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Molecular engineering of twisted dipolar chromophores for efficiency boosted BHJ solar cells

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Experimental Section

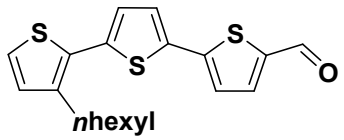
Materials, methods and measurements

All commercially available reagents were used without further purification unless otherwise stated. All organic reagents and catalysts were purchased from Sigma-Aldrich Pvt. Ltd. Solutions in organic solvents were dried with anhydrous sodium sulphate or magnesium sulphate. Solvents were evaporated under reduced pressure. Column chromatography was performed using thick-walled glass columns along with a mixture of petroleum ether and ethyl acetate on silica gel (100-200 mesh, SRL, India). The relative proportions of solvents in chromatographic solvent mixtures refer to the volume to volume (*V*/*V*) ratio. Analytical TLC was performed on precoated plastic sheets of silica gel G/UV-254 of 0.2 mm thickness (Macherey-Nagel, Germany) using analytical grade solvents and visualized with iodine spray (10% w/w I_2 in silica gel), UV light (λ = 254 and 365 nm) and alkaline $KMnO_4$ solution. Melting points were recorded on micro controller-based melting point apparatus using open capillaries. Infrared (IR) spectra for all solid compounds were recorded on a Bruker Optik GmbH, TENSOR 27 FT-IR spectrophotometer as KBr pellets. ^{1}H and ^{13}C NMR spectra were obtained in acetone-d_6 and $CDCl_3$ on a BRUKER spectrometer at 400, 500 and 100, 125 MHz respectively. Proton chemical shifts (δ) are relative to tetramethylsilane (TMS, δ = 0.00) as internal standard and expressed in parts per million. The number of protons (n) for a given resonance was indicated as nH. Spin multiplicities are given as s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet). Coupling constants (*J*) are given in hertz. High-resolution mass spectra (HRMS) were obtained using a Q-TOF and JEOL-GCMate II mass spectrometer. GC-MS spectra were obtained using a PerkinElmer instrument. UV-Visible spectra for all solution and thin film phase were recorded in chloroform solution and as thin film on SHIMADZU UV-3600 plus UV-VIS-NIR spectrometer. Photoluminescence spectra were recorded in Jasco spectrofluorometer FP-8500. Cyclic voltammetry (CV) experiments were performed with Autolab potentiostat galvanostat (Model PGSTAT-30). All CV measurements were carried out at room temperature with a conventional three-electrode configuration employing a glassy carbon electrode as the working electrode, silver wire as the pseudo-reference electrode and a Pt wire as the counter electrode. Tetrabutylammonium hexafluorophosphate (0.1 M) as supporting electrolyte was used in argon-purged chloroform with a scan rate 50 mV s^{-1}. Atomic force microscopic images were captured using 5500 Series, Agilent Technologies. Field Emission Scanning Electron Microscopic images were captured using CARL ZEISS SUPRA 55VP. Thermo gravimetric analysis (TGA) and

differential scanning calorimetry (DSC) was carried out on a NETZSCH STA 409PC instrument under purified nitrogen gas flow with a 5 °C min^{-1} heating rate. XRD spectra for **2j** : **PCBM** blend as thinfilm were recorded on a X-Ray Diffractometer Smart Lab Guidance, RIGAKU.Thermal evaporator with a sputtering unit (model No: VRSU04D) and thickness monitor (model No: CTM-200) was used for chemical vapour deposition. The OPV device performance was measured by recording the current voltage characteristics using a potentiostat (keithley 2400) under illumination from a Solar Simulator (Science-Tech) with an AM 1.5G filter set and an illumination intensity of 100 mW/cm^2. For AFM studies, a mixture of **2j** and PCBM in a blend ratio of 1:1 in *o*-dichlorobenzene was prepared. This mixture was then spin-coated at 1000 rpm for 1 minute on an etched ITO electrode and annealed at 100 °C for 5 minutes under vacuum. The topographical and phase images of this film before and after thermal annealing in an area of 5×5 μM was analyzed.

Experimental procedure for the synthesis of 3''-hexyl-[2,2':5',2''-terthiophene]-5-carbaldehyde (III):

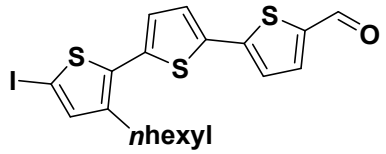
1 g of 5'-iodo-[2,2'-bithiophene]-5-carbaldehyde (0.0031 moL, 1.0 eq.) was dissolved in 25 mL of toluene. With an interval of 10 mins, 1.09 mL of 3-hexylthiopheneboronic acid pinacol ester (0.0037 moL, 2.2 eq.) followed by 20 mL of 2 M K_2CO_3 solution were added under argon atmosphere. Then later a hour, 5 mol% of $(Ph_3P)_4Pd$ was added and then refluxed for 24 h. The crude product was extracted with ethyl acetate and water. The organic fraction was concentrated under reduced pressure and then chromatographed on silica column (100–200 mesh) using 5% EA/PE as an eluent afforded 3''-hexyl-[2,2':5',2''-terthiophene]-5-carbaldehyde.



Yellow semi solid; yield 95 % (1.0 g); R_f = 0.25 (5 % EtOAc−petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 3081, 2928, 1735, 1664, 1524, 1448, 1222, 1148, 1048, 800, 736, 665; ^{1}H NMR (400 MHz, $CDCl_3$, δ in ppm): 0.91 (t, *J* = 4.0 Hz, 3H), 1.31-1.34 (m, 4H), 1.63-1.71 (m, 4H), 2.80 (t, *J* = 8.0 Hz, 2H), 6.97 (d, *J* = 4.0 Hz, 1H), 7.09 (d, *J* = 4.0 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 1H), 7.27 (d, *J* = 4.0 Hz, H), 7.33 (d, *J* = 4.0 Hz, 1H), 7.69 (d, *J* = 4.0 Hz, 1H), 9.88 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, δ in ppm): 14.1, 22.6, 24.7, 29.2, 30.5, 31.6, 118.9, 124.0, 124.5, 126.5, 126.7, 130.2, 135.3, 137.4, 138.3, 140.5, 141.5, 182.5; MS (ESI) : *m*/*z* = 361 $[M+H]^+$

Experimental procedure for the synthesis of 3''-hexyl-5''-iodo-[2,2':5',2''-terthiophene]-5-carbaldehyde (IV):

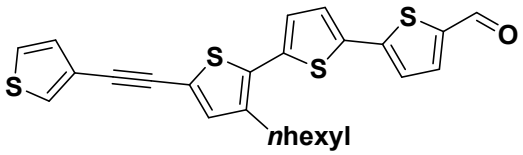
1.2143 g of 3''-hexyl-[2,2':5',2''-terthiophene]-5-carbaldehyde (0.0033 moL, 1.eq.) was taken in 1:1 mixture of acetic acid/chloroform (40 mL + 40 mL). To this mixture was added 887 mg of N-iodosuccinimide (0.0039 moL, 1.2 eq.) and then stirred it room temperature for overnight. The crude product was extracted with ethyl acetate and 5% sodium thiosulphate solution followed by water. The organic fraction was concentrated under reduced pressure and then chromatographed on silica column (100–200 mesh) using 1% EA/PE as an eluent offered 3''-hexyl-5''-iodo-[2,2':5',2''-terthiophene]-5-carbaldehyde.



Yellowish orange solid; yield 98 % (1.33 g); Mp: 90-93°C; R_f = 0.34 (5% EtOAc−petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 3074, 2924, 2853, 1742, 1664, 1441, 1223, 1097, 1044, 799, 662; ^{1}H NMR (400 MHz, $CDCl_3$, δ in ppm): 0.91 (t, *J* = 8.0 Hz, 3H), 1.21-1.48 (m, 7H), 1.63 (p, *J* = 8.0 Hz, 1H), 2.73 (t, *J* = 8.0 Hz, 2H), 7.01 (d, *J* = 4.0 Hz, 1H), 7.10 (s, 1H), 7.25 (d, *J* = 4.0 Hz, 1H), 7.30 (d, *J* = 4.0 Hz, 1H), 7.68 (d, *J* = 4.0 Hz, 1H), 9.88 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, δ in ppm): 14.1, 22.6, 29.0, 29.1, 30.5, 31.6, 72.7, 124.2, 126.4, 127.1, 135.6, 136.6, 137.4, 139.9, 141.7, 142.2, 146.5, 182.4; MS (ESI) : *m*/*z* = 487 $[M+H]^+$

Experimental procedure for the synthesis of 3''-hexyl-5''-(thiophen-2-ylethynyl)-[2,2':5',2''-terthiophene]-5-carbaldehyde (VI):

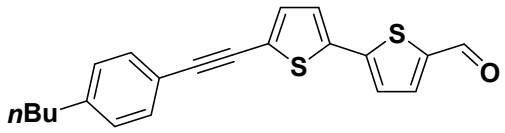
690 mg of iodo precursor (1.4184 mmoL, 1.0 eq.) synthesised from the previous step, 5 mol% of $Pd(Ph_3P)_2Cl_2$, 5 mol% of copper(I) iodide were taken in a dried round flask under argon atmosphere. To this mixture, 5 mL of triethylamine followed by a slow addition of 0.16 mL of 3-ethynylthophene (1.7020 mmoL, 1.2 eq.) and stirred at room temperature for 12 h. Then the reaction mixture was extracted with ethyl acetate (3 × 25 mL) and the combined organic extract was dried over anhydrous $MgSO_4$, concentrated under reduced pressure and column chromatographed on silica gel (100-200 mesh) using 5% ethyl acetate/petroleum ether as eluent to afford the pure product.



