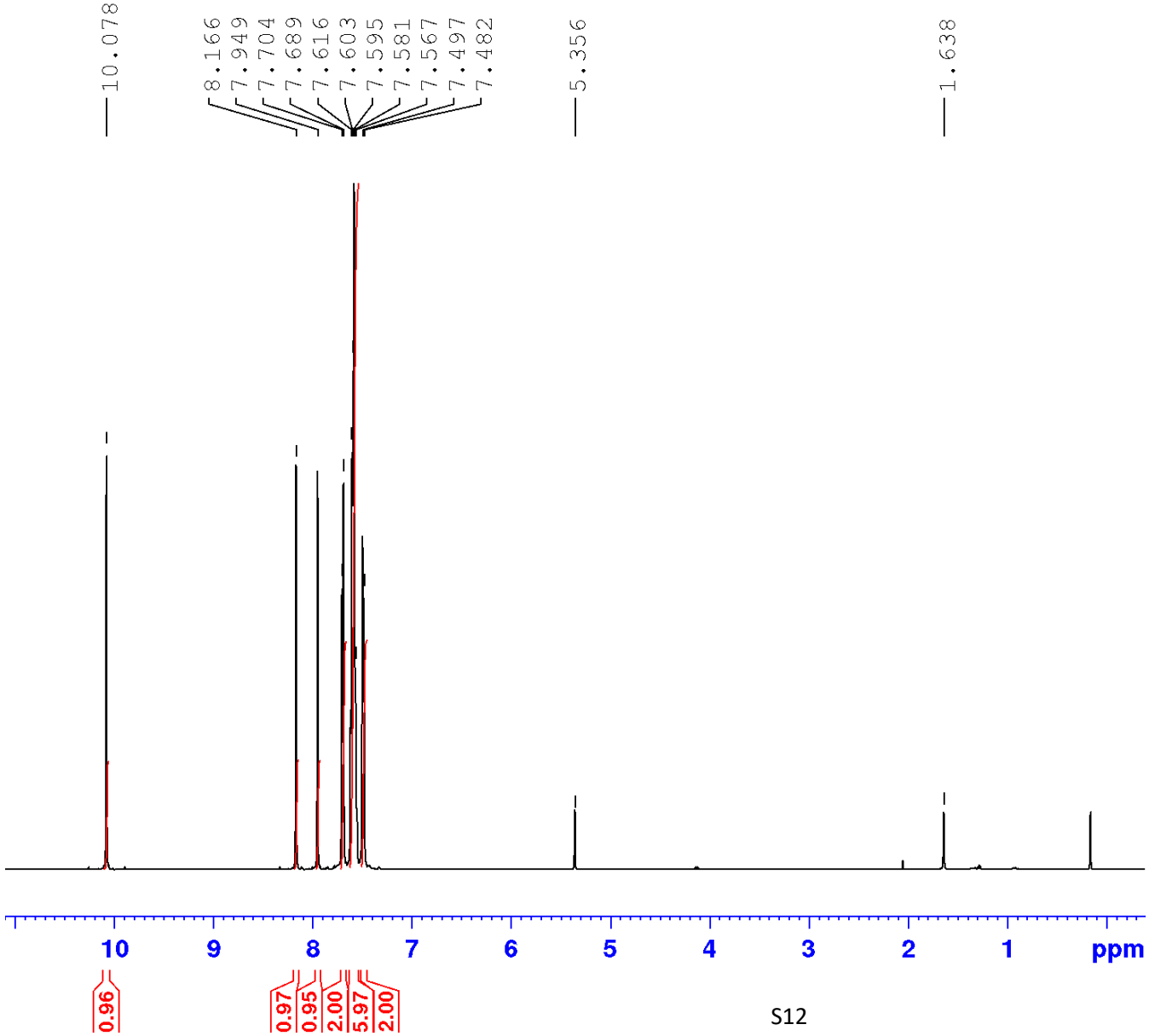
F2 - Acquisition Parameters
Date_           20200310
Time               16.15
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG             jmod
TD                 65536
SOLVENT           CD2Cl2
NS                 11264
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                295.6 K
CNST2        145.0000000
CNST11         1.0000000
D1           2.00000000 sec
D20          0.00689655 sec
TD0                    1

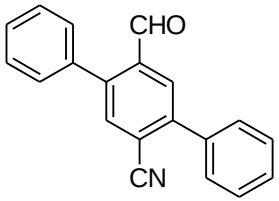
======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                10.00 usec
P2                20.00 usec
PLW1         50.27999878 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         26.98999977 W
PLW12         0.33320999 W

F2 - Processing parameters
SI                 32768
SF           100.6127507 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

^{1}H NMR spectrum of 5'-formyl-[1,1':4',1''-terphenyl]-2'-carbonitrile (3)



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Current Data Parameters
NAME                  DPP
EXPNO                 118
PROCNO                  4

F2 - Acquisition Parameters
Date_           20200707
Time                6.16
INSTRUM            spect
PROBHD   5 mm PATBI 1H/
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                     8
DS                     2
SWH           10000.000 Hz
FIDRES          0.152588 Hz
AQ             3.2767999 sec
RG                 98.58
DW                50.000 usec
DE                 6.50 usec
TE        0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                   1H
P1                10.00 usec
PLW1          8.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.2000000 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```
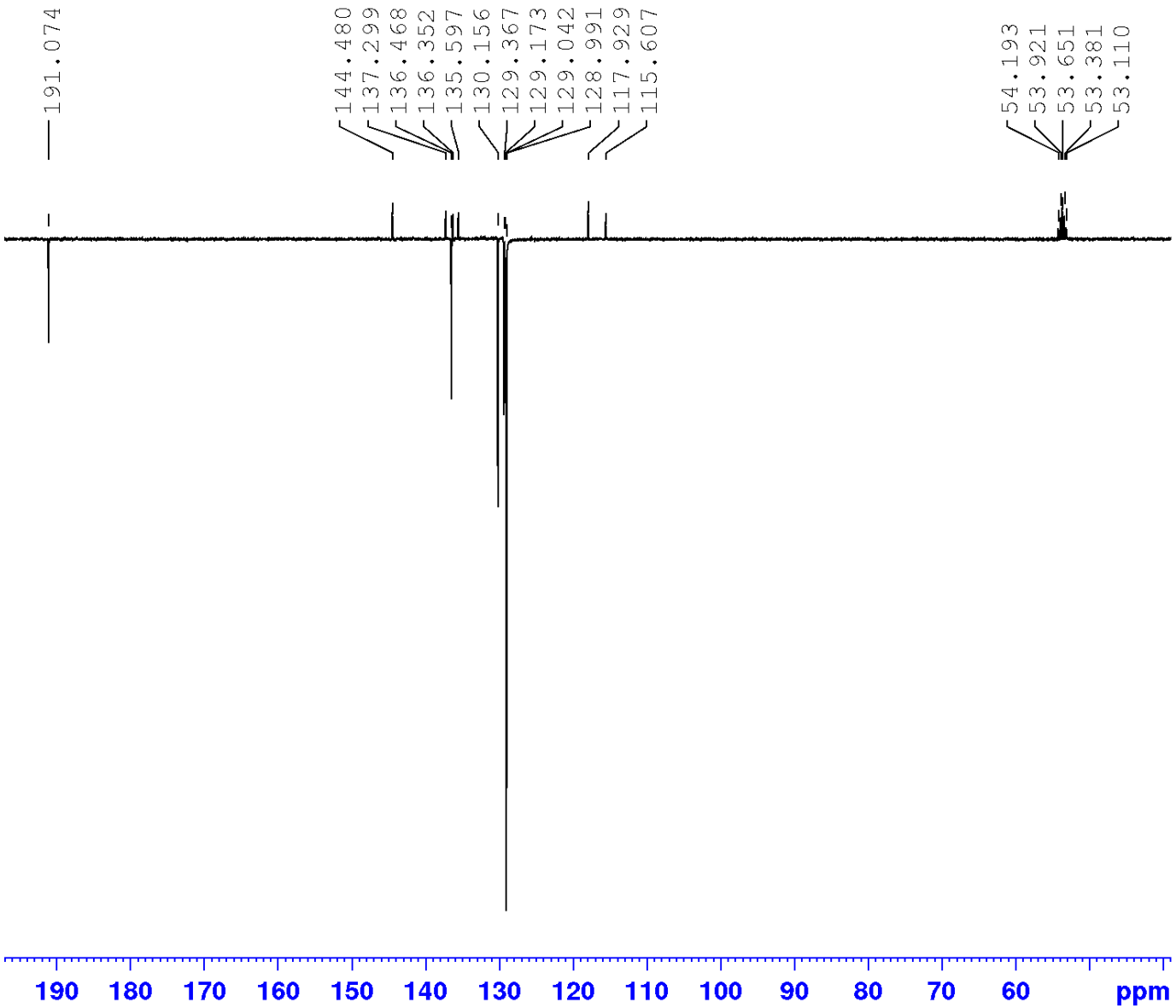
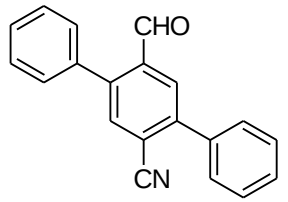
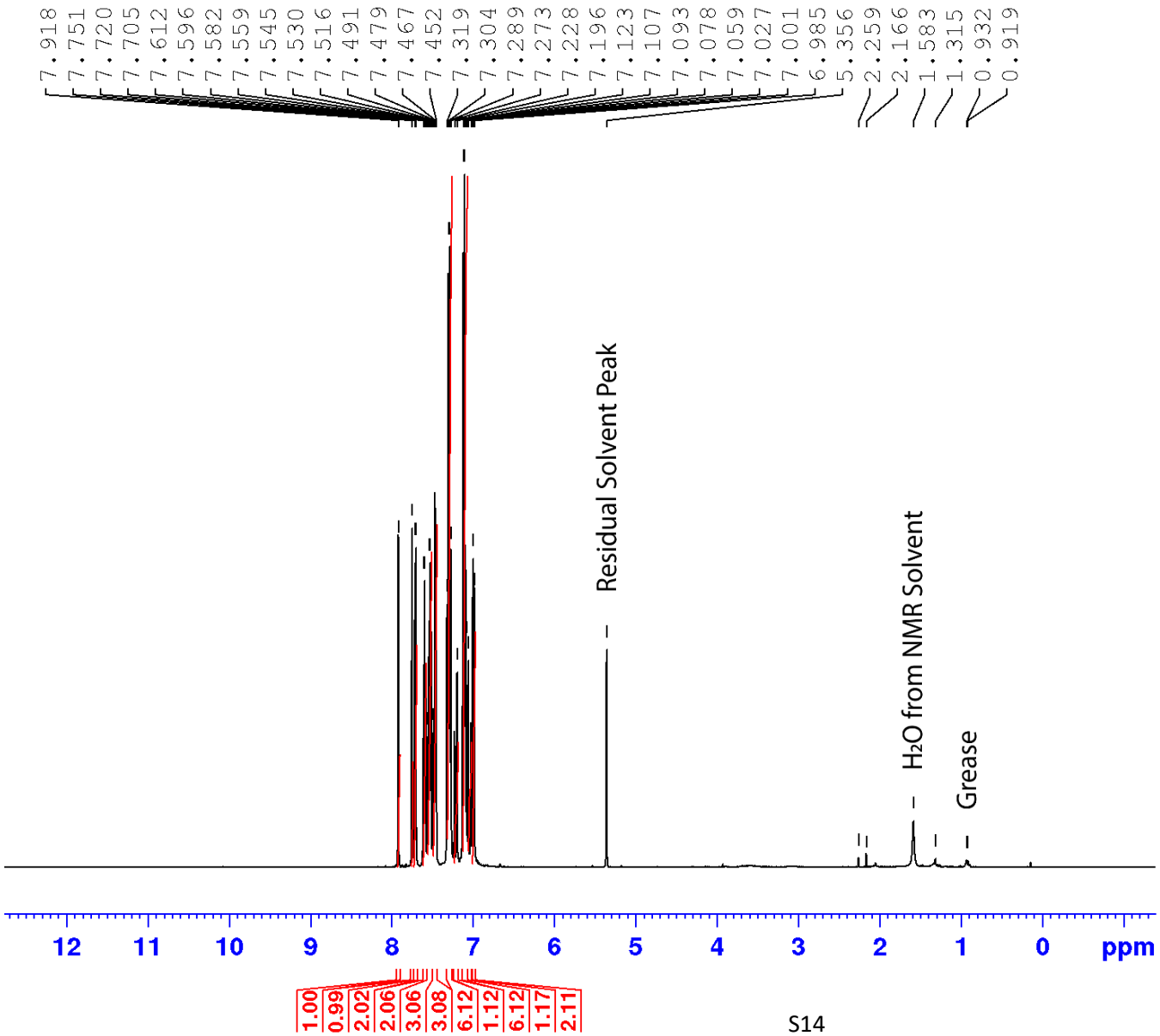

^{13}C NMR spectrum of 5'-formyl-[1,1':4',1''-terphenyl]-2'-carbonitrile (3)

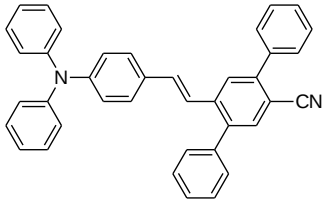





```
Current Data Parameters
NAME                   DPP
EXPNO                  310
PROCNO                   1

F2 - Acquisition Parameters
Date_           20200708
Time                6.35
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             jmod
TD                 65536
SOLVENT           CD2Cl2
NS                  1033
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                296.0 K
CNST2        145.0000000
CNST11         1.0000000
D1            2.00000000 sec
D20           0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                10.00 usec
P2                20.00 usec
PLW1         50.27999878 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         26.98999977 W
PLW12         0.33320999 W

F2 - Processing parameters
SI                 32768
SF           100.6127507 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

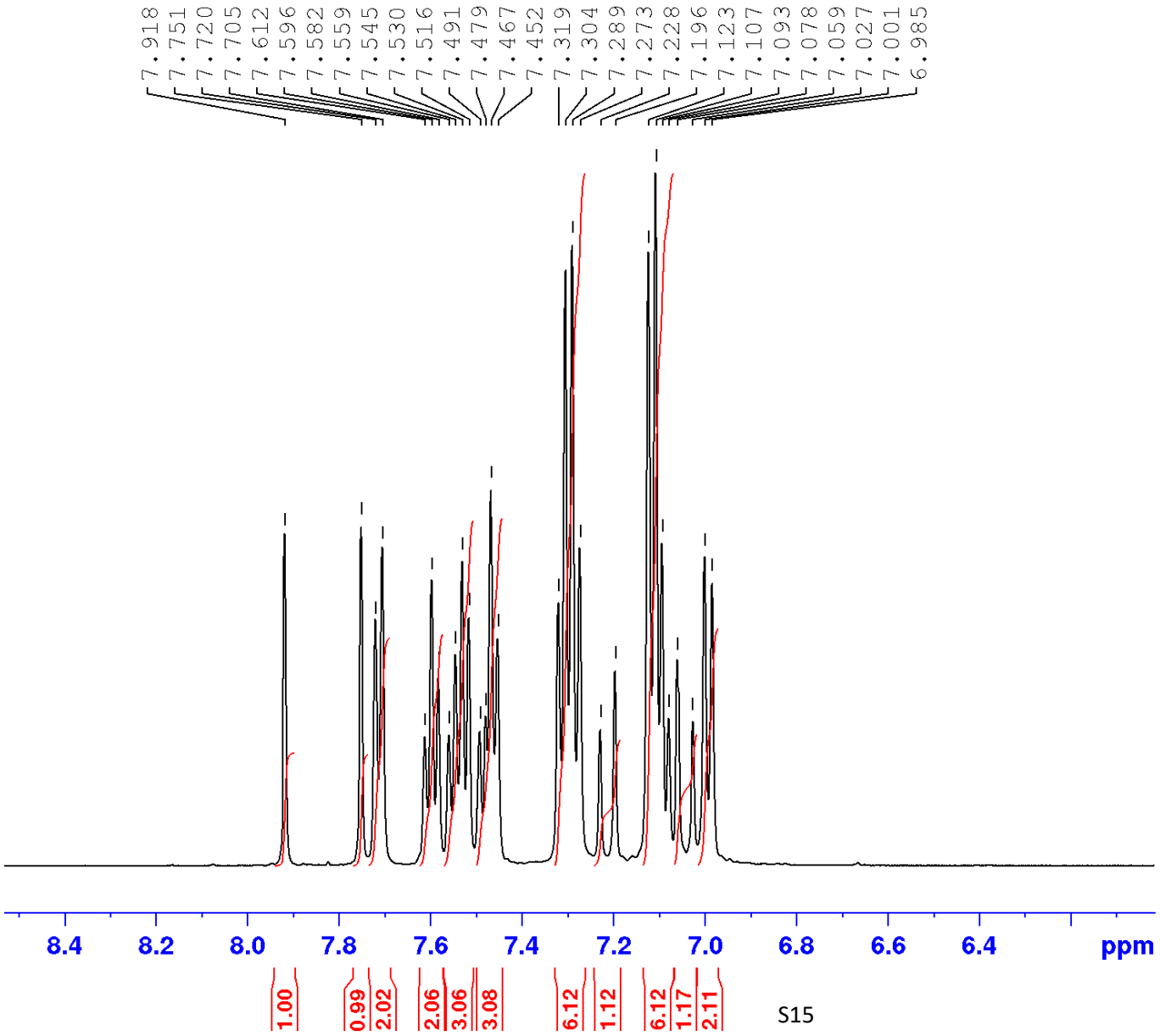
^{1}H NMR spectrum of (*E*)-5'-(4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-carbonitrile (**DPA-DPS-CN**)

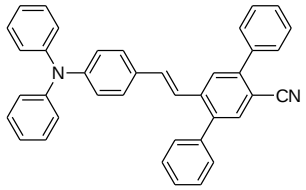





```
Current Data Parameters
NAME                  DPP
EXPNO                 107
PROCNO                  4

F2 - Acquisition Parameters
Date_           20200610
Time                7.24
INSTRUM            spect
PROBHD   5 mm PATBI 1H/
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                     8
DS                     2
SWH           10000.000 Hz
FIDRES          0.152588 Hz
AQ             3.2767999 sec
RG                103.54
DW                50.000 usec
DE                 6.50 usec
TE       0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        500.2030889 MHz
NUC1                   1H
P1                10.00 usec
PLW1          8.00000000 W

F2 - Processing parameters
SI                 65536
SF          500.2000000 MHz
WDW                   EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
```

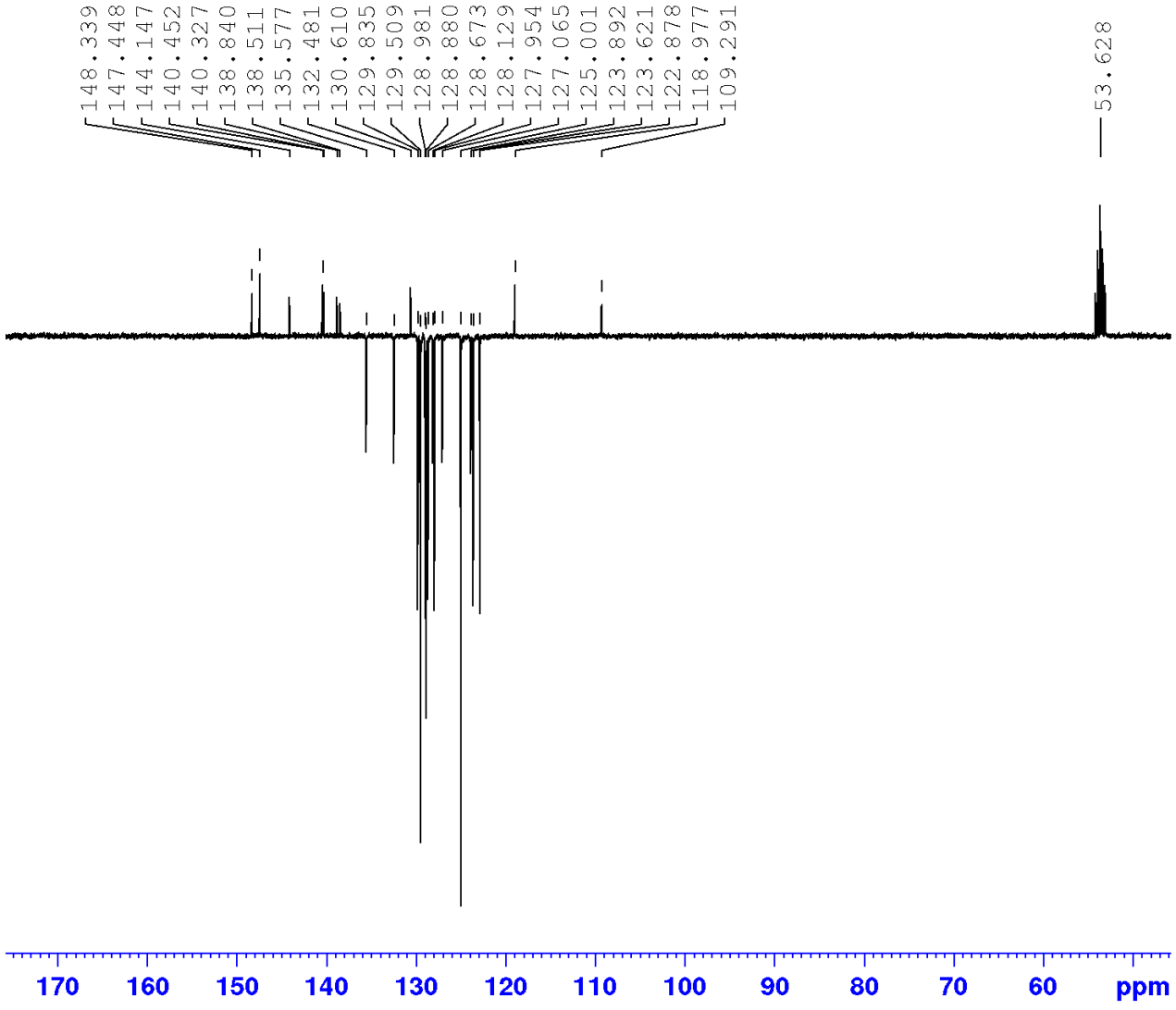
^{1}H NMR spectrum of aromatic part of (*E*)-5'-(4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-carbonitrile (**DPA-DPS-CN**)

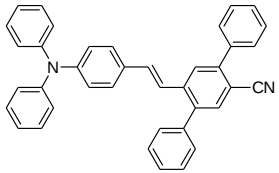





```
Current Data Parameters
NAME                   DPP
EXPNO                  107
PROCNO                   4

F2 - Acquisition Parameters
Date_           20200610
Time               7.24
INSTRUM           spect
PROBHD   5 mm PATBI 1H/
PULPROG            zg30
TD                65536
SOLVENT           CD2Cl2
NS                    8
DS                    2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ            3.2767999 sec
RG                103.54
DW                50.000 usec
DE                 6.50 usec
TE       0 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        500.2030889 MHz
NUC1                1H
P1                10.00 usec
PLW1         8.00000000 W

F2 - Processing parameters
SI                65536
SF          500.2000000 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

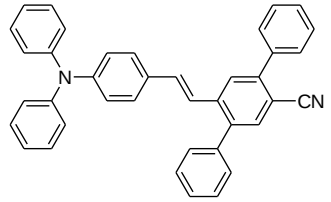
^{13}C NMR spectrum of (*E*)-5'-(4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-carbonitrile (**DPA-DPS-CN**)

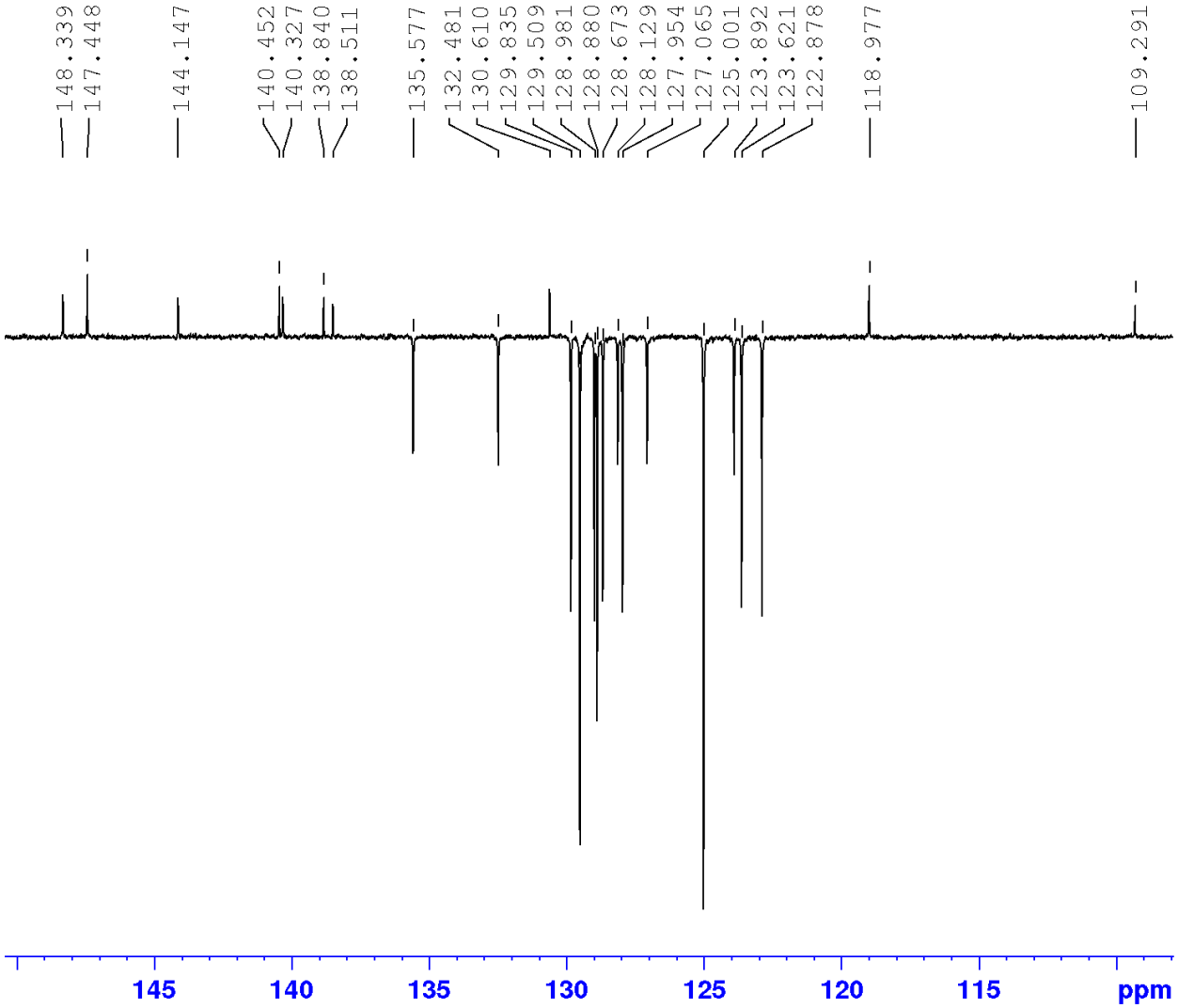





```
Current Data Parameters
NAME                   DPP
EXPNO                  306
PROCNO                   1

F2 - Acquisition Parameters
Date_           20200610
Time                6.19
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG             jmod
TD                 65536
SOLVENT           CD2Cl2
NS                  1026
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                294.4 K
CNST2        145.0000000
CNST11         1.0000000
D1           2.00000000 sec
D20          0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                10.00 usec
P2                20.00 usec
PLW1         50.27999878 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         26.98999977 W
PLW12         0.33320999 W

F2 - Processing parameters
SI                 32768
SF           100.6127507 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

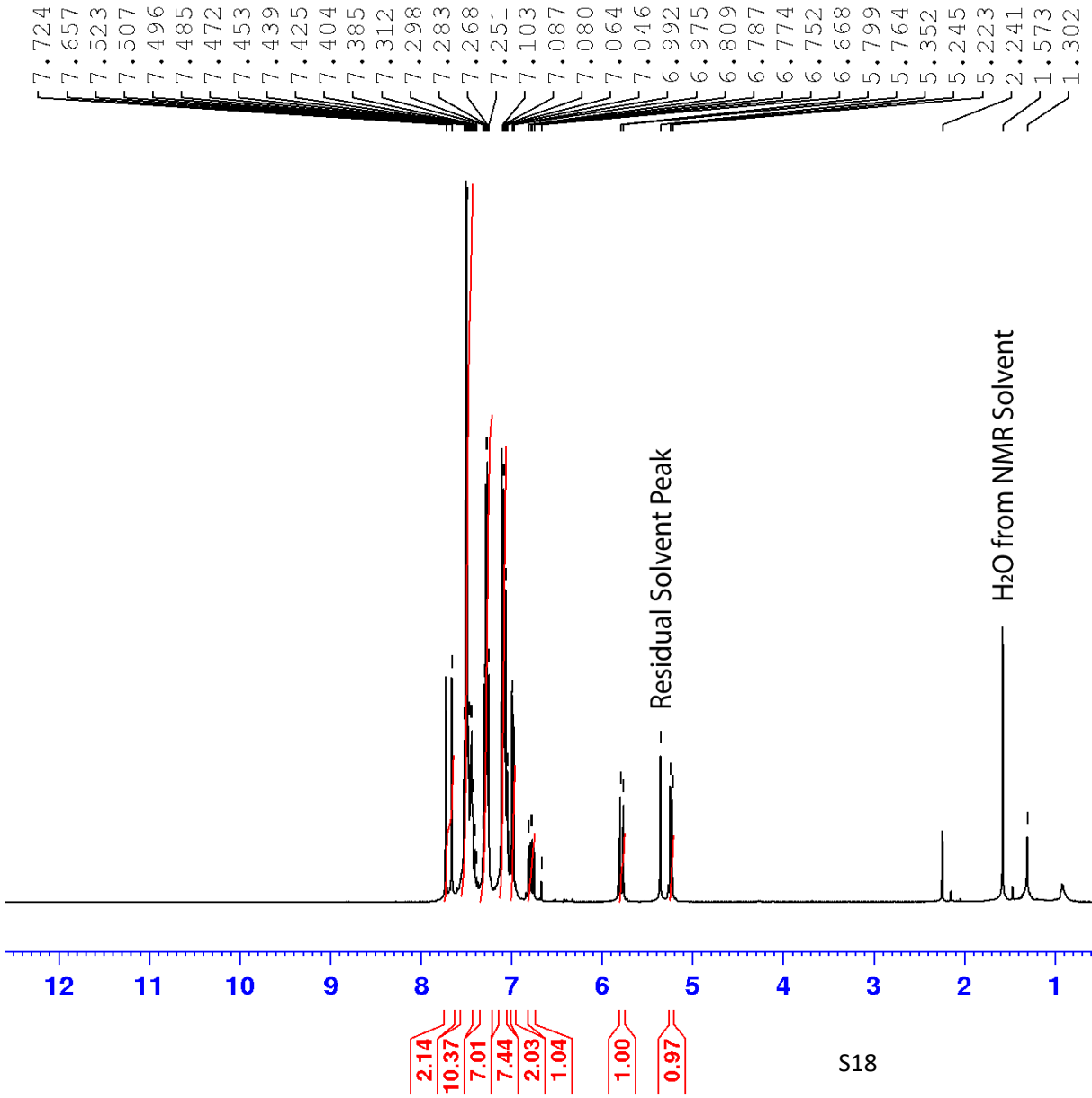
^{13}C NMR spectrum of aromatic part of (*E*)-5'-(4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-carbonitrile (**DPA-DPS-CN**)

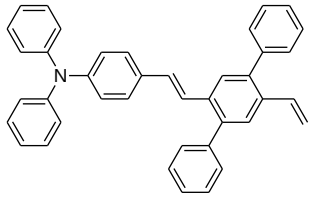





```
Current Data Parameters
NAME                   DPP
EXPNO                  306
PROCNO                   1

F2 - Acquisition Parameters
Date_           20200610
Time                6.19
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             jmod
TD                 65536
SOLVENT            CD2Cl2
NS                  1026
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                  2050
DW                 20.800 usec
DE                  6.50 usec
TE                 294.4 K
CNST2         145.0000000
CNST11          1.0000000
D1              2.00000000 sec
D20             0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                  13C
P1                  10.00 usec
P2                  20.00 usec
PLW1          50.27999878 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          26.98999977 W
PLW12          0.33320999 W

F2 - Processing parameters
SI                 32768
SF            100.6127507 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

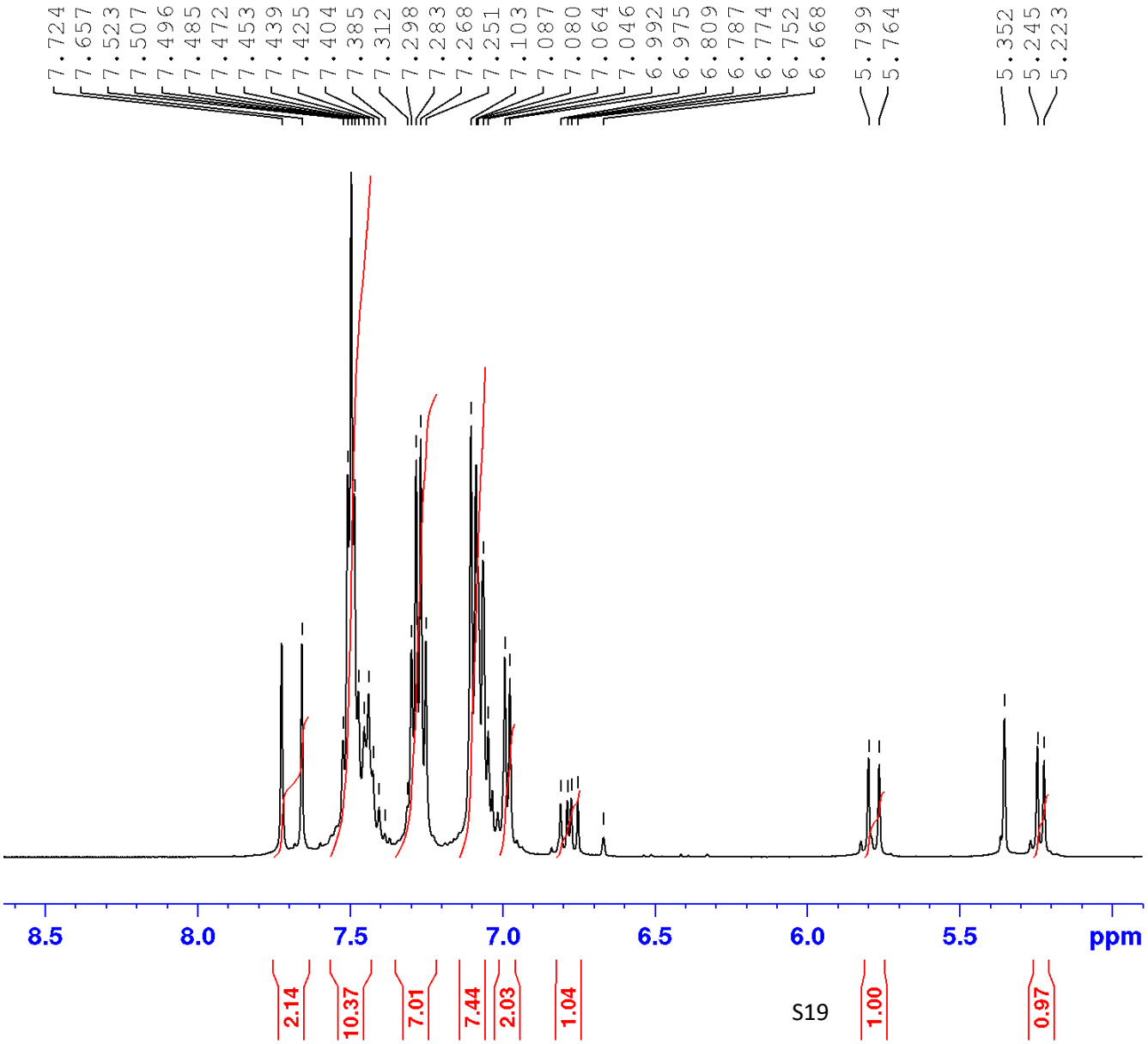
^{1}H NMR spectrum of (*E*)-N,N-diphenyl-4-(2-(5'-vinyl-[1,1':4',1''-terphenyl]-2'-yl)vinyl)aniline (**DPA-DPS-V**)

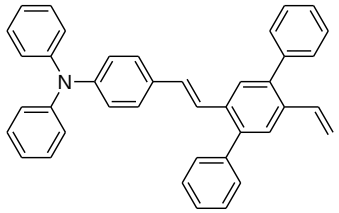





```
Current Data Parameters
NAME                   DPP
EXPNO                   79
PROCNO                   4

F2 - Acquisition Parameters
Date_           20191023
Time                6.37
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                     8
DS                     2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ            3.2767999 sec
RG                  33.7
DW                50.000 usec
DE                10.00 usec
TE                292.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                   1H
P1                12.00 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.2000000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

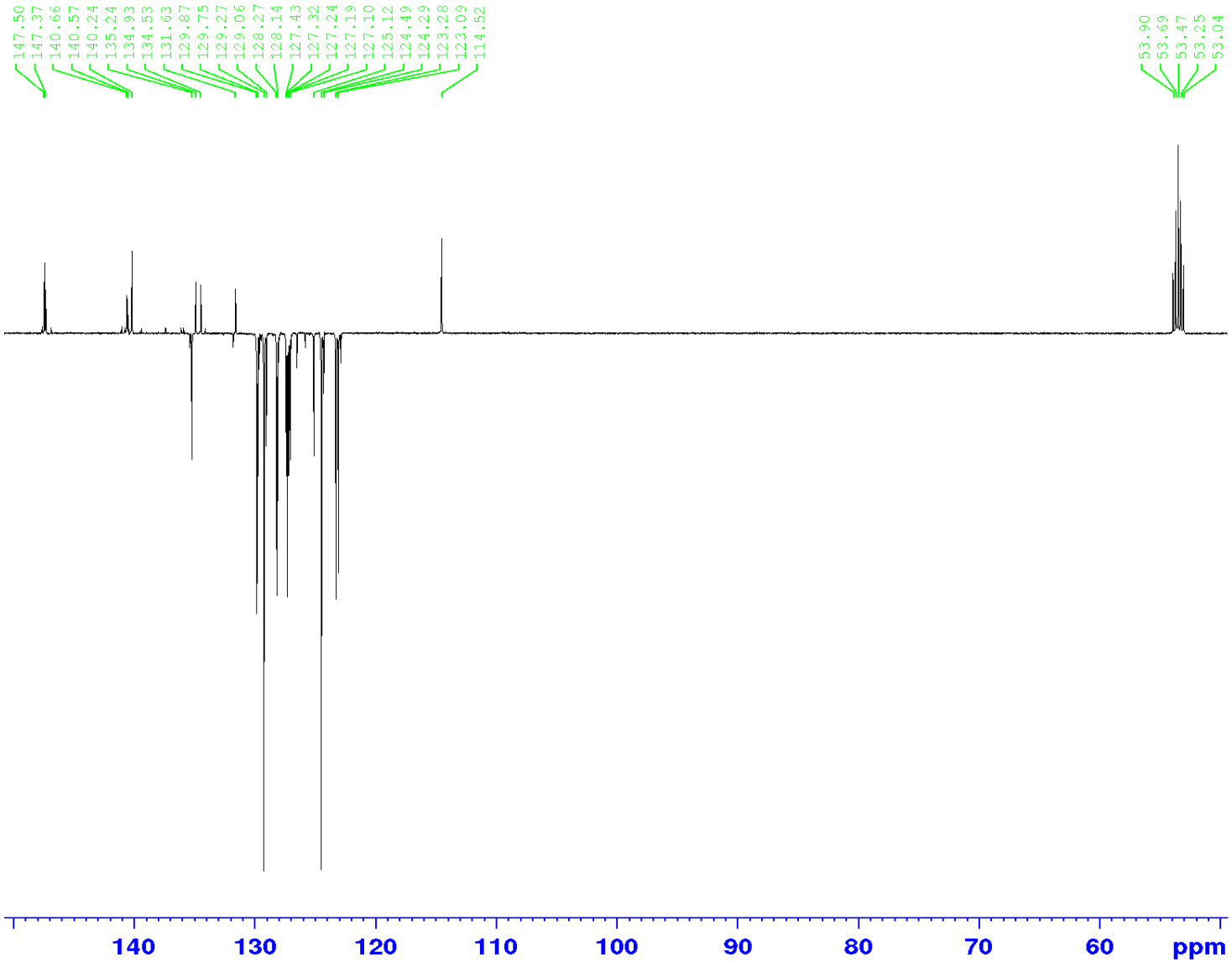
^{1}H NMR spectrum of aromatic part of (*E*)-N,N-diphenyl-4-(2-(5'-vinyl-[1,1':4',1''-terphenyl]-2'-yl)vinyl)aniline (**DPA-DPS-V**)

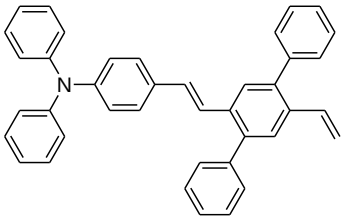