Brown semi solid; yield 80 % (768 mg); R_f = 0.30 (5% EtOAc−petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 3099, 2925, 2856, 1662, 1446, 1221, 1092, 1041, 863, 799, 672; ^{1}H NMR (400 MHz, $CDCl_3$, δ in ppm): 0.92 (t, *J* = 8.0 Hz, 3H), 1.30-1.47 (m, 6H), 1.64-1.71 (m, 2H), 2.77 (t, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 4.0 Hz, 1H), 7.13 (s, 1H), 7.20 (d, *J* = 4.0 Hz, 1H), 7.21 (d, *J* = 4.0 Hz, 1H), 7.28 (s, 1H), 7.34 (d, *J* = 4.0 Hz, 1H), 7.55 (d, *J* = 4.0 Hz, 1H), 7.70 (d, *J* = 4.0 Hz, 1H), 9.89 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, δ in ppm): 14.1, 22.6, 29.1, 29.3, 30.3, 31.6, 81.9, 89.6, 121.7, 121.8, 124.1, 125.6, 126.5, 127.0, 128.9, 129.6, 131.4, 134.9, 135.7, 137.3, 137.4, 140.3, 141.7, 146.8, 182.4; MS (ESI) : *m*/*z* = 467 $[M+H]^+$

Experimental procedure for the synthesis of 5'-((4-butylphenyl)ethynyl)-[2,2'-bithiophene]-5-carbaldehyde (IX):

1 g of 5'-iodo-[2,2'-bithiophene]-5-carbaldehyde (0.0031 moL, 1.0 eq.), 5 mol% of $Pd(Ph_3P)_2Cl_2$, 5 mol% of copper(I) iodide were taken in a dried round flask under argon atmosphere. To this mixture, 5 mL of triethylamine followed by a slow addition of 0.65 mL of 1-butyl-4-ethynylbenzene (0.0037 moL, 1.2 eq.) and stirred at room temperature for 12 h. Then the reaction mixture was extracted with ethyl acetate (3 × 25 mL) and the combined organic extract was dried over anhydrous $MgSO_4$, concentrated under reduced pressure and column chromatographed on silica gel (100-200 mesh) using 5% ethyl acetate/petroleum ether as eluent to afford the pure product.

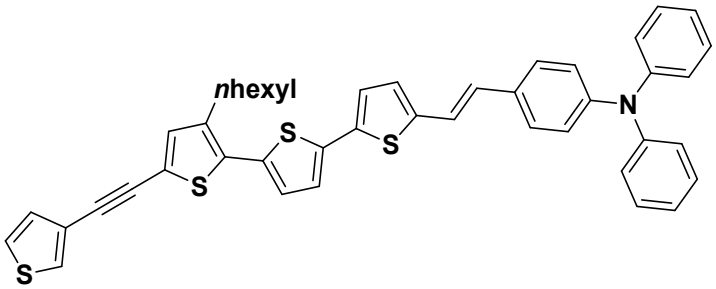


Yellow solid; yield 72 % (787 mg); Mp: 110-112°C; R_f = 0.39 (10% EtOAc - petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 3087, 2927, 2857, 1735, 1651, 1506, 1449, 1338, 1223, 1117, 1051, 883, 800, 748, 664, 575, 483; ^{1}H NMR (400 MHz, $CDCl_3$, δ in ppm): 0.96 (t, *J* = 8.0 Hz, 3H), 1.37 (q, *J* = 8.0 Hz, 2H), 1.63 (p, *J* = 8.0 Hz, 2H), 2.65 (t, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 4.0 Hz, 2H), 7.28 (d, *J* = 4.0 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.69 (d, *J* = 4.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, δ in ppm): 13.9, 22.3, 33.3, 35.6, 81.5, 95.9, 119.5, 124.5, 125.3, 126.0, 128.6, 131.4, 132.7, 136.7, 137.3, 142.0, 144.1, 146.3, 182.5; MS (ESI) : *m*/*z* = 351 $[M+H]^+$

Experimental procedure for the synthesis of (*E*)-4-(2-(3''-hexyl-5''-(thiophen-3-ylethynyl)-[2,2':5',2''-terthiophen]-5-yl)vinyl)-N,N-diphenylaniline (1i):

548.7 mg of N,N-diphenylamino-N-(4-(benzyl)triphenylphosphonium bromide (0.9176 mmoL, 1.1 eq.) was dissolved in 10 mL of DMF and 253.3 mg of anhydrous potassium

carbonate (1.8352 mmoL, 2.2 eq.) was added and allowed to stir at room temperature for 15 min. Then, 2 drops of 18-crown-6 was added and continue stirring for another 15 mins. 389.6 mg of aldehyde precursor (0.8343 mmoL, 1 eq.) synthesized from previous step was added and stirred at room temperature for 2 h. Then the reaction mixture was extracted with ethyl acetate (3 × 25 mL) and the combined organic layer was dried over anhydrous $MgSO_4$, concentrated under reduced pressure to afford crude mixture of *E/Z* isomers. The Crude mixture was taken in 10 mL of chloroform and refluxed with 5 mol% of iodine for 5 h to carry out the isomerization. This reaction mixture was quenched with 10% of sodium thiosulphate solution (3 × 25 mL) and extracted with ethyl acetate (3 X 10 mL). The organic extract was dried over anhydrous $MgSO_4$, concentrated under reduced pressure and chromatographed on silica gel (100-200 mesh) using ethyl acetate/petroleum ether as eluent to afford the pure product.

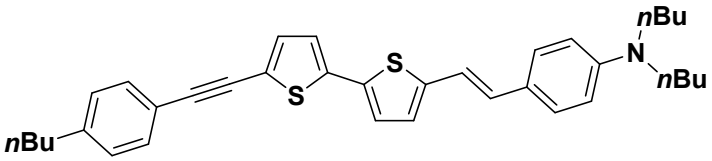


Brown semi solid; yield 71% (754 mg); R_f = 0.50 (5% EtOAc−petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 3029, 2923, 2857, 1587, 1494, 1277, 1179, 945, 787, 695; ^{1}H NMR (400 MHz, $CDCl_3$, δ in ppm): 0.94 (t, *J* = 4.0 Hz, 3H), 1.32 – 1.36 (m, 6H), 1.68 (p, *J* = 8.0 Hz, 2H), 2.78 (t, *J* = 8.0 Hz, 2H), 6.85 (d, *J* = 16.0 Hz, 2H), 6.95 (d, *J* = 4.0 Hz, 2H), 7.05 (t, *J* = 4.0 Hz, 3H), 7.07 (d, *J* = 4.0 Hz, 3H), 7.10 (d, *J* = 4.0 Hz, 2H), 7.12 (d, *J* = 4.0 Hz, 4H), 7.21 (d, *J* = 4.0 Hz, 1H), 7.27 (s, 1H), 7.29 (d, *J* = 4.0 Hz, 3H), 7.37 (s, 1H), 7.54 (d, *J* = 4.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, δ in ppm): 14.1, 22.6, 29.1, 29.3, 30.4, 31.6, 82.9, 89.2, 119.8, 120.9, 121.9, 123.1, 123.4, 123.8, 124.2, 124.6, 125.5, 126.7, 126.9, 127.2, 128.1, 128.8, 129.3, 129.7, 130.8, 132.2, 134.2, 134.9, 135.0, 137.6, 139.6, 142.6, 147.4, 147.5; MS (ESI) : *m*/*z* = 708 $[M+H]^+$

Experimental procedure for the synthesis of 5'-((4-butylphenyl)ethynyl)-[2,2'-bithiophene]-5-carbaldehyde (1j):

476.8 mg of N,N-dibutyl-N-(4-(benzyl)triphenylphosphonium iodide (0.78562 mmoL, 1.1 eq.) was dissolved in 10 mL of DMF and 216.8 mg of anhydrous potassium carbonate (1.57124 mmoL, 2.2 eq.) was added and allowed to stir at room temperature for 15 min.

Then, 2 drops of 18-crown-6 was added and continue stirring for another 15 mins. 250 mg of aldehyde precursor (0.7142 mmoL, 1 eq.) synthesized from previous step was added and stirred at room temperature for 2 h. Then the reaction mixture was extracted with ethyl acetate (3 × 25 mL) and the combined organic layer was dried over anhydrous $MgSO_4$, concentrated under reduced pressure to afford crude mixture of *E/Z* isomers. The Crude mixture was taken in 10 mL of chloroform and refluxed with 5 mol% of iodine for 5 h to carry out the isomerization. This reaction mixture was quenched with 10% of sodium thiosulphate solution (3 × 25 mL) and extracted with ethyl acetate (3 X 10 mL). The organic extract was dried over anhydrous $MgSO_4$, concentrated under reduced pressure and chromatographed on silica gel (100-200 mesh) using ethyl acetate/petroleum ether as eluent to afford the pure product.

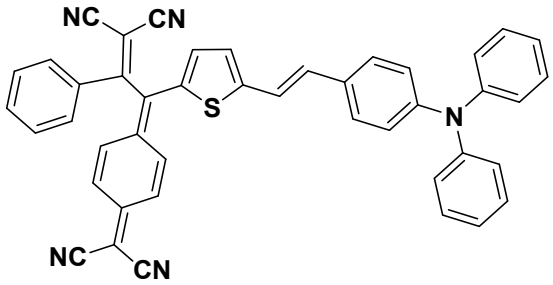


Yellowish brown solid; yield 74 % (584 mg); Mp: 91- 92°C; R_f = 0.66 (10% EtOAc – petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 3071, 3013, 2925, 2859, 1595, 1517, 1456, 1369, 1280, 1184, 1104, 937, 800, 734, 522; ^{1}H NMR (400 MHz, $CDCl_3$, δ in ppm): 0.64 (t, *J* = 4.0 Hz, 9H), 0.90 – 1.03 (m, 5H), 1.08 – 1.24 (m, 9H), 2.14 (t, *J* = 8.0 Hz, 2H), 2.84 (t, *J* = 8.0 Hz, 2H), 6.41 (d, *J* = 8.0 Hz, 2H), 6.61 (d, *J* = 4.0 Hz, 2H), 6.66 (d, *J* = 4.0 Hz, 2H), 6.83 (d, *J* = 4.0 Hz, 2H), 6.85 (d, *J* = 4.0 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, δ in ppm): 12.9, 12.9, 19.3, 21.3, 28.6, 32.3, 34.6, 49.7, 81.9, 94.0, 111.0, 116.0, 119.5, 121.0, 122.3, 123.6, 123.9, 124.7, 127.6, 128.8, 130.6, 132.0, 132.9, 138.5, 142.5, 143.2; MS (ESI) : *m*/*z* = 351 $[M+H]^+$

General procedure for the synthesis of 2a-2h:

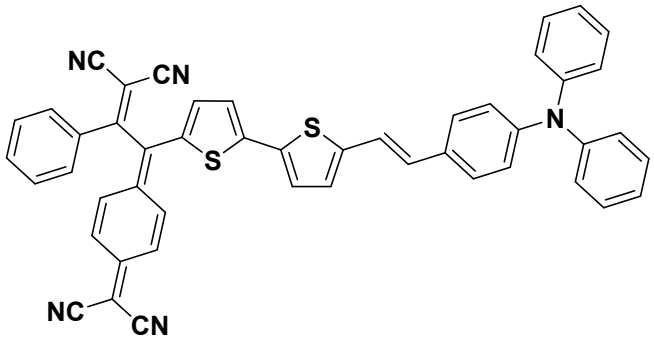
1.0 mmoL of previously synthesized compound 1a-h was taken in 10 mL of 1,2-dichloroethane. Then 1.0 mmoL of tetracyanoquinodimethane was added, refluxed it for overnight. The reaction mixture was concentrated under reduced pressure and chromatographed on silica gel column chromatography using 20% ethyl acetate / petroleum ether to afford pure product of **2a-h**.

(*E*)-2-(4-(3,3-dicyano-1-(5-(4-(diphenylamino)styryl)thiophen-2-yl)-2-phenylallylidene)cyclohexa-2,5-dien-1-ylidene)malononitrile (2a):



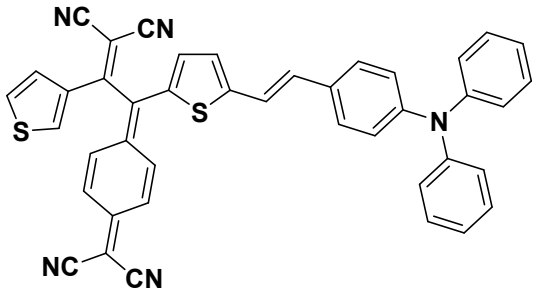
Dark blue solid; yield 92 % (358 mg); Mp: > 250°C; R_f = 0.32 (20% EtOAc−petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 3051, 2927, 2210, 1587, 1498, 1379, 1283, 1180, 1074, 833, 696; ^{1}H NMR (400MHz, Acetone - d_6, δ in ppm): 6.83 (d, *J* = 8.0 Hz, 2H), 7.00 (t, *J* = 8.0 Hz, 7H), 7.12 (t, *J* = 12.0 Hz, 1H), 7.19 – 7.25 (m, 7H), 7.29 (d, *J* = 4.0 Hz, 1H), 7.32 (d, *J* = 4.0 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.44 – 7.56 (m, 3H), 7.59 (d, *J* = 4.0 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 2H), 8.11 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100MHz, Acetone - d_6, δ in ppm): 73.4, 88.7, 112.5, 114.1, 118.6, 121.8, 124.0, 124.9, 125.0, 125.2, 126.3, 128.7, 129.5, 131.3, 133.6, 134.0, 135.1, 136.2, 138.5, 142.3, 147.0, 148.9, 153.3, 154.9, 170.0; HRMS m/*z* calculated for $C_{44}H_{27}N_5S$ MW: 657.1987, found: 657.1986.

(*E*)-2-(4-(3,3-dicyano-1-(5'-(4-(diphenylamino)styryl)-[2,2'-bithiophen]-5-yl)-2-phenylallylidene)cyclohexa-2,5-dien-1-ylidene)malononitrile (**2b**):



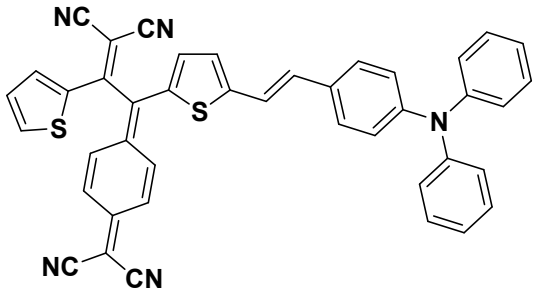
Dark blue solid; yield 90 % (358 mg); Mp: >250°C; R_f = 0.31 (20% EtOAc−petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 3049, 2930, 2858, 2211, 1592, 1494, 1375, 1126, 983, 853, 658, 597; ^{1}H NMR (400MHz, Acetone- d_6, δ in ppm): 6.99 (d, *J* = 8.0 Hz, 2H), 7.09-7.14 (m, 10H), 7.20 (d, *J* = 4.0 Hz, 1H), 7.46-7.50 (m, 3H), 7.52 (d, *J* = 4.0 Hz, 4H), 7.61-7.71 (m, 6H), 7.76 (d, *J* = 4.0 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 8.25 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100MHz, Acetone- d_6, δ in ppm): 74.0, 88.9, 112.5, 112.9, 114.0, 114.1, 119.3, 122.6, 123.6, 124.8, 126.1, 126.5, 127.8, 127.9, 128.0, 129.5, 129.6, 130.1, 130.3, 131.7, 133.2, 133.6, 134.2, 135.1, 136.3, 138.5, 141.9, 146.5, 147.3, 147.6, 148.0, 153.3, 169.7, 176.7; HRMS m/*z* calculated for $C_{48}H_{29}N_5S_2$ MW: 739.1864, found: 739.1862.