```
Current Data Parameters
NAME                  DPP
EXPNO                  79
PROCNO                  4

F2 - Acquisition Parameters
Date_           20191023
Time                6.37
INSTRUM            spect
PROBHD    5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                     8
DS                     2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                  33.7
DW                50.000 usec
DE                10.00 usec
TE                292.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                1H
P1                12.00 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.2000000 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

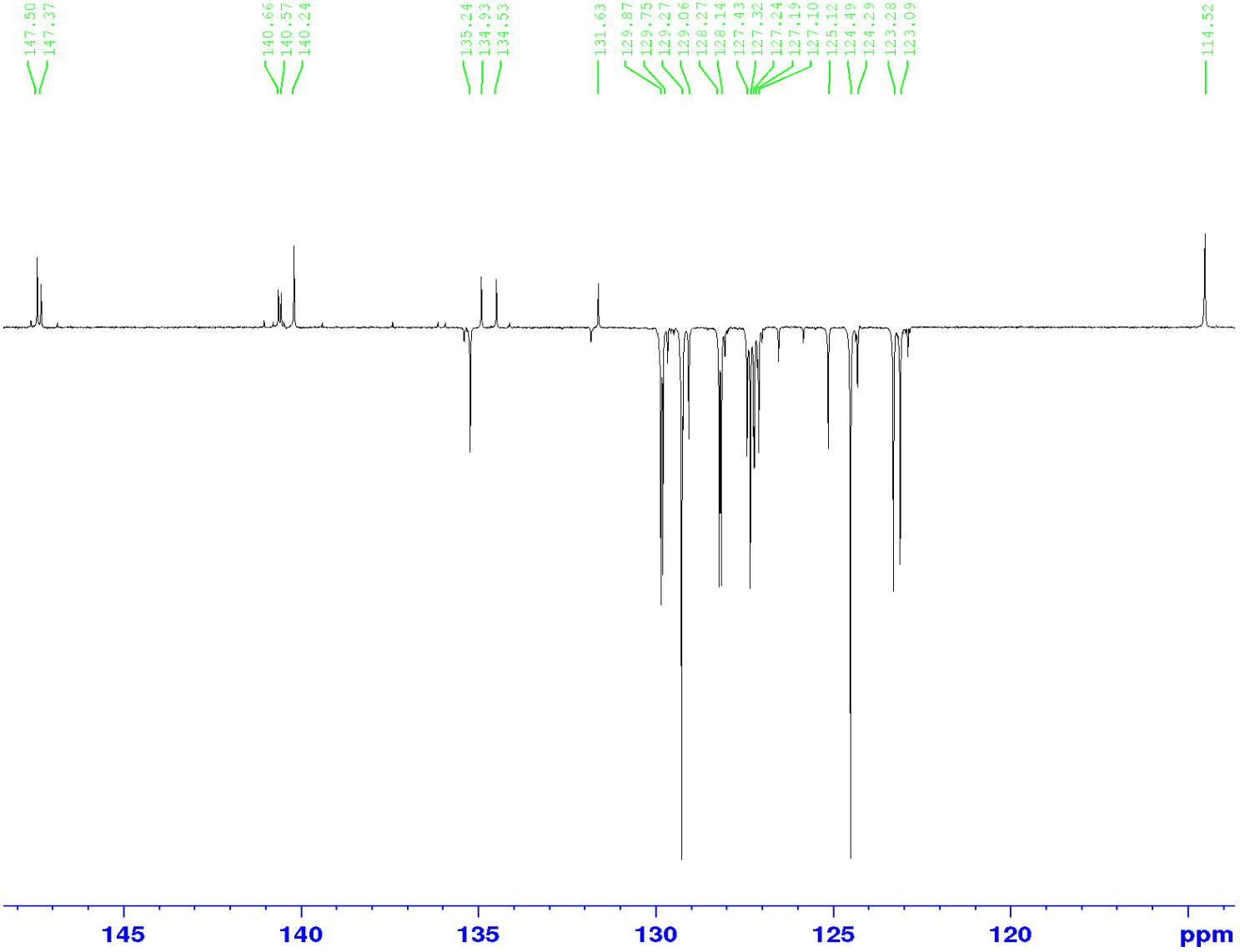
^{13}C NMR spectrum of (*E*)-N,N-diphenyl-4-(2-(5'-vinyl-[1,1':4',1''-terphenyl]-2'-yl)vinyl)aniline (**DPA-DPS-V**)

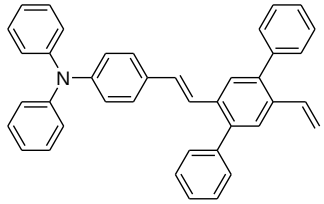





```
Current Data Parameters
NAME                   DPP
EXPNO                   80
PROCNO                   4

F2 - Acquisition Parameters
Date_           20191023
Time                6.43
INSTRUM            spect
PROBHD    5 mm CPPBBO BB
PULPROG             jmod
TD                 65536
SOLVENT           CD2Cl2
NS                   2418
DS                      4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG                   2050
DW                 16.800 usec
DE                 18.00 usec
TE                 292.1 K
CNST2        145.0000000
CNST11         1.0000000
D1            2.00000000 sec
D20           0.00689655 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         125.7879676 MHz
NUC1                  13C
P1                 10.00 usec
P2                 20.00 usec
PLW1         40.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2         13.00000000 W
PLW12         0.29249999 W

F2 - Processing parameters
SI                   32768
SF           125.7753900 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

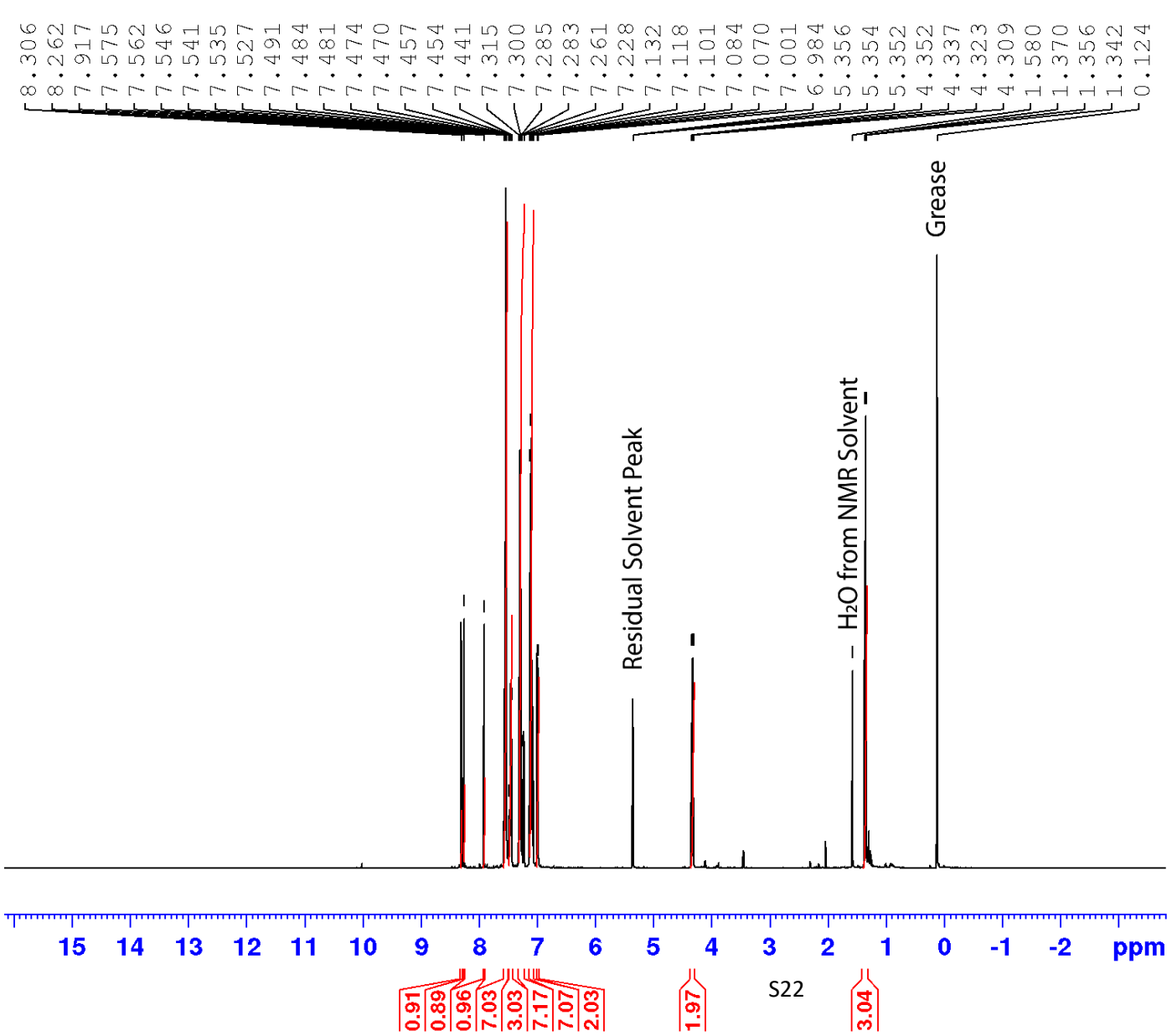
^{13}C NMR spectrum of aromatic part of (*E*)-N,N-diphenyl-4-(2-(5'-vinyl-[1,1':4',1''-terphenyl]-2'-yl)vinyl)aniline (**DPA-DPS-V**)

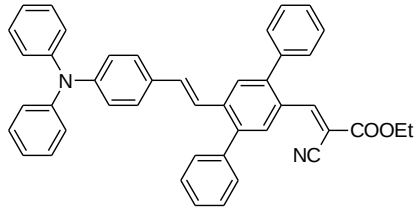





```
Current Data Parameters
NAME                   DPP
EXPNO                   80
PROCNO                   4

F2 - Acquisition Parameters
Date_             20191023
Time                 6.43
INSTRUM             spect
PROBHD    5 mm CPPBBO BB
PULPROG              jmod
TD                  65536
SOLVENT           CD2Cl2
NS                    2418
DS                       4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010048 sec
RG                    2050
DW                  16.800 usec
DE                  18.00 usec
TE                  292.1 K
CNST2           145.0000000
CNST11            1.0000000
D1                2.00000000 sec
D20               0.00689655 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            125.7879676 MHz
NUC1                    13C
P1                    10.00 usec
P2                    20.00 usec
PLW1            40.00000000 W

======== CHANNEL f2 ========
SFO2            500.2020008 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 80.00 usec
PLW2            13.00000000 W
PLW12            0.29249999 W

F2 - Processing parameters
SI                      32768
SF              125.7753900 MHz
WDW                     EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

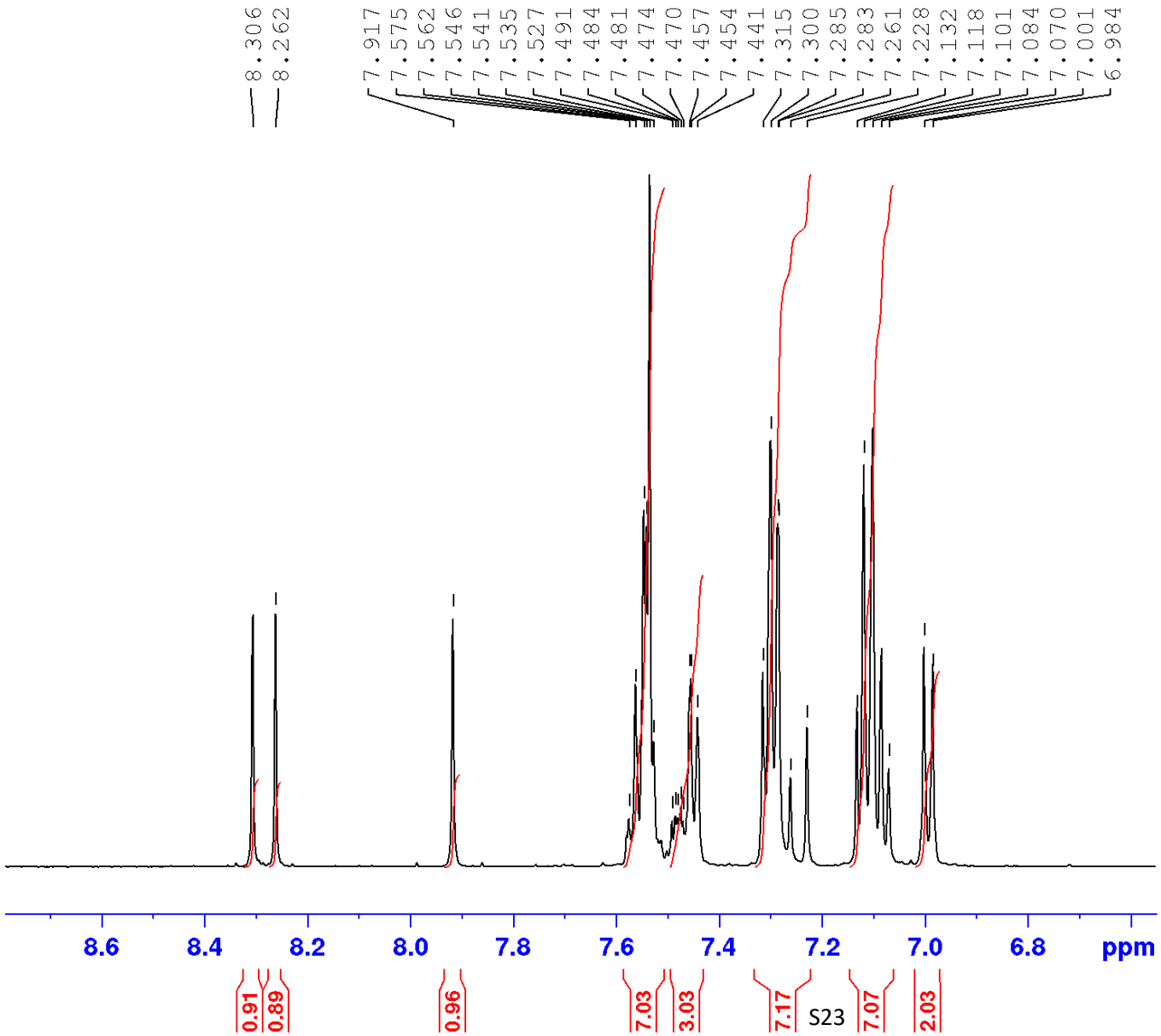
^{1}H NMR spectrum of Ethyl (*E*)-2-cyano-3-(5'-((*E*)-4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)acrylate (**DPA-DPS-CEV**)

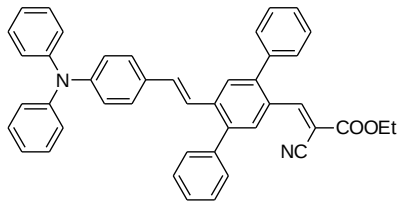





```
Current Data Parameters
NAME                  DPP
EXPNO                 154
PROCNO                  4

F2 - Acquisition Parameters
Date_           20210309
Time               8.30
INSTRUM           spect
PROBHD    5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                     8
DS                     2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ            3.2767999 sec
RG                 38.51
DW                50.000 usec
DE                10.00 usec
TE                291.8 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                1H
P1                12.00 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.2000000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{1}H NMR spectrum of aromatic part of Ethyl (*E*)-2-cyano-3-(5'-((*E*)-4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)acrylate (**DPA-DPS-CEV**)



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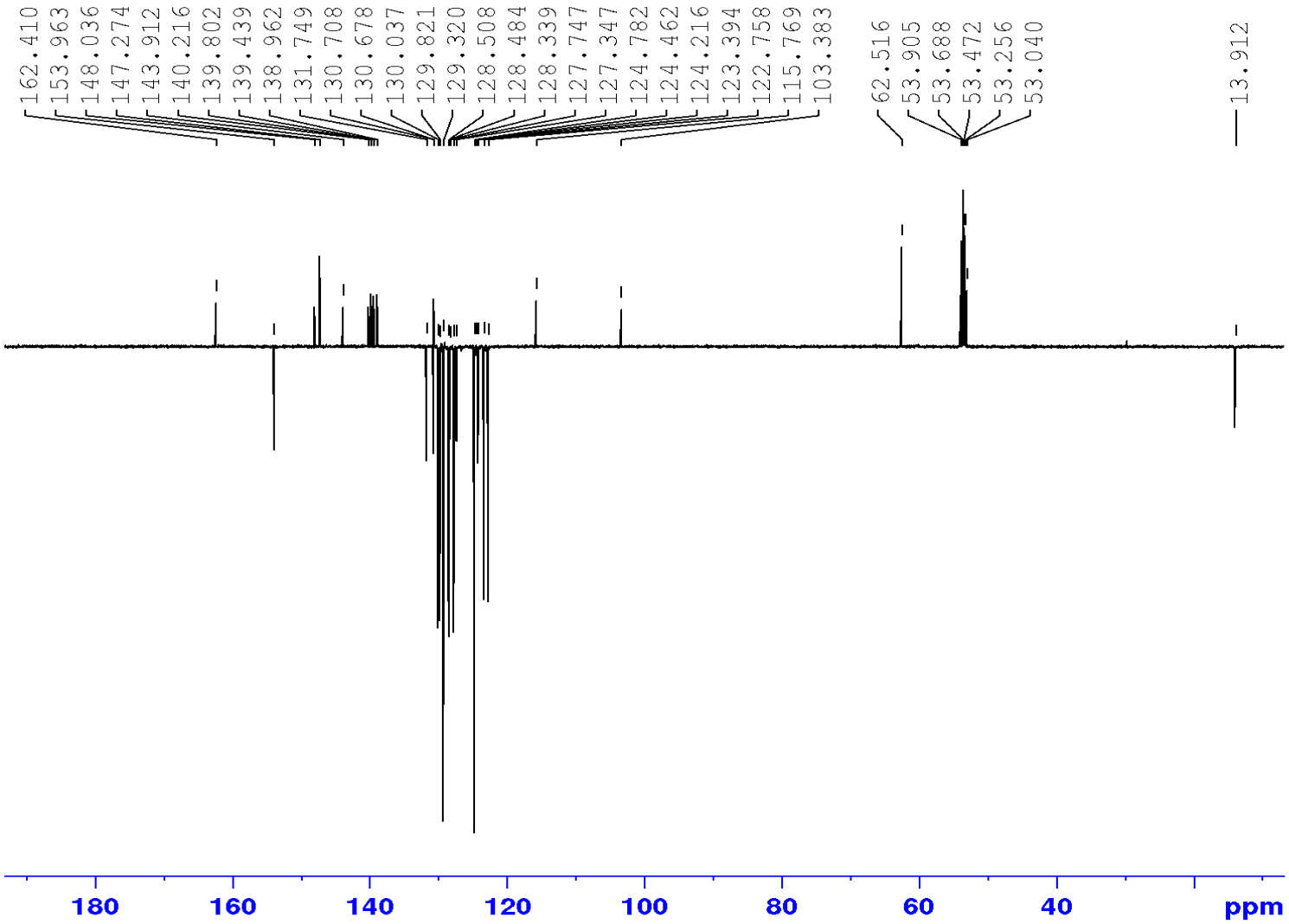
Current Data Parameters
NAME                  DPP
EXPNO                 154
PROCNO                  4

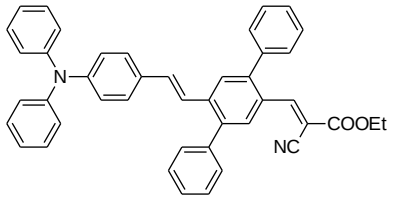
F2 - Acquisition Parameters
Date_           20210309
Time                8.30
INSTRUM            spect
PROBHD    5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                     8
DS                     2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ            3.2767999 sec
RG                 38.51
DW                50.000 usec
DE                10.00 usec
TE                291.8 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                 1H
P1                12.00 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.2000000 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}C NMR spectrum of Ethyl (*E*)-2-cyano-3-(5'-((*E*)-4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)acrylate (**DPA-DPS-CEV**)