(*E*)-2-(4-(3,3-dicyano-1-(5-(4-(diphenylamino)styryl)thiophen-2-yl)-2-(thiophen-3-yl)allylidene)cyclohexa-2,5-dien-1-ylidene)malononitrile (2c):



Dark blue solid; yield 71 % (411 mg); Mp: >250°C; R_f = 0.30 (20% EtOAc−petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 3076, 2206, 1581, 1497, 1376, 1283, 1185, 841, 688, 593; ^{1}H NMR (400MHz, Acetone- d_6, δ in ppm): 6.99 (d, *J* = 8.0 Hz, 2H), 7.13 (t, *J* = 4.0 Hz, 4H), 7.15 (t, *J* = 4.0 Hz, 4H), 7.18 (d, *J* = 4.0 Hz, 1H), 7.35 – 7.38 (m, 6H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 4.0 Hz, 1H), 7.83 (s, 1H), 7.84 (d, *J* = 4.0 Hz, 2H), 8.31 (d, *J* = 4.0 Hz, 1H), 8.47 (t, *J* = 4.0 Hz, 2H); ^{13}C NMR (100MHz, Acetone- d_6, δ in ppm): 67.3, 84.4, 112.4, 112.7, 113.4, 113.6, 118.6, 121.8, 124.0, 124.7, 125.2, 126.1, 127.0, 128.4, 128.7, 129.1, 129.5, 130.3, 133.7, 133.8, 135.1, 137.0, 138.5, 147.0, 148.9, 148.9, 153.3, 165.9, 176.8; HRMS m/*z* calculated for $C_{42}H_{25}N_5S_2$ MW: 663.1551, found: 663.1552.

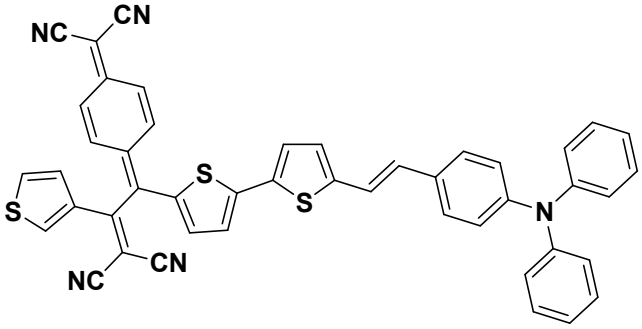
(*E*)-2-(4-(3,3-dicyano-1-(5-(4-(diphenylamino)styryl)thiophen-2-yl)-2-(thiophen-2-yl)allylidene)cyclohexa-2,5-dien-1-ylidene)malononitrile (2d):



Dark blue solid; yield 85 % (492 mg); Mp: >250°C; R_f = 0.24 (20% EtOAc−petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 2921, 2854, 2205, 1583, 1496, 1378, 1272, 1178, 1066, 818, 695, 589; ^{1}H NMR (400MHz, Acetone- d_6, δ in ppm): 6.84 (d, *J* = 8.0 Hz, 2H), 7.01 – 7.05 (m, 6H), 7.04 (d, *J* = 4.0 Hz, 1H), 7.23 – 7.34 (m, 10H), 7.61 (d, *J* = 4.0 Hz, 1H), 7.92 (d, *J* = 4.0 Hz, 1H), 8.14 (d, *J* = 4.0 Hz, 1H), 8.15 (d, *J* = 4.0 Hz, 2H), 8.17 (d, *J* = 4.0 Hz, 1H); ^{13}C NMR (100MHz, Acetone- d_6, δ in ppm): 73.7, 81.7, 113.1, 113.8, 114.5, 114.5, 119.0, 122.2, 124.4, 125.2, 125.6, 126.7, 128.8, 129.2, 129.9, 130.2, 130.6, 134.1, 135.3, 136.7, 137.6,

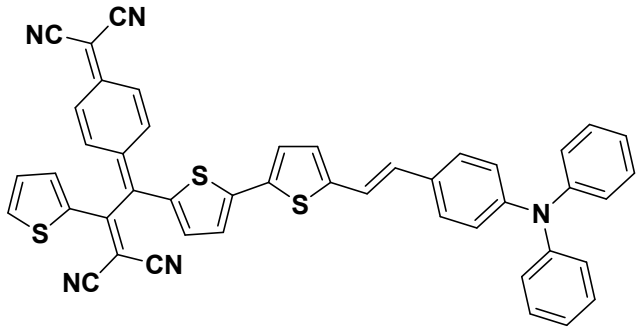
138.1, 138.9, 141.9, 147.4, 149.3, 153.6, 155.4, 161.4; HRMS m/*z* calculated for $C_{42}H_{25}N_5S_2$ MW: 663.1551, found: 663.1549.

(*E*)-2-(4-(3,3-dicyano-2-(5'-(4-(diphenylamino)styryl)-[2,2'-bithiophen]-5-yl)-1-(thiophen-3-yl)allylidene)cyclohexa-2,5-dien-1-ylidene)malononitrile (2e):



Dark blue solid; yield 79 % (654 mg); Mp: >250°C; R_f = 0.27 (20% EtOAc−petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 2918, 2851, 2204, 1587, 1494, 1369, 1278, 1194, 1154, 1085, 949, 884, 86, 750, 694; ^{1}H NMR (400MHz, Acetone- d_6, δ in ppm): 7.00 (d, *J* = 8.0 Hz, 2H), 7.11 (t, *J* = 4.0 Hz, 5H), 7.20 – 7.27 (m, 4H), 7.28 (d, *J* = 4.0 Hz, 1H), 7.49 (d, *J* = 4.0 Hz, 3H), 7.56 (d, *J* = 4.0 Hz, 2H), 7.60 (s, 1H), 7.68 (d, *J* = 4.0 Hz, 2H), 7.83 – 7.89 (m, 4H), 8.31 (d, *J* = 4.0 Hz, 1H), 8.49 (d, *J* = 4.0 Hz, 2H); ^{13}C NMR (100MHz, Acetone- d_6, δ in ppm): 67.7, 74.0, 113.6, 113.8, 114.2, 114.4, 119.7, 123.0, 123.9, 125.1, 125.3, 126.5, 126.7, 127.4, 128.1, 128.3, 128.4, 129.1, 129.5, 129.8, 130.0, 130.5, 130.8, 130.9, 134.1, 135.4, 135.9, 137.4, 138.8, 146.9, 147.7, 153.7, 174.1; HRMS m/*z* calculated for $C_{46}H_{27}N_5S_3$ MW: 745.1429, found: 745.1427.

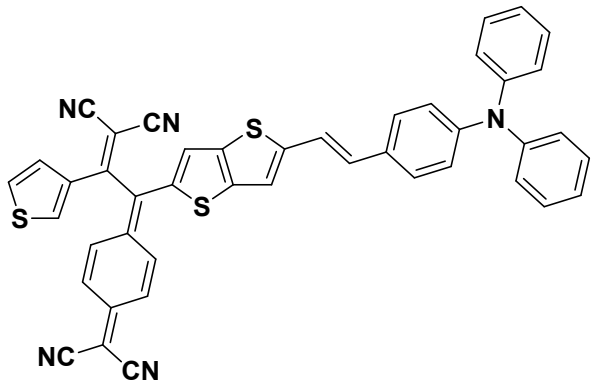
(*E*)-2-(4-(3,3-dicyano-2-(5'-(4-(diphenylamino)styryl)-[2,2'-bithiophen]-5-yl)-1-(thiophen-2-yl)allylidene)cyclohexa-2,5-dien-1-ylidene)malononitrile (2f):



Dark blue solid; yield 81 % (336 mg); Mp: 194-197°C; R_f = 0.23 (20% EtOAc−petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 2959, 2923, 2857, 2205, 1589, 1494, 1373, 1263, 1093, 1032, 806, 696; ^{1}H NMR (400MHz, Acetone-d_6, δ in ppm): 7.00 (d, *J* = 8.0 Hz, 2H), 7.09 – 7.13 (m, 10H), 7.28 (d, *J* = 4.0 Hz, 1H), 7.32 – 7.38 (m, 7H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* =

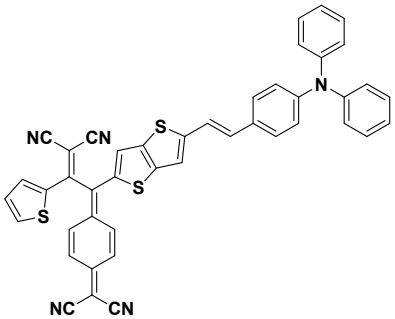
4.0 Hz, 3H), 7.76 (d, *J* = 4.0 Hz, 2H), 7.78 (d, *J* = 4.0 Hz, 1H); ^{13}C NMR (100MHz, Acetone-d_6, δ in ppm): 67.4, 90.2, 112.8, 113.1, 113.3, 113.7, 118.9, 121.5, 123.5, 124.0, 124.5, 124.7, 127.7, 127.8, 128.7, 129.4, 130.6, 131.1, 132.5, 133.3, 136.5, 138.3, 138.4, 138.9, 144.1, 145.4, 146.3, 147.2, 147.3, 167.1, 170.7; HRMS m/*z* calculated for $C_{46}H_{27}N_5S_3$ MW: 745.1429, found: 745.1427.

(*E*)-2-(4-(3,3-dicyano-1-(5-(4-(diphenylamino)styryl)thieno[3,2-b]thiophen-2-yl)-2-(thiophen-3-yl)allylidene)cyclohexa-2,5-dien-1-ylidene)malononitrile (2g):



Dark blue solid; yield 73 % (409 mg); Mp: 221-223°C; R_f = 0.32 (20% EtOAc−petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 2962, 2910, 2847, 2208, 1586, 1494, 1332, 1269, 1189, 805, 697; ^{1}H NMR (400MHz, Acetone- d_6, δ in ppm): 6.99 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 4.0 Hz, 3H), 7.13 (d, *J* = 4.0 Hz, 2H), 7.15 (d, *J* = 4.0 Hz, 1H), 7.19 – 7.23 (m, 2H), 7.31 – 7.40 (m, 4H), 7.43 – 7.52 (m, 3H), 7.54 (s, 1H), 7.58 (s, 1H), 7.80 – 7.87 (m, 3H), 8.09 (s, 1H), 8.28 (d, *J* = 8.0 Hz, 1H), 8.48 (d, *J* = 4.0 Hz, 1H); ^{13}C NMR (100MHz, Acetone- d_6, δ in ppm): 73.1, 84.4, 112.7, 113.4, 114.1, 114.2, 118.7, 119.0, 120.0, 122.2, 123.8, 124.9, 125.0, 126.3, 127.0, 128.1, 128.7, 129.1, 129.2, 129.5, 130.5, 131.9, 134.1, 135.0, 135.6, 137.1, 140.1, 147.2, 148.5, 153.3, 162.6, 173.7; HRMS m/*z* calculated for $C_{44}H_{25}N_5S_3$ MW: 719.1272, found: 719.1270.

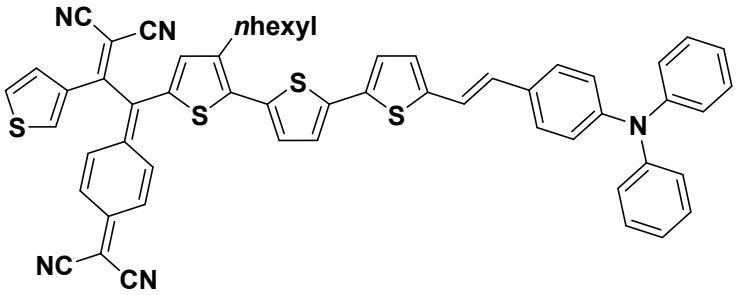
(*E*)-2-(4-(3,3-dicyano-1-(5-(4-(diphenylamino)styryl)thieno[3,2-b]thiophen-2-yl)-2-(thiophen-2-yl)allylidene)cyclohexa-2,5-dien-1-ylidene)malononitrile (2h):



Dark blue solid; yield 77 % (377 mg); Mp: 145-147°C; R_f = 0.28 (20% EtOAc−petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 2961, 2919, 2860, 2206, 1586, 1497, 1383, 1333, 1264, 1185, 1095, 1030, 809, 748, 700, 614, 561, 500; ^{1}H NMR (400MHz, Acetone- d_6, δ in ppm): 6.99 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 4.0 Hz, 4H), 7.20 – 7.23 (m, 3H), 7.33 – 7.42 (m, 5H), 7.46 – 7.52 (m, 3H), 7.54 – 7.60 (m, 3H), 8.04 (s, 1H), 8.08 (d, *J* = 4.0 Hz, 1H), 8.12 (s, 1H), 8.29 (d, *J* = 4.0 Hz, 1H), 8.31 (d, *J* = 4.0 Hz, 1H); ^{13}C NMR (100MHz, Acetone- d_6, δ in ppm): 73.5, 81.4, 112.8, 113.5, 114.1, 114.2, 118.7, 120.0, 122.2, 123.8, 125.0, 126.5, 128.1, 128.7, 129.2, 129.5, 129.8, 130.4, 132.0, 133.9, 134.9, 137.3, 137.8, 138.6, 139.6, 140.2, 142.2, 147.2, 148.5, 153.2, 153.4, 160.9; HRMS m/*z* calculated for $C_{44}H_{25}N_5S_3$ MW: 719.1272, found: 719.1268.

Experimental procedure for the synthesis of (*E*)-2-(4-(3,3-dicyano-1-(5''-(4-(diphenylamino)styryl)-3-hexyl-[2,2':5',2''-terthiophen]-5-yl)-2-(thiophen-3-yl)allylidene)cyclohexa-2,5-dien-1-ylidene)malononitrile (2i):

250 mg of alkyne precursor (0.3541 mmoL, 1 eq.) synthesized from previous step was taken in 10 mL of 1,2-dichloroethane. Then 72.23 mg of tetracyanoquinodimethane (0.3541 mmoL, 1 eq.) was added, refluxed it for overnight. The reaction mixture was concentrated under reduced pressure and chromatographed on silica gel column chromatography using 20% ethyl acetate/petroleum ether to afford pure product of **2i**.

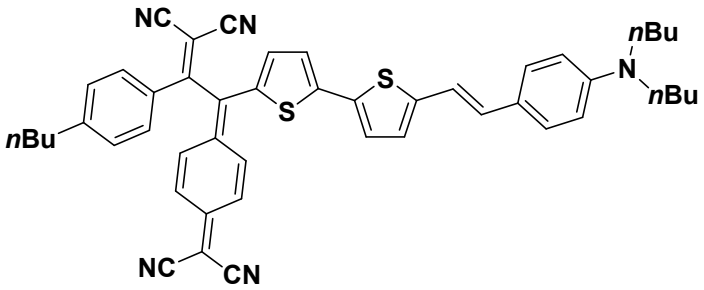


Dark blue solid; yield 88 % (397 mg); Mp: 214-216°C; R_f = 0.46 (20% EtOAc−petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 2924, 2857, 2204, 1680, 1591, 1431, 1365, 1273, 1194, 1089, 803; ^{1}H NMR (500MHz, Acetone- d_6, δ in ppm):0.88 (t, *J* = 5.0 Hz, 3H), 1.22 - 1.25 (m, 8H), 2.13 (t, *J* = 5.0 Hz, 2H), 6.85 (d, *J* = 10.0 Hz, 2H), 6.94 (s, 1H), 6.95 (d, *J* = 10.0 Hz, 2H), 6.99 (d, *J* = 5.0 Hz, 2H), 7.05 (d, *J* = 10.0 Hz, 1H), 7.11 (d, *J* = 5.0 Hz, 1H), 7.13 (d, *J* = 5.0 Hz, 1H), 7.19 (t, *J* = 5.0 Hz, 6H), 7.24 (d, *J* = 5.0 Hz, 1H), 7.32 (d, *J* = 5.0 Hz, 2H), 7.35 (d, *J* = 5.0 Hz, 2H), 7.43 (d, *J* = 10.0 Hz, 1H), 7.58 (s, 1H), 7.66-7.71 (m, 4H), 8.14 (d, *J* = 10.0 Hz, 1H); ^{13}C NMR (125 MHz, Acetone- d_6, δ in ppm): 12.9, 21.8, 24.2, 30.2, 30.8, 31.2, 64.4, 79.0, 112.1, 112.9, 113.4, 113.5, 118.4, 119.2, 122.4, 122.9, 123.4, 124.1, 124.2, 124.5,

125.0, 125.9, 126.5, 126.9, 127.0, 128.2, 128.5, 128.9, 130.2, 130.3, 132.3, 133.4, 134.5, 136.3, 139.7, 141.7, 143.3, 146.9, 147.2, 152.8, 162.0, 173.1; HRMS m/*z* calculated for $C_{56}H_{41}N_5S_4$ MW: 911.2245, found: 911.2244.

Experimental procedure for the synthesis of (*E*)-2-(1-(4-butylphenyl)-2-(5'-(4-(dibutylamino)styryl)-[2,2'-bithiophen]-5-yl)-2-(4-(dicyanomethylene)cyclohexa-2,5-dien-1- ylidene)ethylidene)malononitrile (2j):

100 mg of alkyne precursor (0.1718 mmoL, 1 eq.) synthesized from previous step was taken in 10 mL of 1,2-dichloroethane. Then 35.0 mg of tetracyanoquinodimethane (0.1718 mmoL, 1 eq.) was added, refluxed it for overnight. The reaction mixture was concentrated under reduced pressure and chromatographed on silica gel column chromatography using 20% ethyl acetate/petroleum ether to afford pure product of **2j**.