```
Current Data Parameters
NAME                      DPP
EXPNO                     155
PROCNO                      4

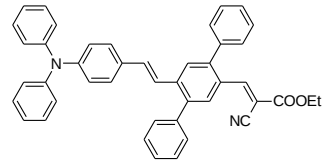
F2 - Acquisition Parameters
Date_              20210309
Time                    8.31
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG                 jmod
TD                     65536
SOLVENT             CD2Cl2
NS                        624
DS                          4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010048 sec
RG                     2050
DW                   16.800 usec
DE                   18.00 usec
TE                   291.8 K
CNST2           145.0000000
CNST11            1.0000000
D1               2.00000000 sec
D20              0.00689655 sec
TD0                         1

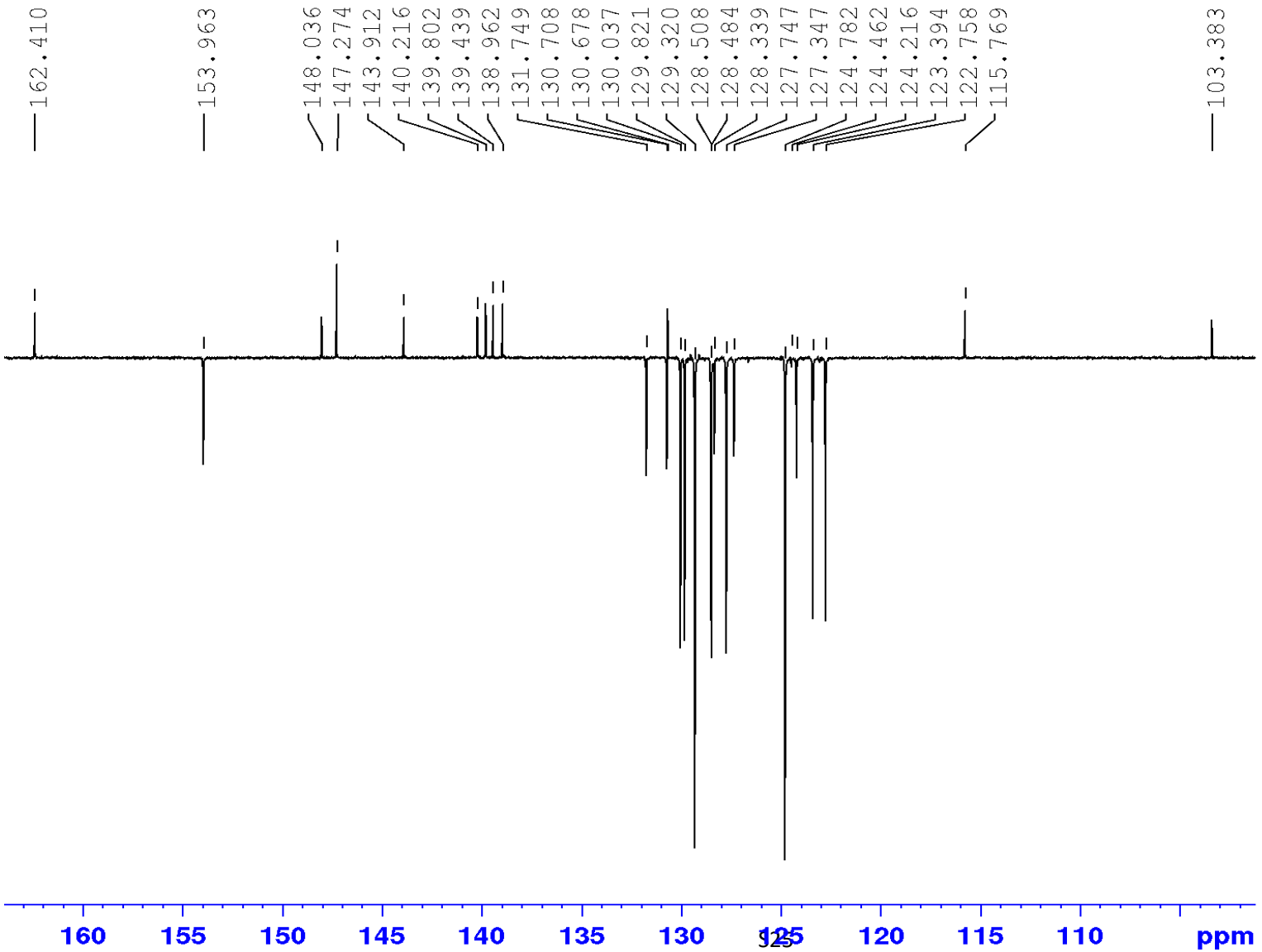
======== CHANNEL f1 ========
SFO1            125.7879676 MHz
NUC1                    13C
P1                   10.00 usec
P2                   20.00 usec
PLW1           40.00000000 W

======== CHANNEL f2 ========
SFO2            500.2020008 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                80.00 usec
PLW2           13.00000000 W
PLW12           0.29249999 W

F2 - Processing parameters
SI                      32768
SF              125.7753900 MHz
WDW                        EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

^{13}C NMR spectrum of aromatic part of Ethyl (*E*)-2-cyano-3-(5'-((*E*)-4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)acrylate (**DPA-DPS-CEV**)






```
Current Data Parameters
NAME                      DPP
EXPNO                     155
PROCNO                      4

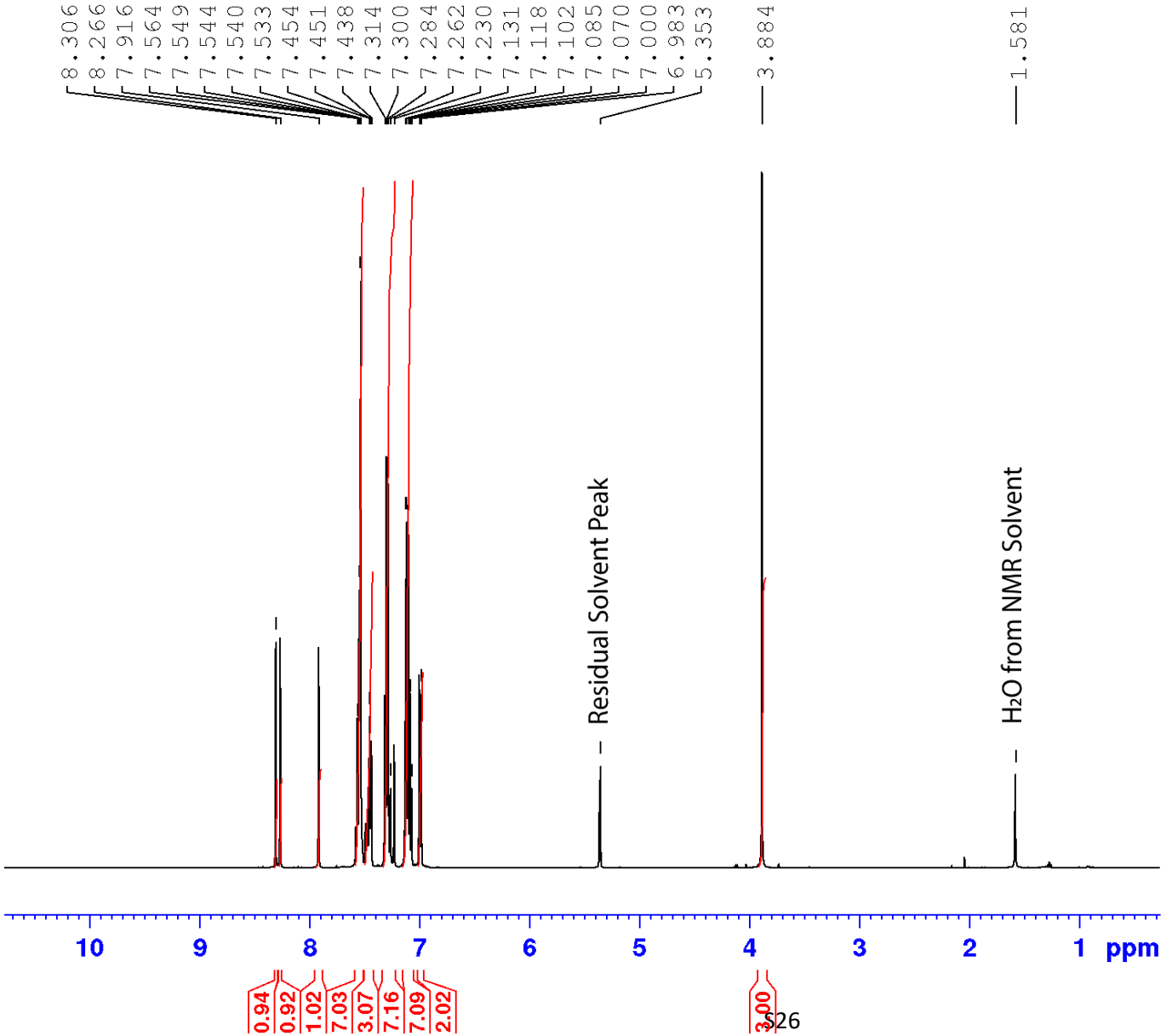
F2 - Acquisition Parameters
Date_              20210309
Time                    8.31
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG                 jmod
TD                     65536
SOLVENT             CD2Cl2
NS                        624
DS                          4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ               1.1010048 sec
RG                       2050
DW                     16.800 usec
DE                     18.00 usec
TE                     291.8 K
CNST2          145.0000000
CNST11           1.0000000
D1              2.00000000 sec
D20             0.00689655 sec
TD0                         1

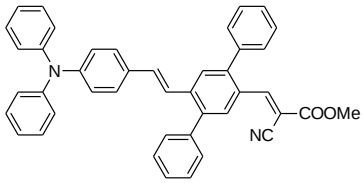
======== CHANNEL f1 ========
SFO1           125.7879676 MHz
NUC1                     13C
P1                    10.00 usec
P2                    20.00 usec
PLW1           40.00000000 W

======== CHANNEL f2 ========
SFO2           500.2020008 MHz
NUC2                     1H
CPDPRG[2           waltz16
PCPD2                 80.00 usec
PLW2           13.00000000 W
PLW12           0.29249999 W

F2 - Processing parameters
SI                       32768
SF             125.7753900 MHz
WDW                         EM
SSB         0
LB                     1.00 Hz
GB          0
PC                     1.40
```

^{1}H NMR spectrum of Methyl (*E*)-2-cyano-3-(5'-((*E*)-4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)acrylate (**DPA-DPS-CMV**)





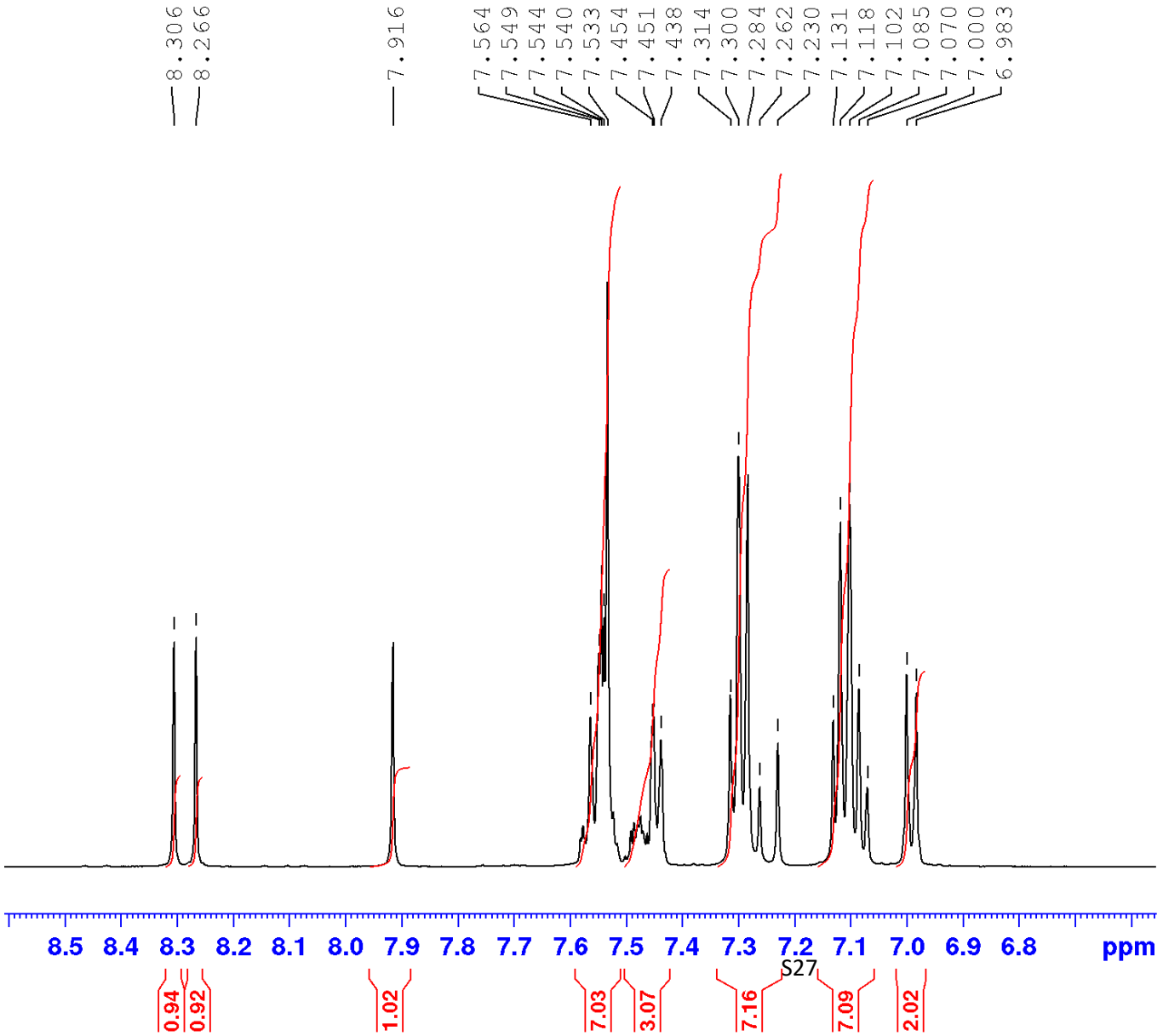

```
Current Data Parameters
NAME                  DPP
EXPNO                 152
PROCNO                  4

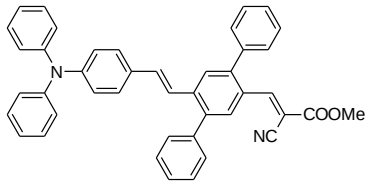
F2 - Acquisition Parameters
Date_           20210309
Time                8.09
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                     8
DS                     2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ            3.2767999 sec
RG                 38.51
DW               50.000 usec
DE               10.00 usec
TE                291.6 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                   1H
P1                12.00 usec
PLW1        13.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.2000000 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{1}H NMR spectrum of aromatic part of Methyl (*E*)-2-cyano-3-(5'-((*E*)-4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)acrylate (**DPA-DPS-CMV**)





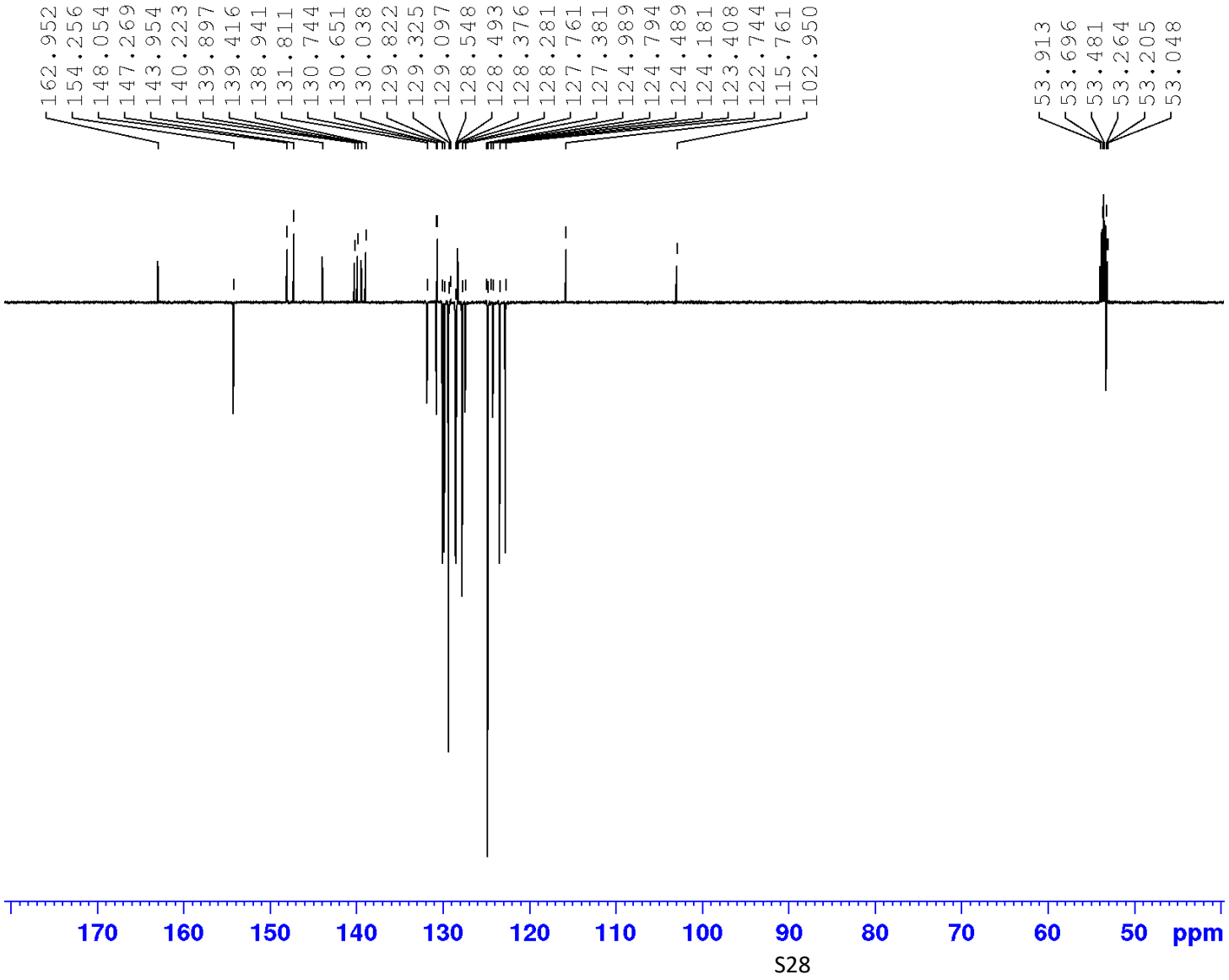

```
Current Data Parameters
NAME                  DPP
EXPNO                 152
PROCNO                  4