Dark blue solid; yield 83 % (285 mg); Mp: 192-193°C; R_f = 0.2 (10% EtOAc – petroleum ether); FT-IR (KBr, cm^{-1}) ν_{max} 3752, 3075, 2926, 2860, 2377, 2202, 1595, 1519, 1372, 1292, 1183, 1086, 941, 886, 813, 735, 653, 467; ^{1}H NMR (500MHz, Acetone-d_6, δ in ppm): 0.92 (t, *J* = 5.0 Hz, 3H), 0.97 (t, *J* = 5.0 Hz, 6H), 1.26-1.44 (m, 8H), 1.59-1.65 (m, 5H), 2.72 (t, *J* = 5.0 Hz, 2H), 3.39 (t, *J* = 5.0 Hz, 3H), 6.71 (d, *J* =10.0Hz, 2H), 6.99 (d, *J* = 10.0 Hz, 2H), 7.11 (d, *J* = 5.0 Hz, 2H), 7.42 (d, *J* = 5.0Hz, 3H), 7.46 (d, *J* = 10.0 Hz, 2H), 7.50 (d, *J* = 5.0 Hz, 1H), 7.52 (d, *J* = 5.0 Hz, 2H), 7.74 (d, *J* = 5.0 Hz, 1H), 7.87 (d, *J* = 10.0 Hz, 3H); ^{13}C NMR (125 MHz, Acetone- d_6, δ in ppm): 12.9, 19.3, 21.9, 24.2, 30.3, 31.2, 32.8, 49.6, 64.4, 66.9, 110.5, 113.2, 118.4, 122.6, 123.4, 123.9, 124.0, 128.2, 129.1, 129.2, 130.55, 130.59, 130.7, 131.2, 132.4, 132.5, 136.9, 137.9, 138.4, 143.5, 145.9, 146.7, 147.1, 166.5, 173.3; HRMS m/*z* calculated for $C_{48}H_{45}N_5S_2$ MW: 755.3116, found: 755.3114.

Procedure for small molecule organic solar cell fabrication

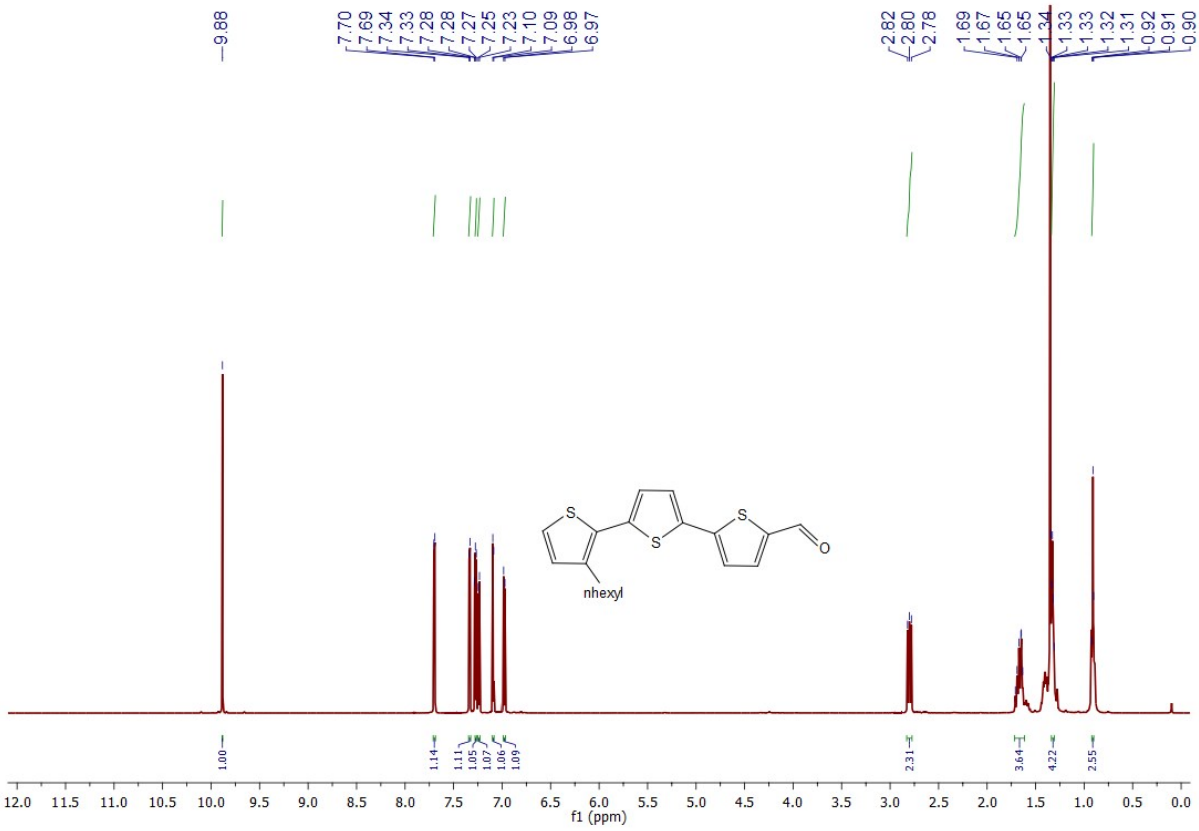
To unravel the solar cell performance of all chromophores (**2a-j**), inverted bulk heterojunction devices (ITO/ZnO/BHJ/V_2O_5/Ag) were constructed. The 0.5 cm area at middle of indium tin oxide (ITO) electrodes (1.5 x 1.5 cm) were masked with polymeric tape

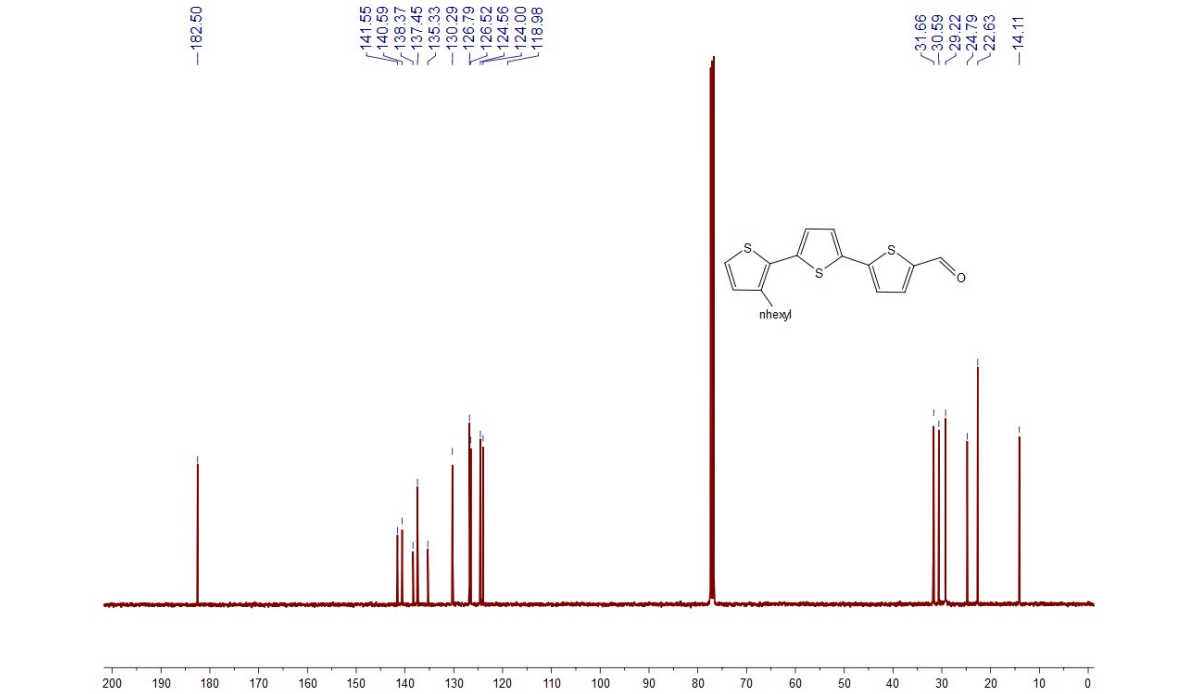
and etched with Zn powder and 20 % HCl. It was then cleaned sequentially with demineralized water, acetone followed by isopropanol under sonication before a final UV-ozone treatment. To deposit the ZnO on the cleaned ITO surface, the reaction was carried out between ethanolamine (0.28 g) and zinc acetate (1.0 g) in ethylene glycol (10 mL) at 70 ^{o}C for overnight. The aliquate obtained from the previous chemical composition was spin casted on the ITO surface at 3000 rpm for a minute and then the electrodes were heated at 270 ^{o}C. Afterward, the bulk heterojunction blend obtained from 1:1 ratio of chromophore **2a-j** (5 mg) and PCBM (5 mg) in 1,2-dichlorobenzene (1 mL) under pulse imposed stirring for 15 min were coated on the ZnO surface for 1 min at 1000 rpm and dried under vacuum at 140 ^{o}C for 30 min. Then of V_2O_5 at a thickness of ~5–7 nm at 0.1 Å s^{-1} and silver at a thickness of ~140–160 nm at 10 Å s^{-1}, respectively, were coated over the BHJ surface by chemical vapour deposition (CVD). The as-prepared cells were encapsulated in air and the photocurrent of the fabricated devices was measured with a sweeping voltage using a source measurement unit controlled by a computer under simulated solar light illumination (AM 1.5G; 100 mW cm^{-2}). The incident light intensity was calibrated to 1 Sun (100 mW cm^{-2}) with a standard silicon photodiode. The current vs. voltage (*J–V*) characteristics were measured for an area (0.2 x 0.5 cm) of 0.1 cm^2.