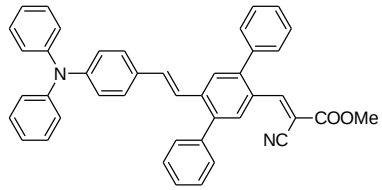
F2 - Acquisition Parameters
Date_           20210309
Time                8.09
INSTRUM            spect
PROBHD    5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                     8
DS                     2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ              3.2767999 sec
RG                 38.51
DW                50.000 usec
DE                10.00 usec
TE                291.6 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                  1H
P1                 12.00 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.2000000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C NMR spectrum of Methyl (*E*)-2-cyano-3-(5'-((*E*)-4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)acrylate (**DPA-DPS-CMV**)






```
Current Data Parameters
NAME                      DPP
EXPNO                     153
PROCNO                      4

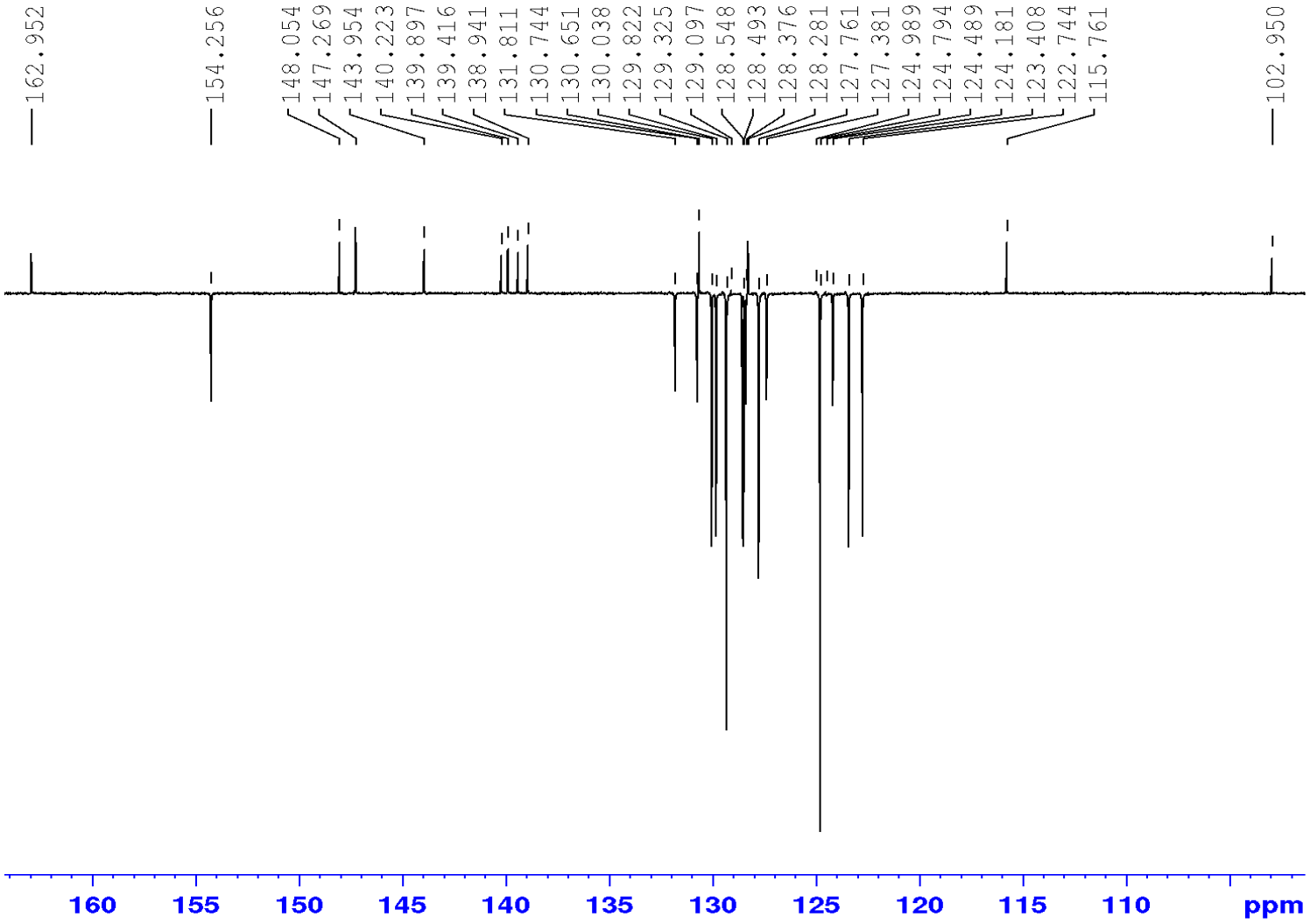
F2 - Acquisition Parameters
Date_                20210309
Time                     8.09
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG                 jmod
TD                     65536
SOLVENT             CD2Cl2
NS                        343
DS                          4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010048 sec
RG                       1820
DW                     16.800 usec
DE                     18.00 usec
TE                     291.6 K
CNST2             145.0000000
CNST11              1.0000000
D1                 2.00000000 sec
D20                0.00689655 sec
TD0                         1

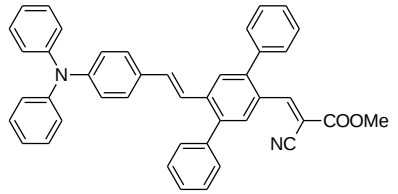
======== CHANNEL f1 ========
SFO1              125.7879676 MHz
NUC1                      13C
P1                     10.00 usec
P2                     20.00 usec
PLW1              40.00000000 W

======== CHANNEL f2 ========
SFO2              500.2020008 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                  80.00 usec
PLW2              13.00000000 W
PLW12              0.29249999 W

F2 - Processing parameters
SI                        32768
SF                125.7753900 MHz
WDW                         EM
SSB           0
LB                      1.00 Hz
GB            0
PC                      1.40
```

^{13}C NMR spectrum of aromatic part of Methyl (*E*)-2-cyano-3-(5'-((*E*)-4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)acrylate (**DPA-DPS-CMV**)






```
Current Data Parameters
NAME                      DPP
EXPNO                     153
PROCNO                      4

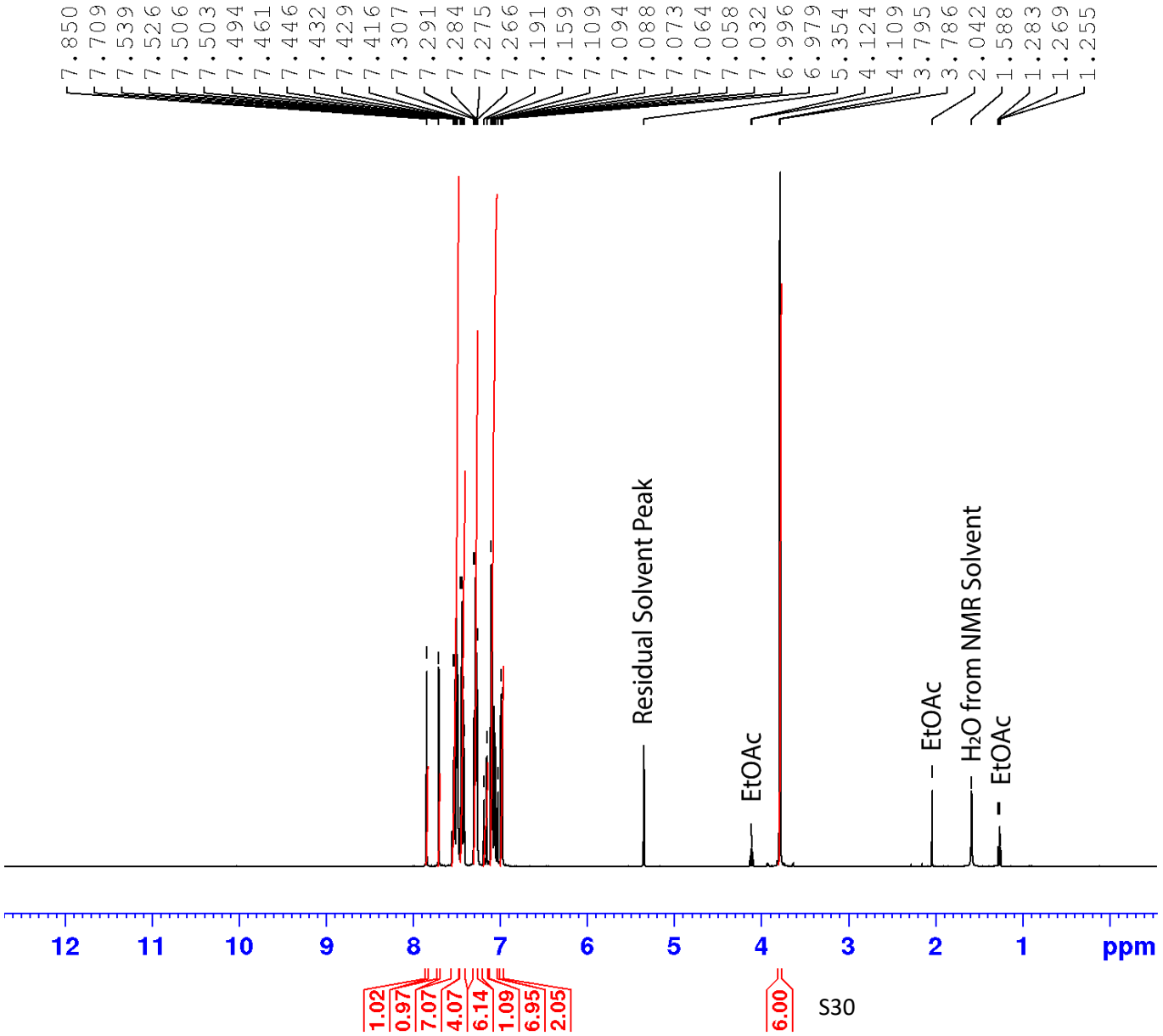
F2 - Acquisition Parameters
Date_                20210309
Time                     8.09
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG                 jmod
TD                     65536
SOLVENT             CD2Cl2
NS                        343
DS                          4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010048 sec
RG                       1820
DW                     16.800 usec
DE                     18.00 usec
TE                     291.6 K
CNST2             145.0000000
CNST11              1.0000000
D1                 2.00000000 sec
D20                0.00689655 sec
TD0                         1

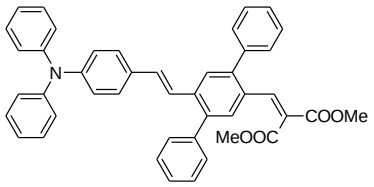
======== CHANNEL f1 ========
SFO1              125.7879676 MHz
NUC1                      13C
P1                     10.00 usec
P2                     20.00 usec
PLW1              40.00000000 W

======== CHANNEL f2 ========
SFO2              500.2020008 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                  80.00 usec
PLW2              13.00000000 W
PLW12              0.29249999 W

F2 - Processing parameters
SI                        32768
SF                125.7753900 MHz
WDW                          EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

^{1}H NMR spectrum of Dimethyl (*E*)-2-((5'-(4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)methylene)malonate (**DPA-DPS-DMV**)





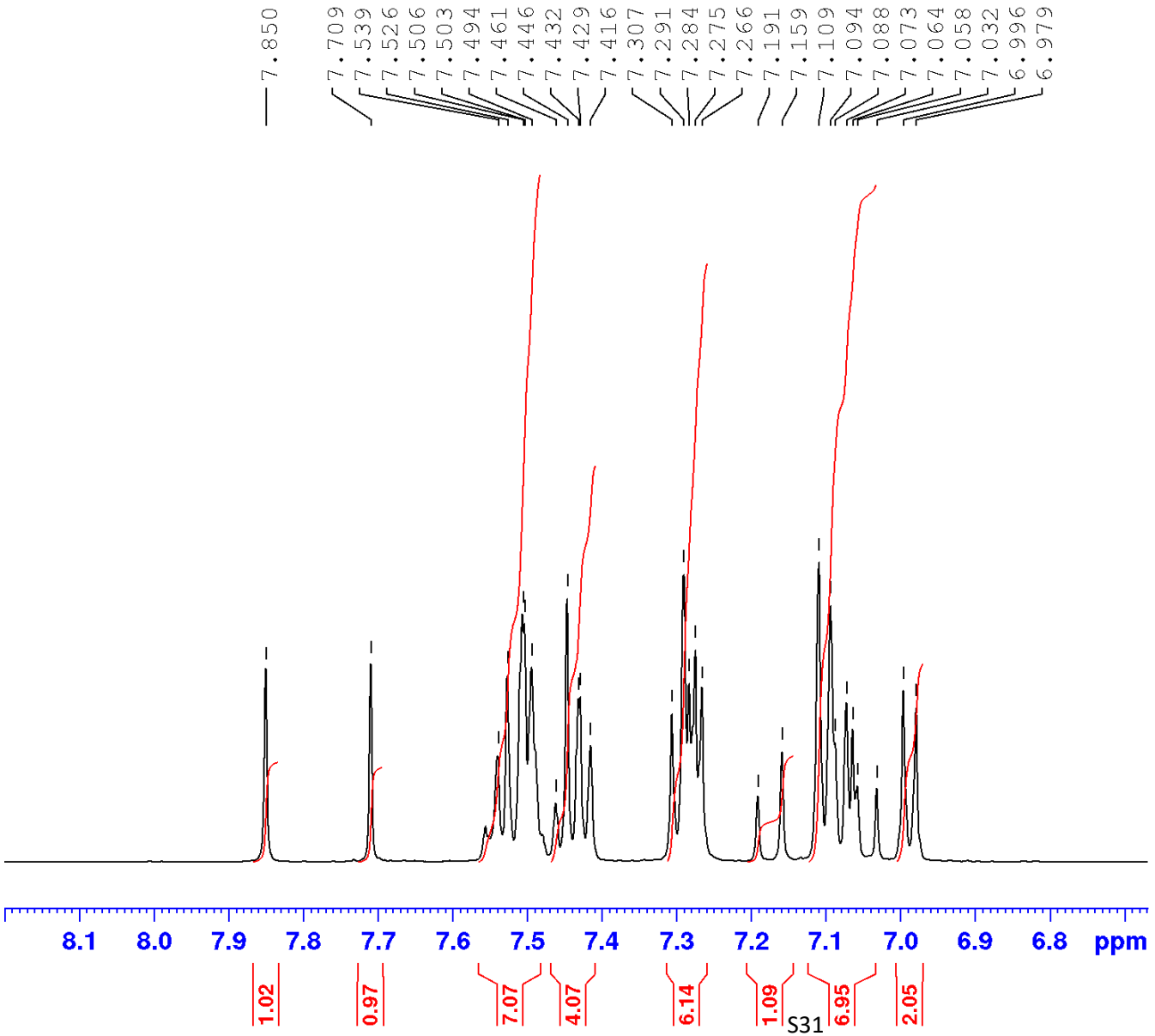

```
Current Data Parameters
NAME                  DPP
EXPNO                 150
PROCNO                  4

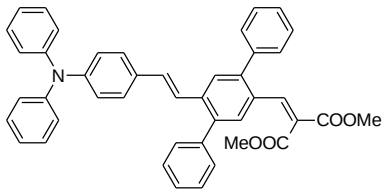
F2 - Acquisition Parameters
Date_           20210309
Time               7.23
INSTRUM           spect
PROBHD    5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT           CD2C12
NS                     8
DS                     2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ            3.2767999 sec
RG                 38.51
DW                50.000 usec
DE                10.00 usec
TE                291.5 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                1H
P1                12.00 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.2000000 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{1}H NMR spectrum of aromatic part of Dimethyl (*E*)-2-((5'-(4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)methylene)malonate (**DPA-DPS-DMV**)





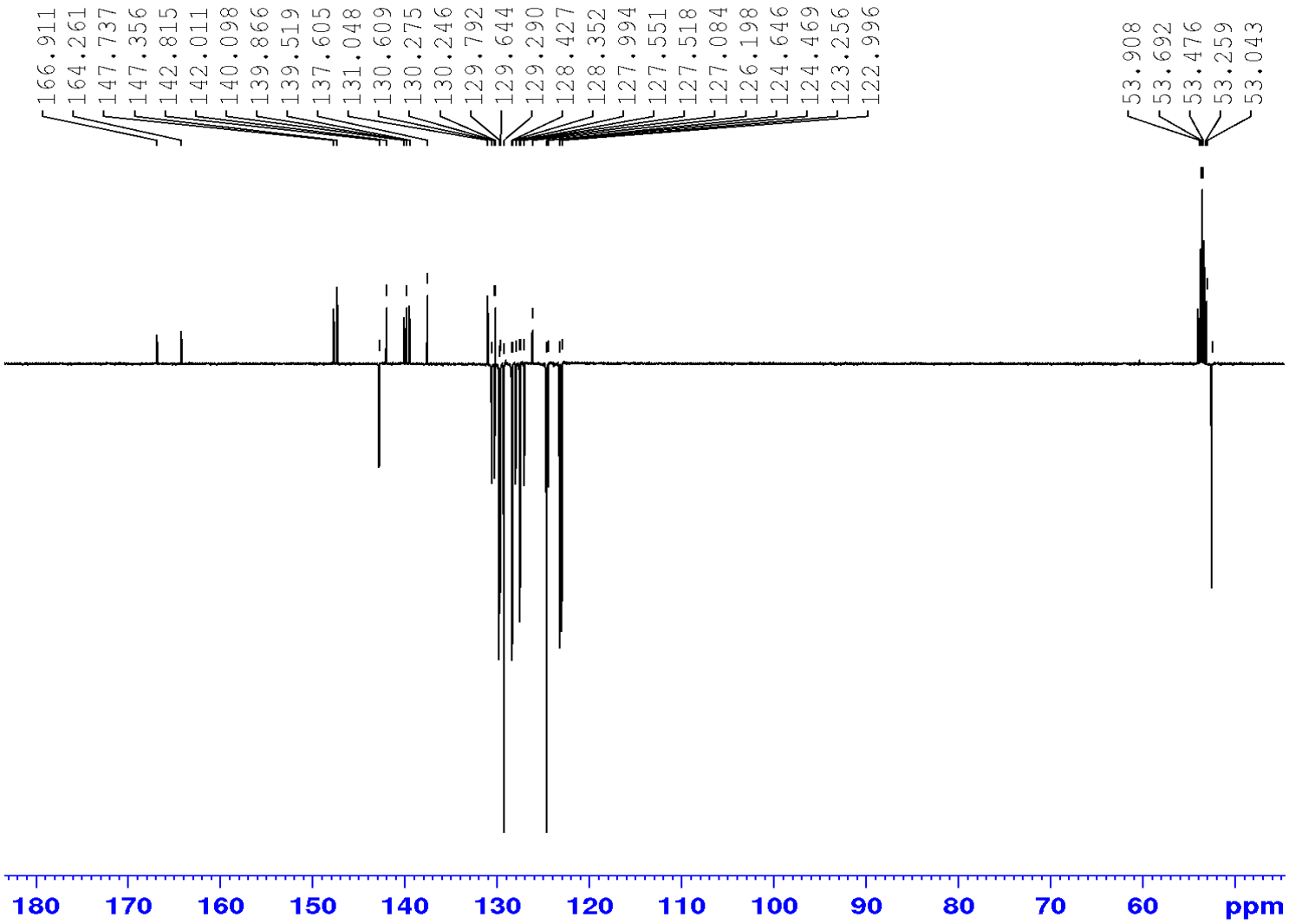

```
Current Data Parameters
NAME                   DPP
EXPNO                  150
PROCNO                   4

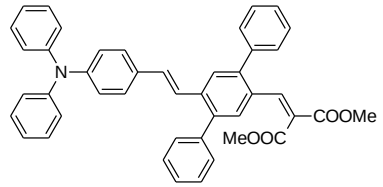
F2 - Acquisition Parameters
Date_           20210309
Time               7.23
INSTRUM           spect
PROBHD   5 mm CPPBBO BB
PULPROG            zg30
TD                65536
SOLVENT           CD2Cl2
NS                    8
DS                    2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                 38.51
DW                50.000 usec
DE                10.00 usec
TE                291.5 K
D1             1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1               1H
P1                12.00 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI                65536
SF           500.2000000 MHz
WDW                EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C NMR spectrum of Dimethyl (*E*)-2-((5'-(4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)methylene)malonate (**DPA-DPS-DMV**)






```
Current Data Parameters
NAME                   DPP
EXPNO                  151
PROCNO                   4

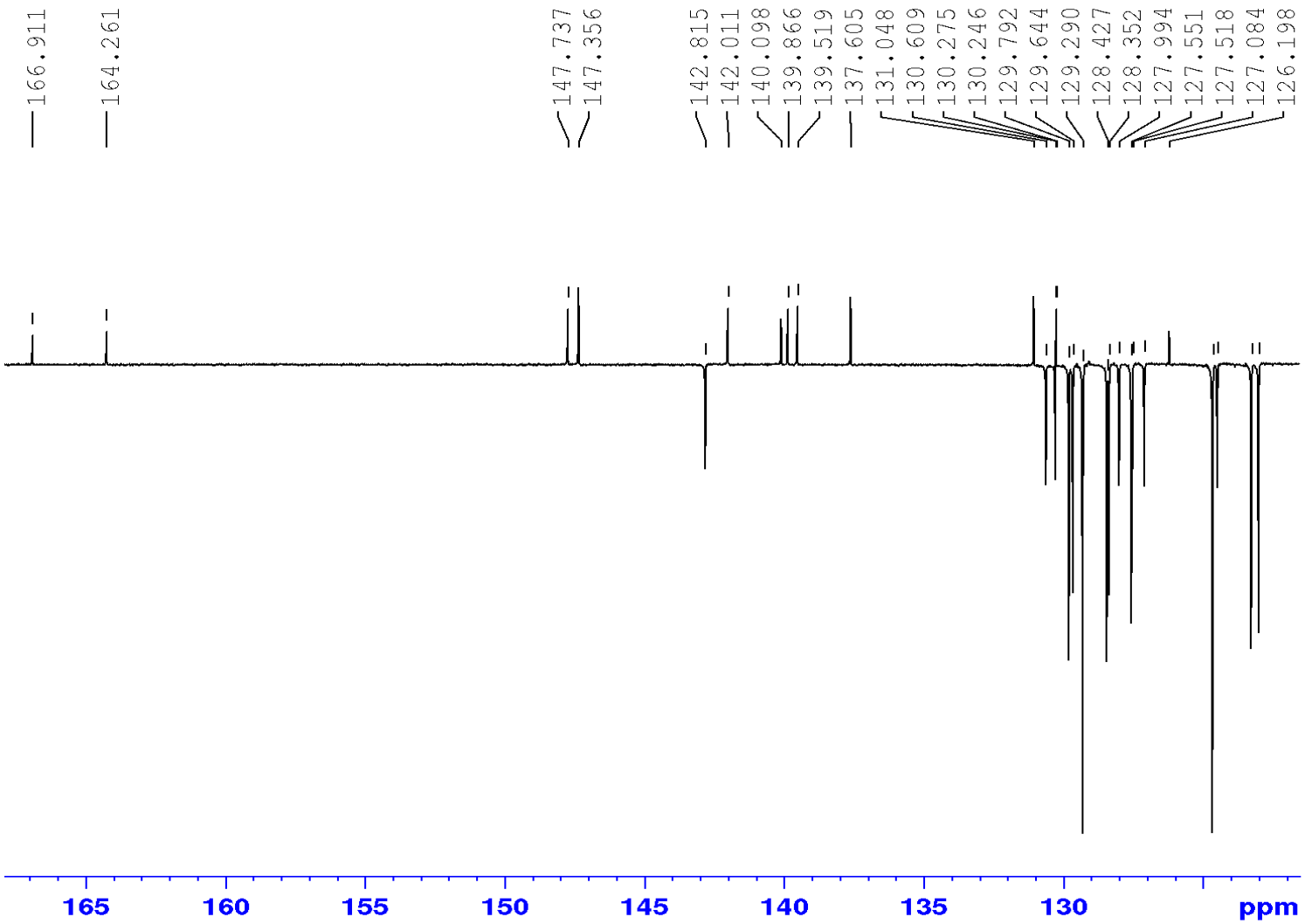
F2 - Acquisition Parameters
Date_             20210309
Time                 7.24
INSTRUM             spect
PROBHD    5 mm CPPBBO BB
PULPROG              jmod
TD                  65536
SOLVENT            CD2Cl2
NS                    785
DS                      4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ             1.1010048 sec
RG                   1820
DW                 16.800 usec
DE                 18.00 usec
TE                 291.6 K
CNST2         145.0000000
CNST11          1.0000000
D1             2.00000000 sec
D20            0.00689655 sec
TD0                     1

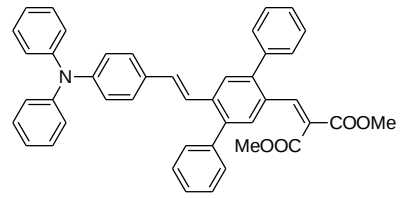
======== CHANNEL f1 ========
SFO1          125.7879676 MHz
NUC1                  13C
P1                 10.00 usec
P2                 20.00 usec
PLW1          40.00000000 W

======== CHANNEL f2 ========
SFO2          500.2020008 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2              80.00 usec
PLW2          13.00000000 W
PLW12          0.29249999 W

F2 - Processing parameters
SI                   32768
SF            125.7753900 MHz
WDW                     EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

^{13}C NMR spectrum of Dimethyl (*E*)-2-((5'-(4-(diphenylamino)styryl)-[1,1':4',1''-terphenyl]-2'-yl)methylene)malonate (**DPA-DPS-DMV**)






```
Current Data Parameters
NAME                   DPP
EXPNO                  151
PROCNO                   4

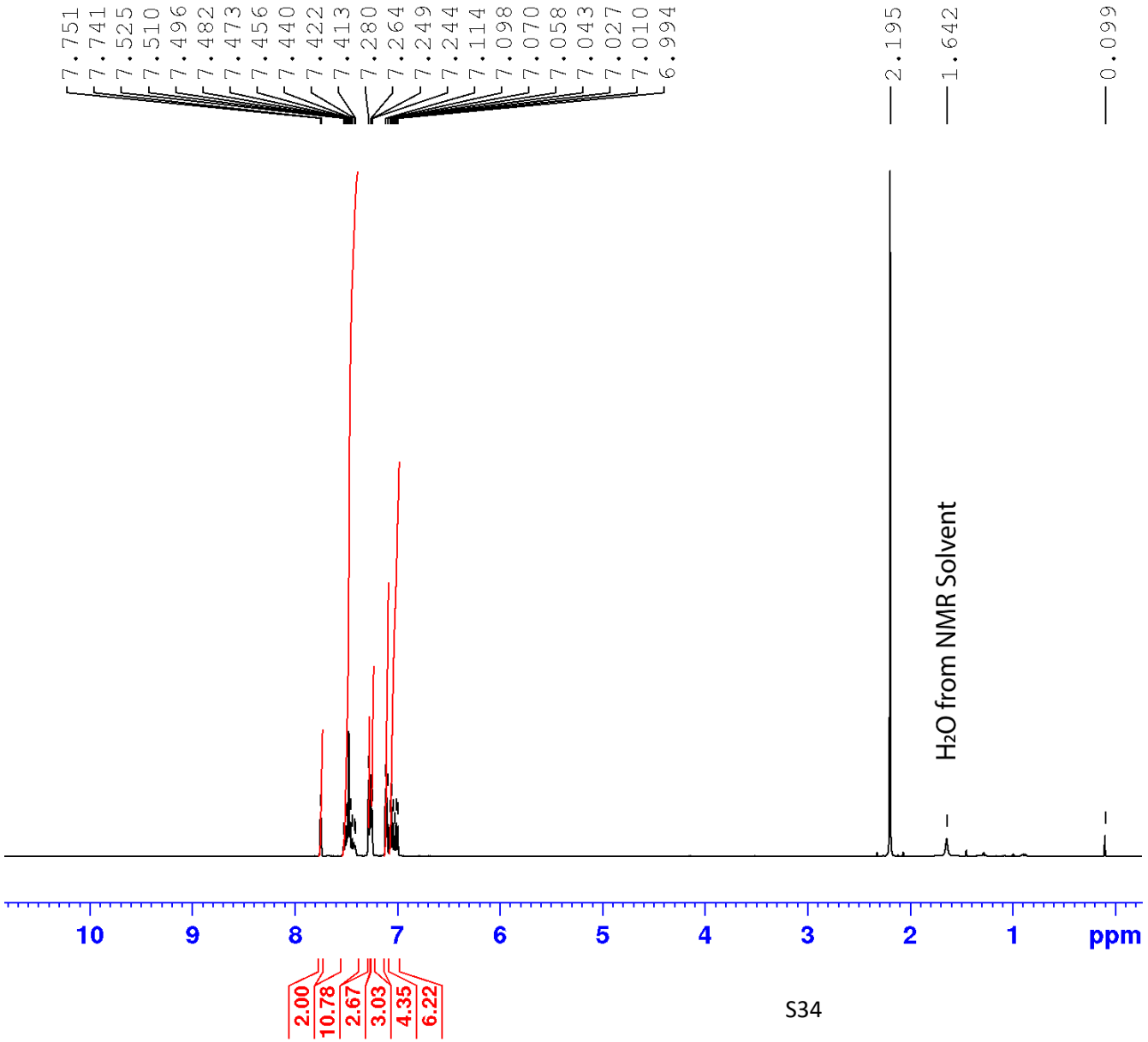
F2 - Acquisition Parameters
Date_             20210309
Time                 7.24
INSTRUM             spect
PROBHD    5 mm CPPBBO BB
PULPROG              jmod
TD                  65536
SOLVENT           CD2Cl2
NS                    785
DS                      4
SWH             29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                   1820
DW                 16.800 usec
DE                 18.00 usec
TE                 291.6 K
CNST2          145.0000000
CNST11           1.0000000
D1               2.00000000 sec
D20              0.00689655 sec
TD0                     1

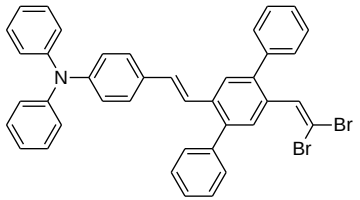
======== CHANNEL f1 ========
SFO1          125.7879676 MHz
NUC1                  13C
P1                 10.00 usec
P2                 20.00 usec
PLW1          40.00000000 W

======== CHANNEL f2 ========
SFO2          500.2020008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          13.00000000 W
PLW12          0.29249999 W

F2 - Processing parameters
SI                    32768
SF            125.7753900 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

^{1}H NMR spectrum of (*E*)-4-(2-(5'-(2,2-dibromovinyl)-[1,1':4',1''-terphenyl]-2'-yl)vinyl)-*N*,*N*-diphenylaniline (**DPA-DPS-DBV**)





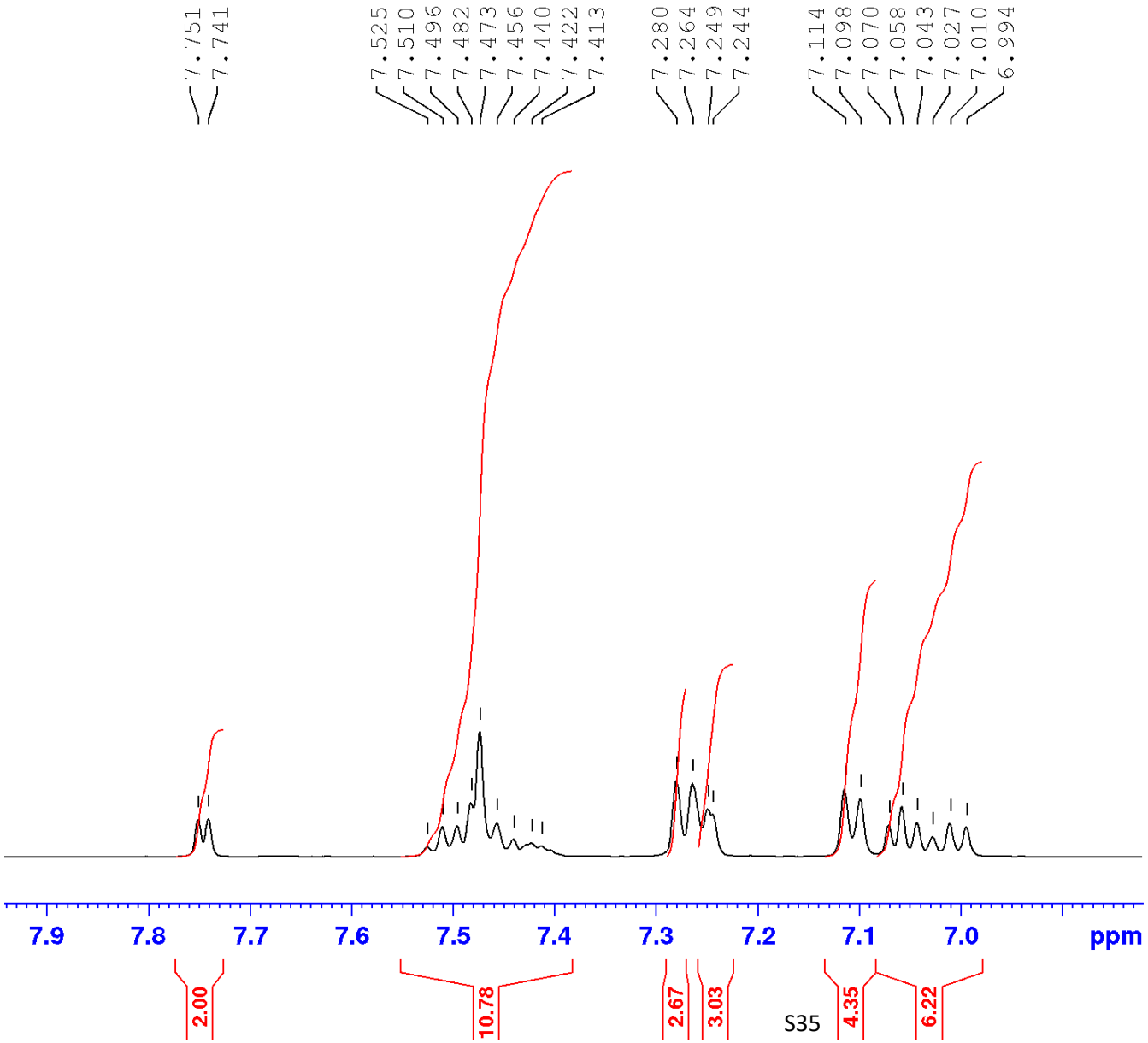

```
Current Data Parameters
NAME                   DPP
EXPNO                  115
PROCNO                   4

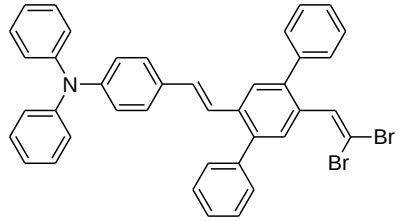
F2 - Acquisition Parameters
Date_           20200616
Time               11.23
INSTRUM            spect
PROBHD   5 mm PATBI 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                     8
DS                     2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ            3.2767999 sec
RG                 131.1
DW                50.000 usec
DE                 6.50 usec
TE        0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                1H
P1                10.00 usec
PLW1          8.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.2000000 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{1}H NMR spectrum of (*E*)-4-(2-(5'-(2,2-dibromovinyl)-[1,1':4',1''-terphenyl]-2'-yl)vinyl)-*N*,*N*-diphenylaniline (**DPA-DPS-DBV**)



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EXPNO                 115
PROCNO                  4

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PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                 131.1
DW                50.000 usec
DE                 6.50 usec
TE        0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
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NUC1                1H
P1                10.00 usec
PLW1          8.00000000 W

F2 - Processing parameters
SI                 65536
SF          500.2000000 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```
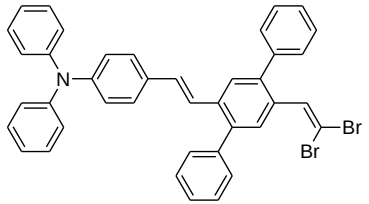
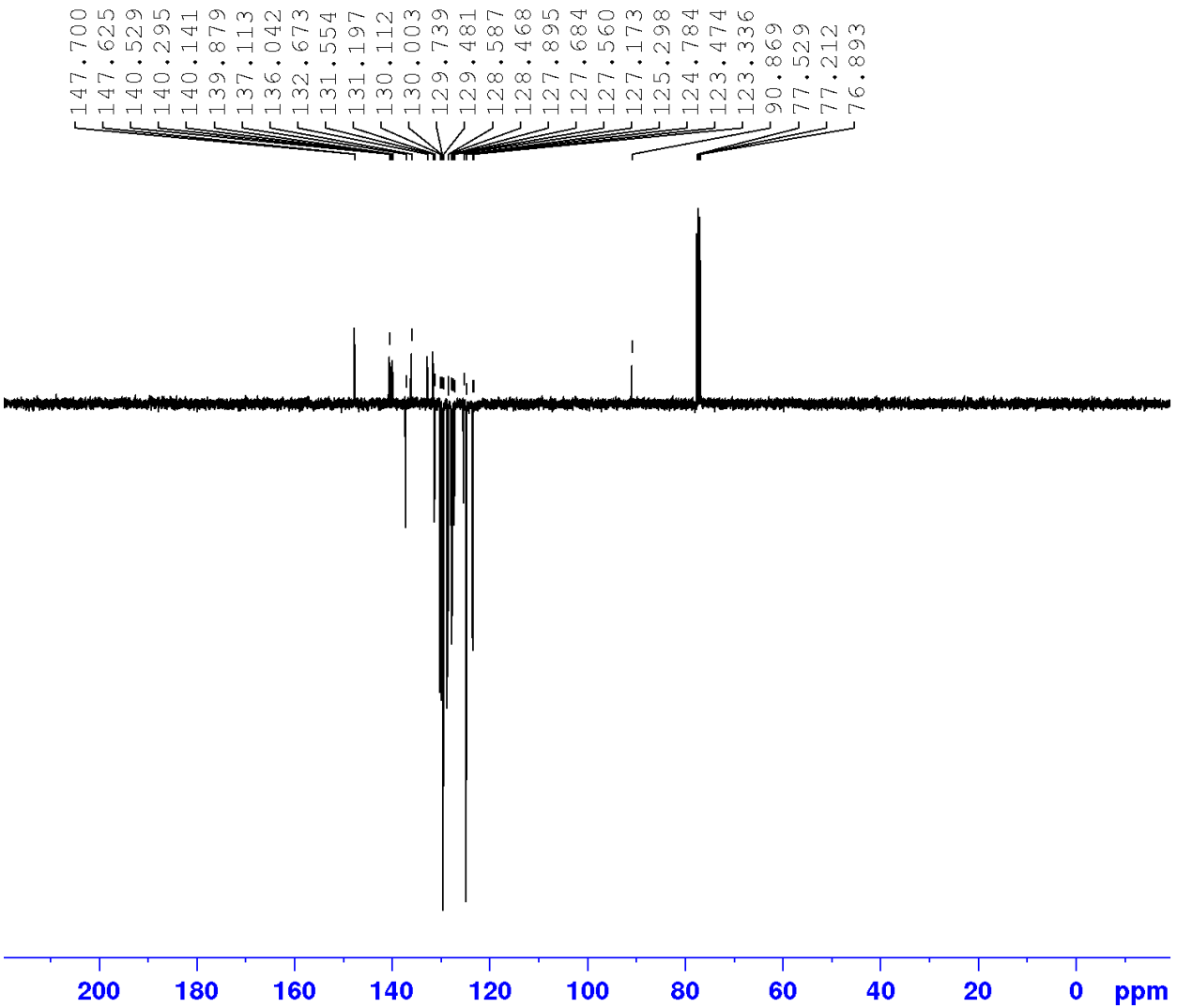

^{13}C NMR spectrum of (*E*)-4-(2-(5'-(2,2-dibromovinyl)-[1,1':4',1''-terphenyl]-2'-yl)vinyl)-*N*,*N*-diphenylaniline (**DPA-DPS-DBV**)



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Current Data Parameters
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EXPNO                 307
PROCNO                  1