Table S1: Solubility data of **2a-2j** in acetone and chloroform

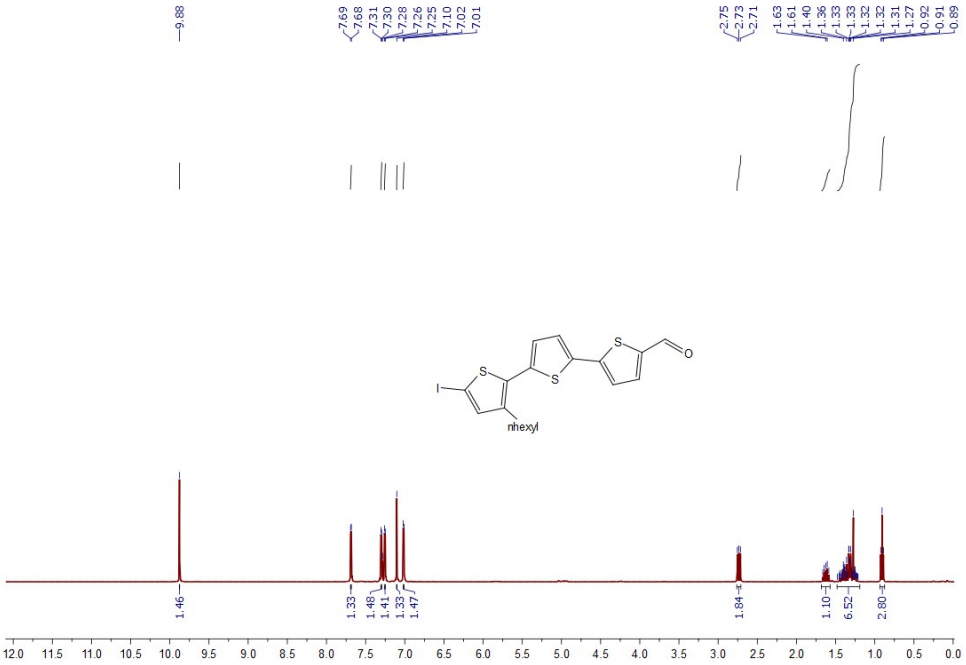
Sl. No.	Compound	Acetone	Chloroform
1	**2a**	12 mg/mL	8 mg/mL
2	**2b**	15 mg/mL	12 mg/mL
3	**2c**	9 mg/mL	6 mg/mL
4	**2d**	16 mg/mL	13 mg/mL
5	**2e**	14 mg/mL	10 mg/mL
6	**2f**	10 mg/mL	7 mg/mL
7	**2g**	13 mg/mL	11 mg/mL
8	**2h**	13 mg/mL	12 mg/mL
9	**2i**	21 mg/mL	19 mg/mL
10	**2j**	29 mg/mL	26 mg/mL

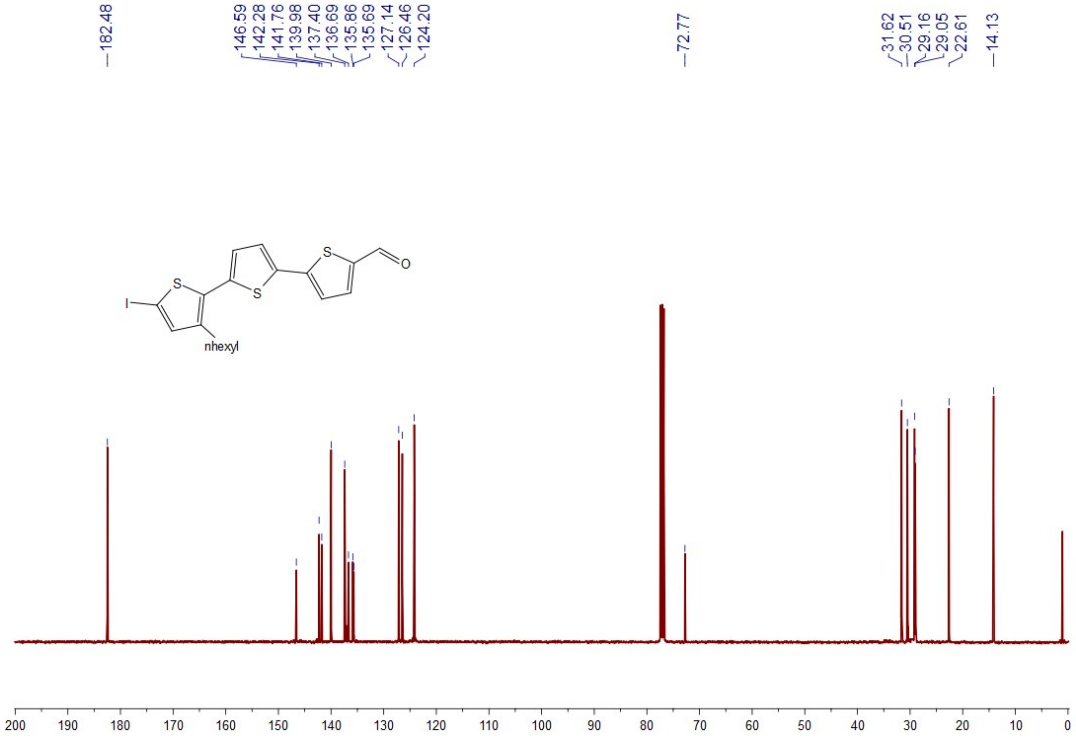
^{1}H NMR & ^{13}C NMR spectrum of compound III in $CDCl_3$