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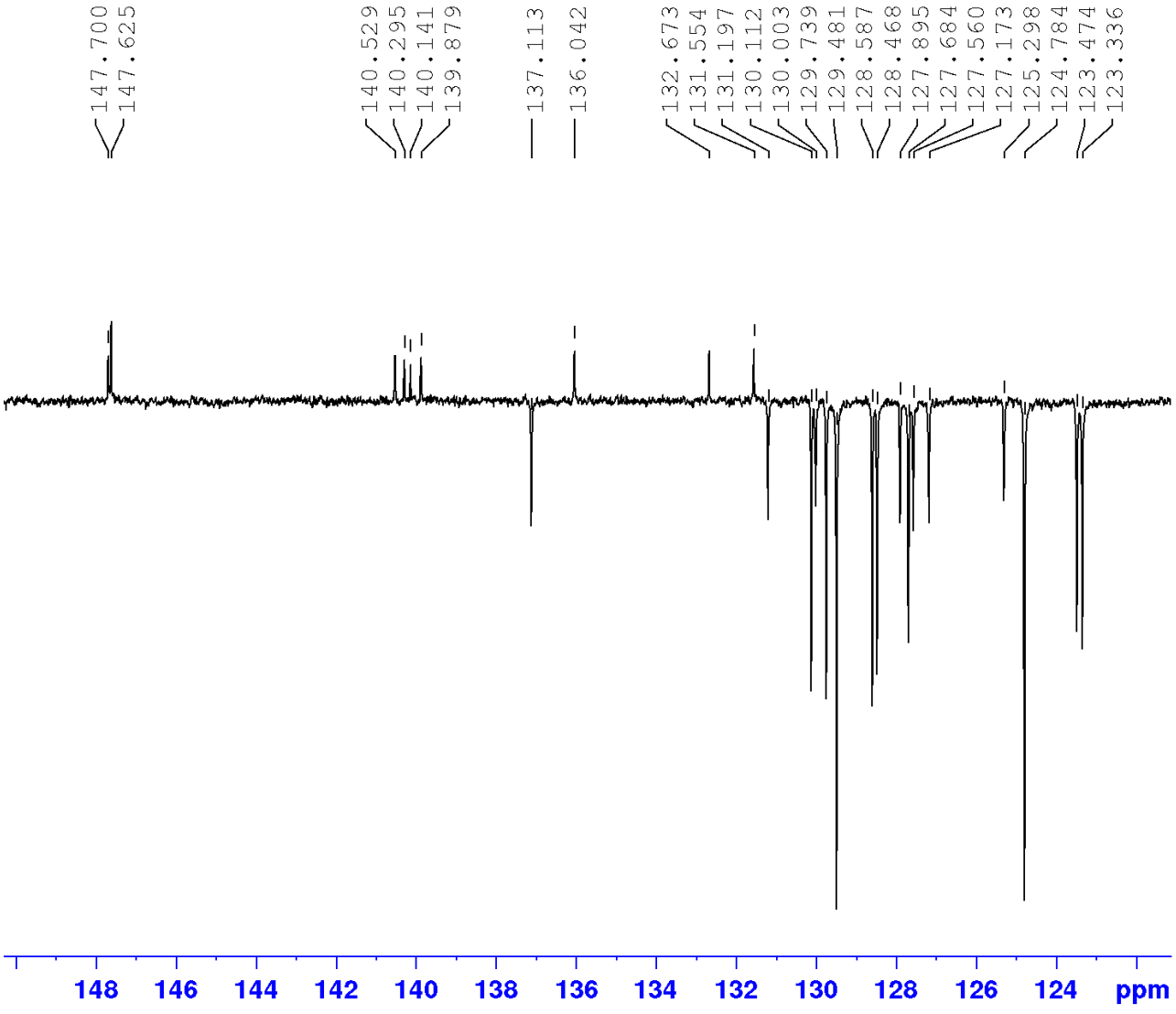
PULPROG             jmod
TD                 65536
SOLVENT            CDCl3
NS                  1389
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                296.1 K
CNST2        145.0000000
CNST11         1.0000000
D1           2.00000000 sec
D20          0.00689655 sec
TD0                    1

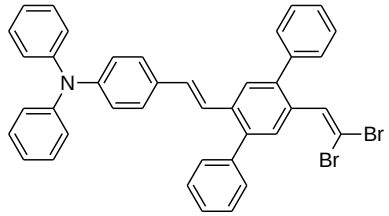
======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                10.00 usec
P2                20.00 usec
PLW1         50.27999878 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         26.98999977 W
PLW12         0.33320999 W

F2 - Processing parameters
SI                 32768
SF           100.6127507 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

^{13}C NMR spectrum of aromatic part of(*E*)-4-(2-(5'-(2,2-dibromovinyl)-[1,1':4',1''-terphenyl]-2'-yl)vinyl)-*N,N*-diphenylaniline (**DPA-DPS-DBV**)



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Current Data Parameters
NAME                   DPP
EXPNO                  307
PROCNO                   1

F2 - Acquisition Parameters
Date_           20200617
Time                6.31
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG             jmod
TD                 65536
SOLVENT            CDCl3
NS                  1389
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                296.1 K
CNST2         145.0000000
CNST11          1.0000000
D1            2.00000000 sec
D20           0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                10.00 usec
P2                20.00 usec
PLW1         50.27999878 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         26.98999977 W
PLW12         0.33320999 W

F2 - Processing parameters
SI                 32768
SF           100.6127507 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```
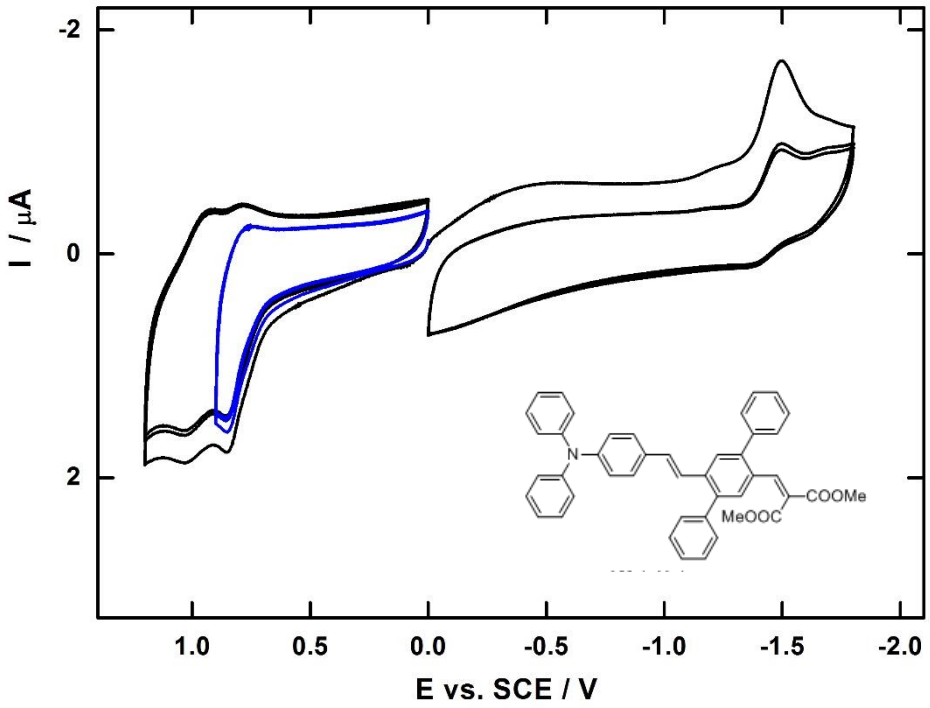
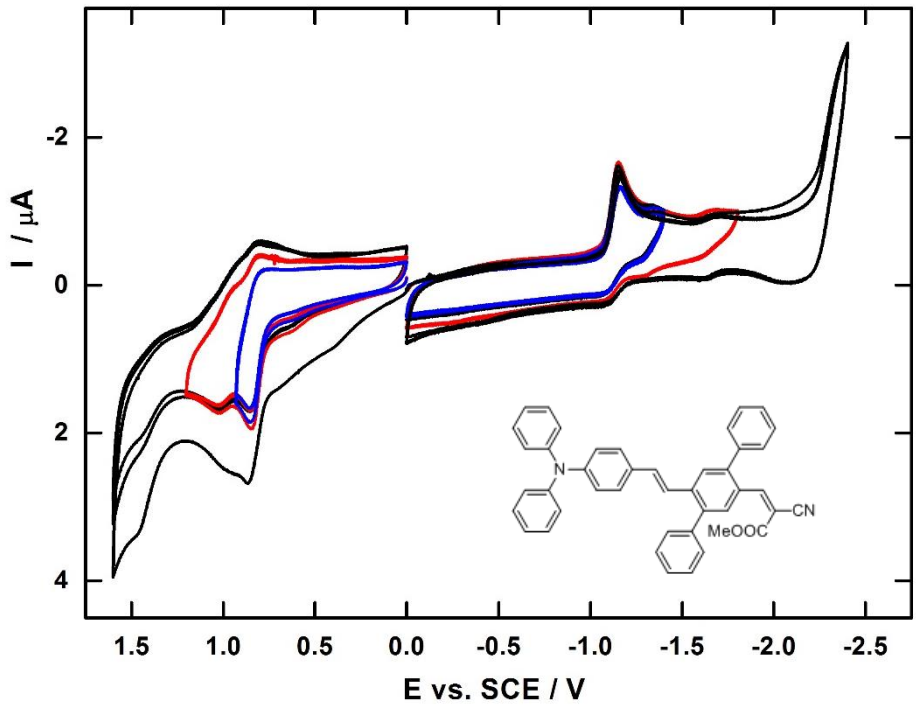

Electrochemical measurements

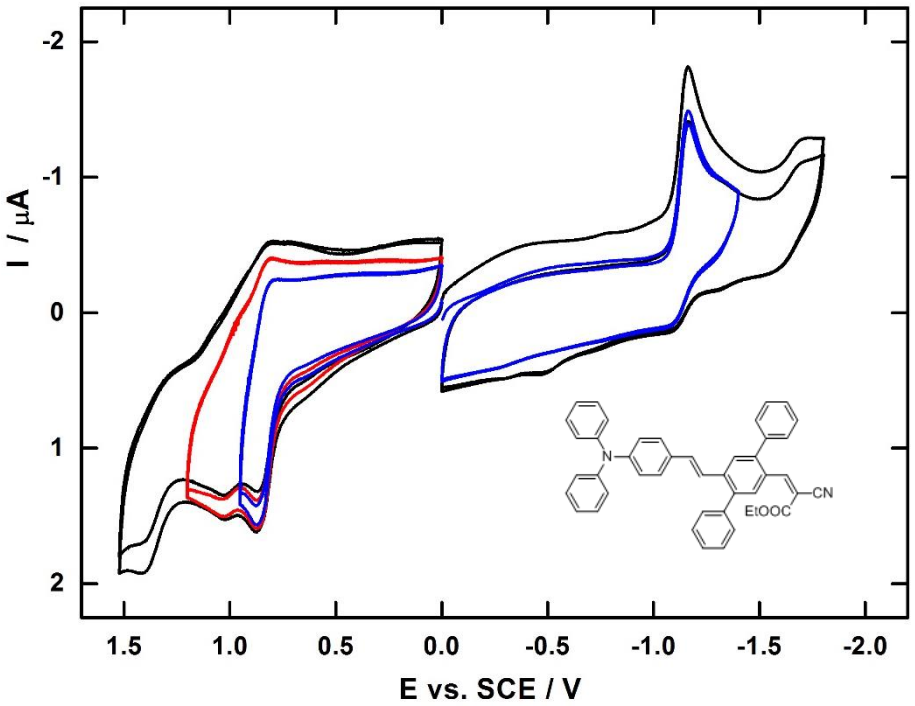
Electrochemical measurements were carried out in acetonitrile containing 0.1 M Bu_4NPF_6 in a three-electrode cell by cyclic voltammetry (CV), and rotating disk voltammetry (RDV). The working electrode was a glassy carbon disk (3 mm in diameter) for CV and RDV experiments. A saturated calomel electrode (SCE) separated by a bridge filled with supporting electrolyte and Pt wire were used as the reference and auxiliary electrodes. All potentials are given vs. SCE. Voltammetric measurements were performed using a potentiostat PGSTAT 128N (AUTOLAB, Metrohm Autolab B.V., Utrecht, The Netherlands) operated via NOVA 1.11 software.



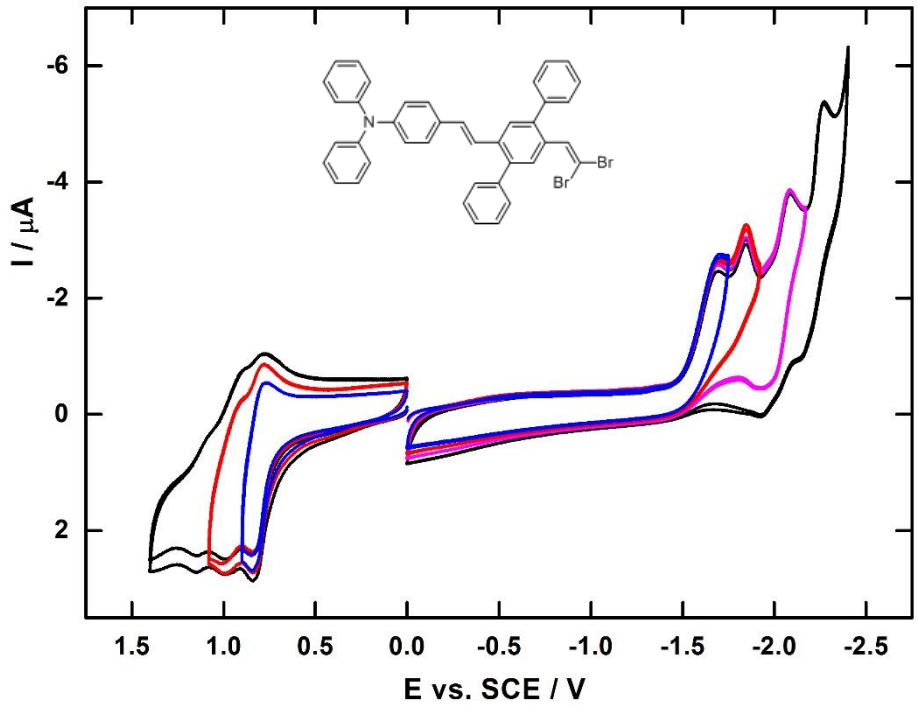
Representative CV curves of the oxidation and reduction of **DPA-DPS-DMV** at glassy carbon electrode in acetonitrile containing 0.1 M Bu_4NPF_6.; v = 100 $mV.s^{-1}$.



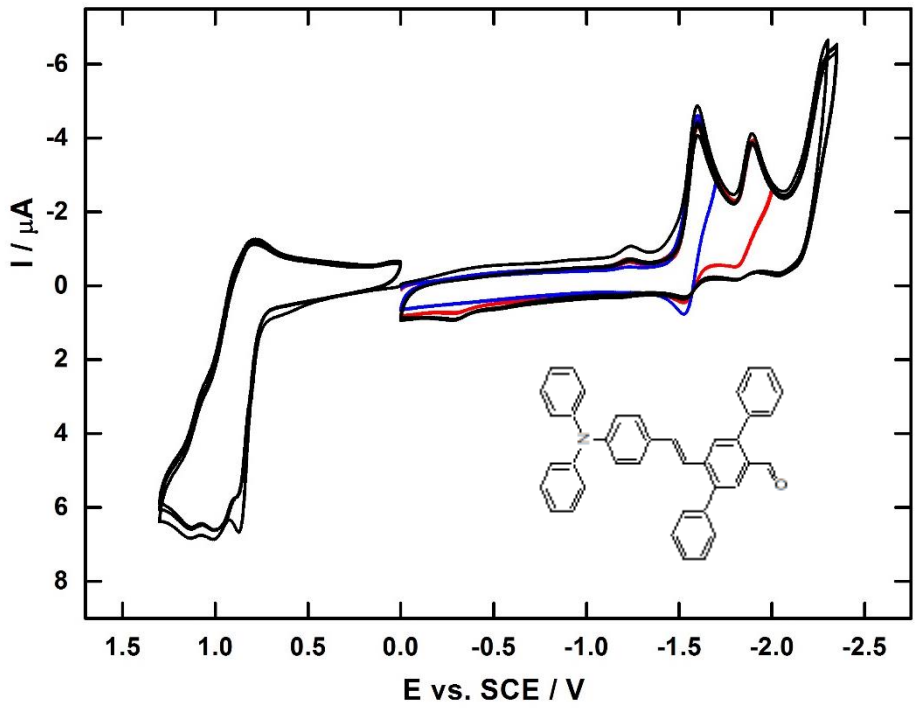
Representative CV curves of the oxidation and reduction of **DPA-DPS-CMV** at glassy carbon electrode in acetonitrile containing 0.1 M Bu_4NPF_6.; v = 100 $mV.s^{-1}$.



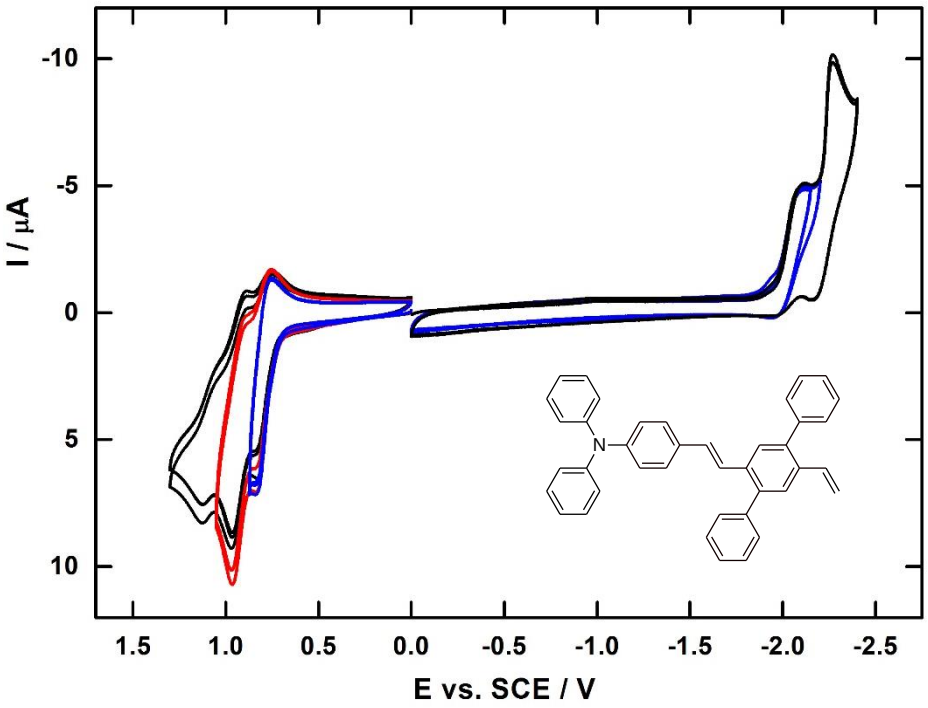
Representative CV curves of the oxidation and reduction of **DPA-DPS-CEV** compound at glassy carbon electrode in acetonitrile containing 0.1 M Bu_4NPF_6.; v = 100 $mV.s^{-1}$.



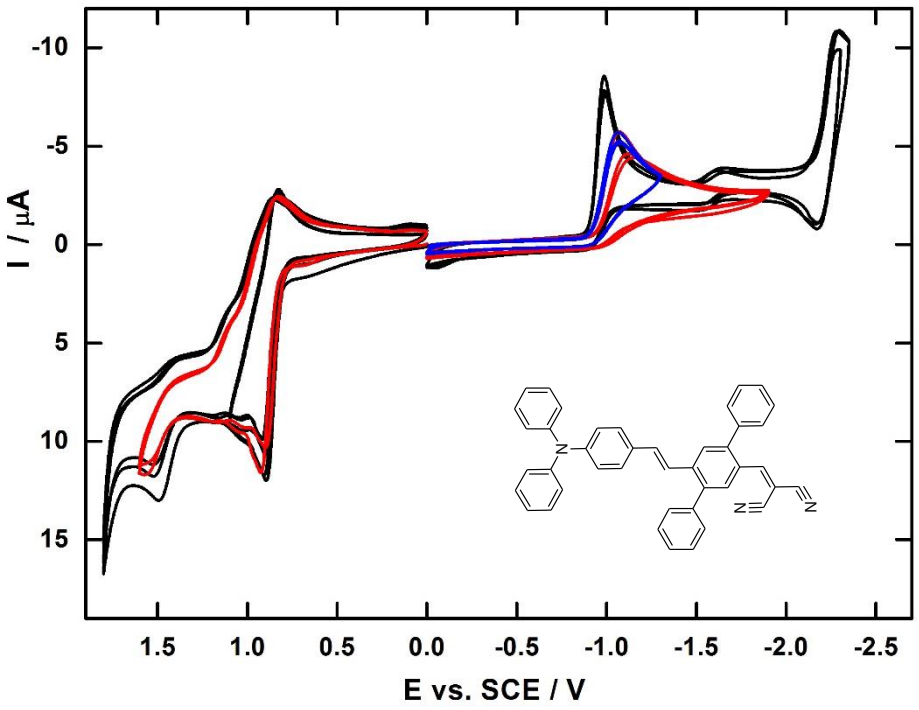
Representative CV curves of the oxidation and reduction of **DPA-DPS-DBV** compound at glassy carbon electrode in acetonitrile containing 0.1 M Bu_4NPF_6.; v = 100 $mV.s^{-1}$.



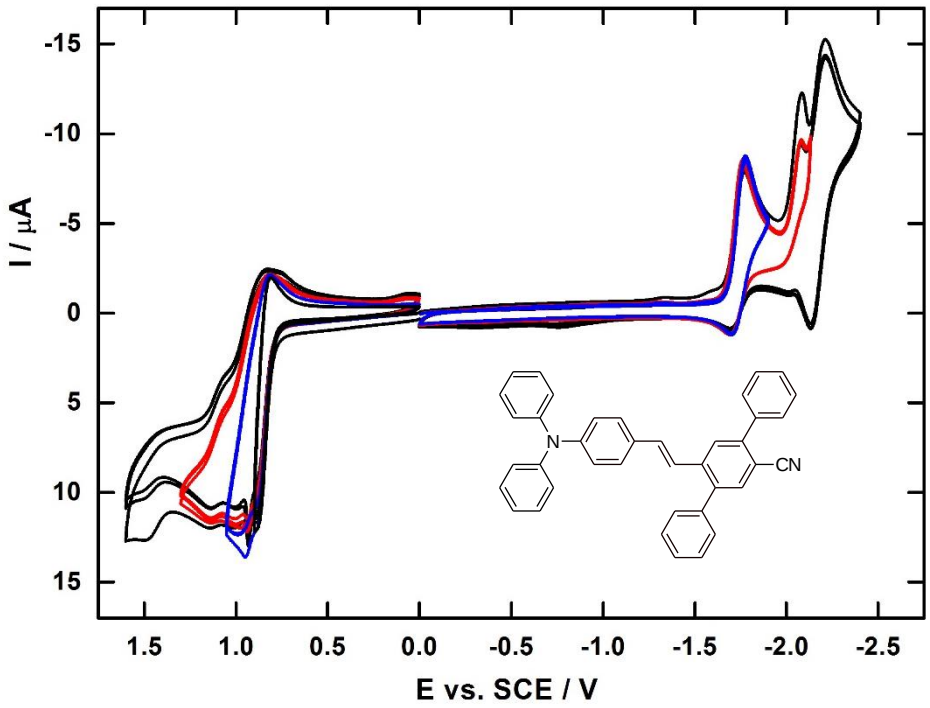
Representative CV curves of the oxidation and reduction of **DPA-DPS-CHO** compound at glassy carbon electrode in acetonitrile containing 0.1 M Bu_4NPF_6.; v = 100 $mV.s^{-1}$.



Representative CV curves of the oxidation and reduction of **DPA-DPS-V** compound at glassy carbon electrode in acetonitrile containing 0.1 M Bu_4NPF_6.; v = 100 $mV.s^{-1}$.



Representative CV curves of the oxidation and reduction of **DPA-DPS-DCV** compound at glassy carbon electrode in acetonitrile containing 0.1 M Bu_4NPF_6.; v = 100 $mV.s^{-1}$.



Representative CV curves of the oxidation and reduction of **DPA-DPS-CN** compound at glassy carbon electrode in acetonitrile containing 0.1 M Bu_4NPF_6.; v = 100 $mV.s^{-1}$.

Single crystal XRD

Full-sets of diffraction data for **DPA-DPS-CMV** and **DPA-DPS-DMV** were collected at 150(2)K with a Bruker D8-Venture diffractometer equipped with Cu (Cu/K_α radiation; λ =1.54178 Å) or Mo (Mo/K_α radiation; λ = 0.71073 Å) microfocus X-ray (IμS) sources, Photon CMOS detector and Oxford Cryosystems cooling device was used for data collection.

The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. Data were corrected for absorption effects using the Multi-Scan method (SADABS). Obtained data were treated by XT-version 2017/1 and SHELXL-2014/7 software implemented in APEX3 v2017.1-0 (Bruker AXS) system [G. M. Sheldrick, SHELXT. *Acta Cryst*. 2015, A71, 3].

Hydrogen atoms were mostly localized on a difference Fourier map, however to ensure uniformity of treatment of crystal, all hydrogen were recalculated into idealized positions (riding model) and assigned temperature factors $H_{iso}(H)$ = 1.2 (1.5 for methyl) U_{eq} (pivot atom). H atoms in methyl, vinylidene moieties and hydrogen atoms in aromatic rings were placed with C-H distances of 0.98 and 0.95 Å.

$R_{int} = \sum | F_o^2 - F_{o,mean}^2 | / \sum F_o^2$, GOF = $[\sum(w(F_o^2 - F_c^2)^2)/(N_{diffrs} - N_{params})]^{½}$ for all data, $R(F) = \sum | | F_o | - | F_c | | / \sum | F_o |$ for observed data, $wR(F^2) = [\sum(w(F_o^2 - F_c^2)^2)/(\sum w(F_o^2)^2)]^{½}$ for all data.

Crystallographic data for structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC nos. 2118685-2118686. Copies of this information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge CB2 1EY, UK (fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or www: http://www.ccdc.cam.ac.uk).

Deposition Number 2118685-2118686

Summary of Data - Deposition Number 2118685

Compound Name:
Data Block Name: data_ai201214O2
Unit Cell Parameters: a 15.070(3) b 9.7398(13) c 22.418(3) P21/c
---

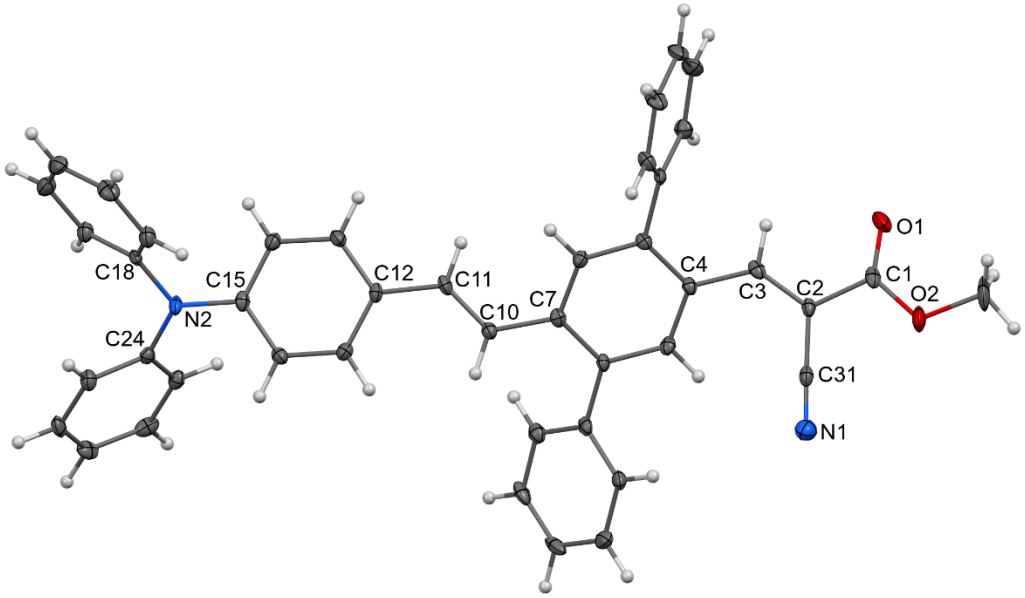
Summary of Data - Deposition Number 2118686

Compound Name:
Data Block Name: data_ai210301O4
Unit Cell Parameters: a 8.614(2) b 19.486(4) c 20.323(4) P212121

Table S1: Experimental details for **DPA-DPS-CMV**

Crystal data	
Chemical formula	$C_{43}H_{32}N_2O_2$
M_r	608.70
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, b, c (Å)	15.070 (3), 9.7398 (13), 22.418 (3)
β (°)	97.637 (8)
V (Å^3)	3261.3 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.41 × 0.29 × 0.22
Data collection	
Diffractometer	Bruker D8 - Venture
Absorption correction	Multi-scan *SADABS2016*/2 - Bruker AXS area detector scaling and absorption correction
T_{min}, T_{max}	0.540, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	39500, 6190, 4272
R_{int}	0.147
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.104, 0.147, 1.19
No. of reflections	6190
No. of parameters	425
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.30

Computer programs: Bruker Instrument Service vV6.2.3, *APEX3* v2016.5-0 (Bruker AXS), *SAINT* V8.37A (Bruker AXS Inc., 2015), XT, VERSION 2014/5, *SHELXL2014*/7 (Sheldrick, 2014), *PLATON* (Spek, 2009).



O1—C1 1.199 (4), N1—C31 1.140 (4), C1—O2 1.333 (4), N2—C15 1.410 (4), N2—C24 1.420 (4), N2—C18 1.427 (4), C2—C3 1.342 (4), C10—C11 1.332 (4), O1—C1—O2 124.5 (3), O1—C1—C2 123.8 (3), O2—C1—C2 111.7 (3), C2—C3—C4 130.0 (3), C3—C2—C1 118.6 (3), C3—C2—C31 124.2 (3).

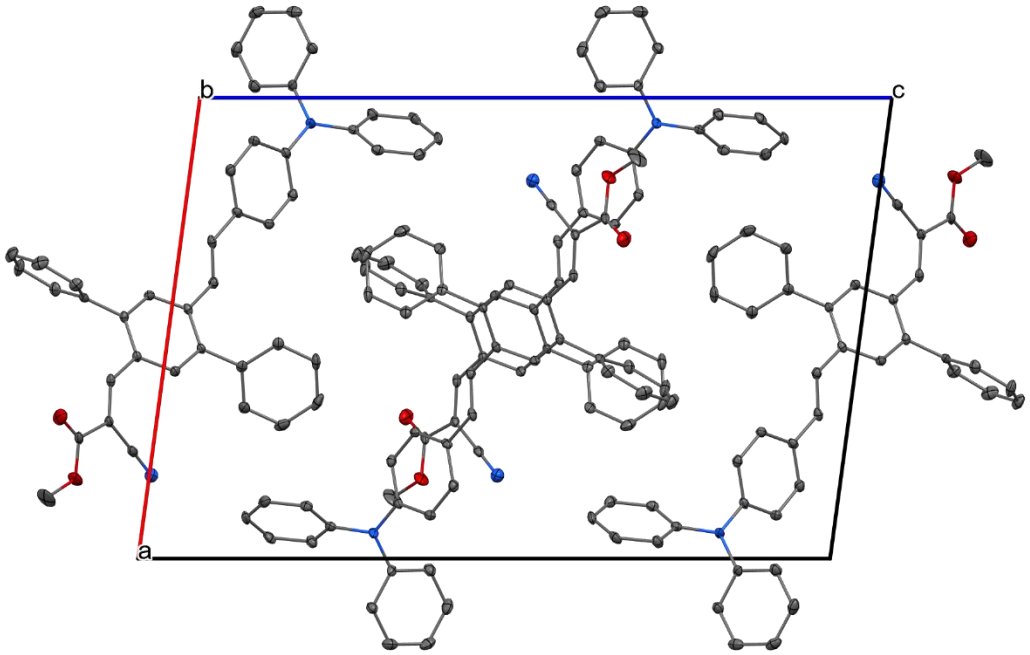
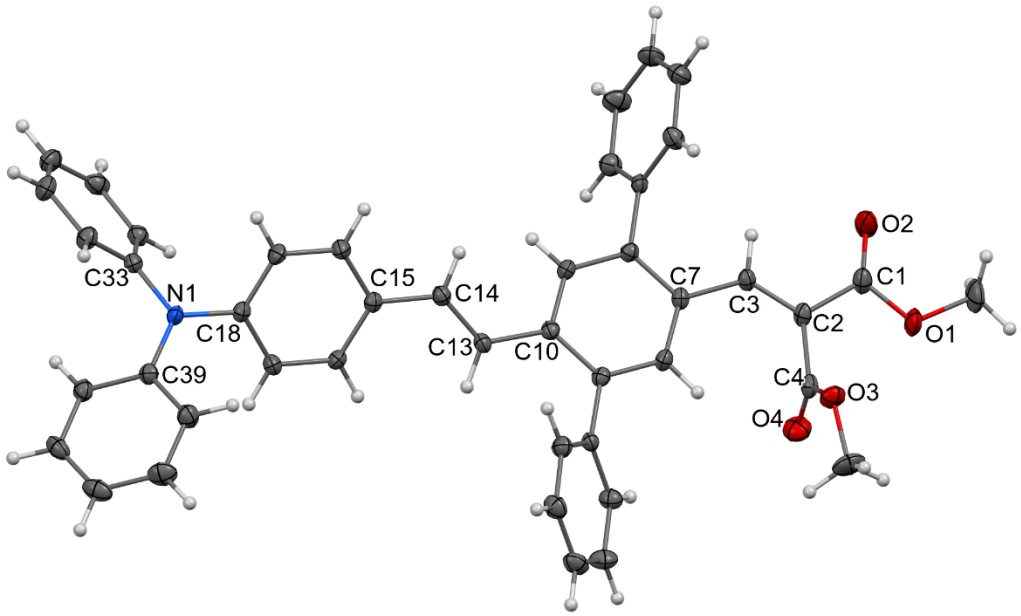


Table S2: Experimental details for **DPA-DPS-DMV**

Crystal data	
Chemical formula	$C_{44}H_{35}NO_4$
M_r	641.73
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	150
a, b, c (Å)	8.614 (2), 19.486 (4), 20.323 (4)
V (Å^3)	3411.2 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.55 × 0.36 × 0.03
Data collection	
Diffractometer	Bruker D8 - Venture
Absorption correction	Multi-scan *SADABS2016*/2 - Bruker AXS area detector scaling and absorption correction
T_{min}, T_{max}	0.632, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25860, 6525, 5003
R_{int}	0.103
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.062, 0.097, 1.04
No. of reflections	6525
No. of parameters	445
No. of restraints	381
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.19
Absolute structure	Flack x determined using 1721 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).

Computer programs: Bruker Instrument Service vV6.2.3, *APEX3* v2016.5-0 (Bruker AXS), *SAINT* V8.37A (Bruker AXS Inc., 2015), XT, VERSION 2014/5, *SHELXL2014*/7 (Sheldrick, 2014), *PLATON* (Spek, 2009).



O1—C1 1.337 (4), O1—C5 1.451 (4), N1—C39 1.418 (4), N1—C33 1.419 (4), N1—C18 1.421 (4), C1—O2 1.206 (4), C2—C3 1.342 (4), O3—C4 1.332 (4), O3—C6 1.451 (4), C4—O4 1.204 (4), C13—C14 1.338 (4), O2—C1—O1 123.7 (3), O2—C1—C2 125.9 (3), O1—C1—C2 110.4 (3), C3—C2—C1 118.1 (3), C3—C2—C4 126.1 (3), C25—C24—C23 120.4 (3), C1—C2—C4 115.7 (3).

Spectral and photophysical measurements

Table S3: Photophysical properties of DPA-DPS-V

	λ_A (nm)	λ_A (eV)	$\varepsilon(\lambda_A) \times 10^3$ ($l \cdot mol^{-1} \cdot cm^{-1}$)	λ_{PL} (nm)	λ_{PL} (eV)	Stokes (eV)	PLQY (%)	τ (ns)
Toluene	387	3.20	44.3(3)	444	2.79	0.411	83(4)	1.43
Chloroform	380	3.26	41.0(1.1)	469	2.64	0.619	56(1)	1.66
Dichloromethane	378	3.28	29.4(1.2)	483	2.57	0.713	83(3)	1.96
Acetonitrile	378	3.28	43.6(1)	504	2.46	0.820	82(6)	2.29
Solid state	440[b]	2.82	-	475	2.61	0.208	12(1)	2.19[a]

[a] weighted average

[b] maximum of PL excitation spectrum.

Table S4: Photophysical properties of DPA-DPS-DBV

	λ_A (nm)	λ_A (eV)	$\varepsilon(\lambda_A) \times 10^3$ ($l \cdot mol^{-1} \cdot cm^{-1}$)	λ_{PL} (nm)	λ_{PL} (eV)	Stokes (eV)	PLQY (%)	τ (ns)
Chloroform	388	3.20	41.1(1)	499	2.48	0.711	10(1)	0.12;1.23
Dichloromethane	386	3.21	40.0(1.5)	502	2.47	0.742	48(7)	1.64
Solid state	463[b]	2.68	-	498	2.49	0.188	11(1)	0.42[a]

[a] weighted average

[b] maximum of PL excitation spectrum.

Table S5: Photophysical properties of DPA-DPS-CN

	λ_A (nm)	λ_A (eV)	$\varepsilon(\lambda_A) \times 10^3$ ($l \cdot mol^{-1} \cdot cm^{-1}$)	λ_{PL} (nm)	λ_{PL} (eV)	Stokes (eV)	PLQY (%)	τ (ns)
Chloroform	396	3.13	21.1(2)	517	2.40	0.733	44(1)	1.59
Dichloromethane	393	3.16	18.0(2)	530	2.34	0.816	62(4)	1.98
Solid state	481[b]	2.58	-	529	2.34	0.234	18(2)	2.38[a]

[a] weighted average

[b] maximum of PL excitation spectrum.

Table S7: Photophysical properties of DPA-DPS-DMV

	λ_A (nm)	λ_A (eV)	$\varepsilon(\lambda_A) \times 10^3$ ($l \cdot mol^{-1} \cdot cm^{-1}$)	λ_{PL} (nm)	λ_{PL} (eV)	Stokes (eV)	PLQY (%)	τ (ns)
Chloroform	407	3.05	36.9(6)	627	1.98	1.069	21(2)	0.53
Dichloromethane	406	3.05	29.9(1.3)	663	1.87	1.184	46(4)	1.45
Solid state	516[b]	2.4	-	574	2.16	0.243	20(3)	3.12[a]

[a] weighted average

[b] maximum of PL excitation spectrum.

Table S8: Photophysical properties of DPA-DPS-CEV

	λ_A (nm)	λ_A (eV)	$\varepsilon(\lambda_A) \times 10^3$ ($l \cdot mol^{-1} \cdot cm^{-1}$)	λ_{PL} (nm)	λ_{PL} (eV)	Stokes (eV)	PLQY (%)	τ (ns)
Toluene	443	2.80	28.9(1)	579	2.14	0.657	98(7)	-
Chloroform	447	2.77	30(1)	664	1.87	0.907	97(7)	3.05
Dichloromethane	442	2.81	27.9(7)	716	1.73	1.074	58(5)	2.03
Solid state	556[b]	2.23	-	627	1.98	0.253	9(1)	1.90[a]

[a] weighted average

[b] maximum of PL excitation spectrum.

Table S9: Photophysical properties of DPA-DPS-CMV

	λ_A (nm)	λ_A (eV)	$\varepsilon(\lambda_A) \times 10^3$ ($l \cdot mol^{-1} \cdot cm^{-1}$)	λ_{PL} (nm)	λ_{PL} (eV)	Stokes (eV)	PLQY (%)	τ (ns)
Chloroform	452	2.74	32.5(5)	673	1.84	0.901	100(9)	3.05
Dichloromethane	445	2.79	28.2(9)	729	1.70	1.086	44(3)	1.85
Solid state	564[b]	2.20	-	637	1.95	0.252	35(4)	10.05[a]

[a] weighted average

[b] maximum of PL excitation spectrum.