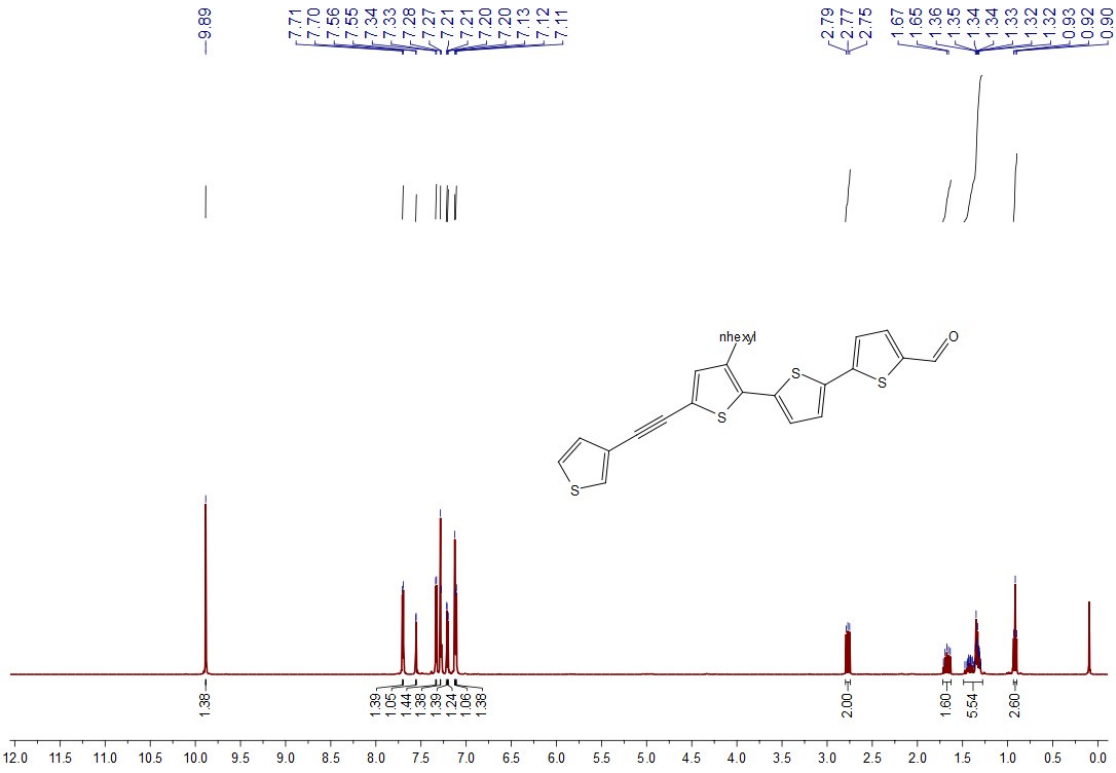


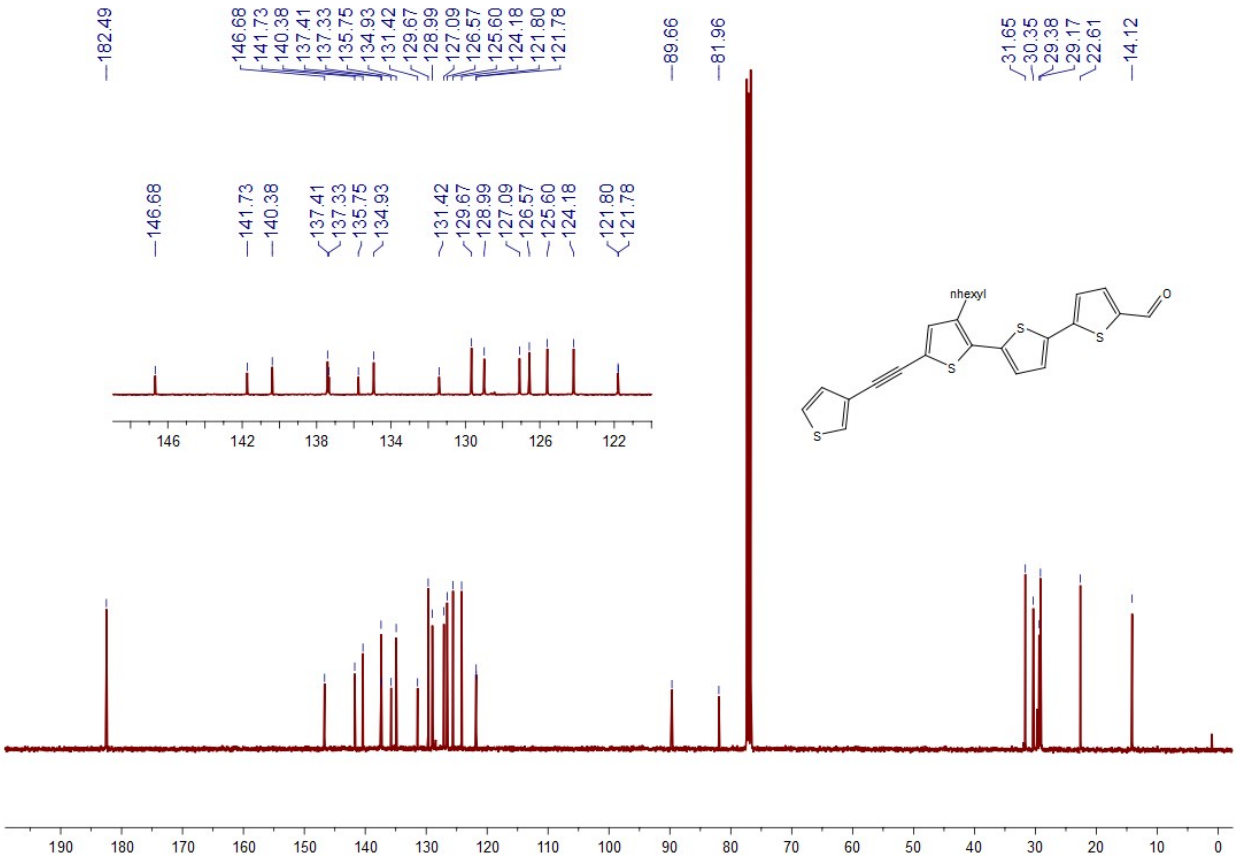
^{1}H NMR & ^{13}C NMR spectrum of compound IV in $CDCl_3$



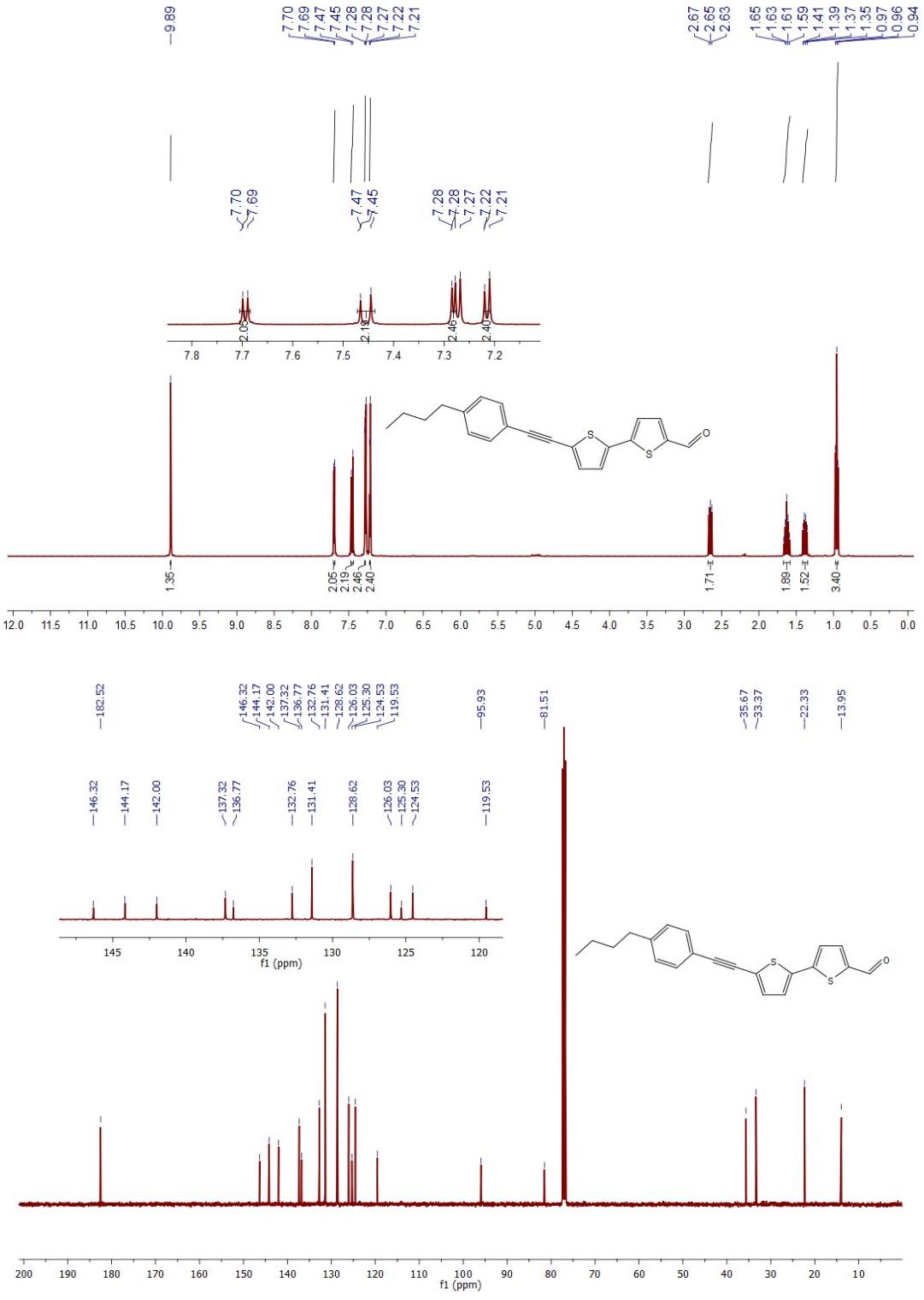


^{1}H NMR & ^{13}C NMR spectrum of compound VI in $CDCl_3$

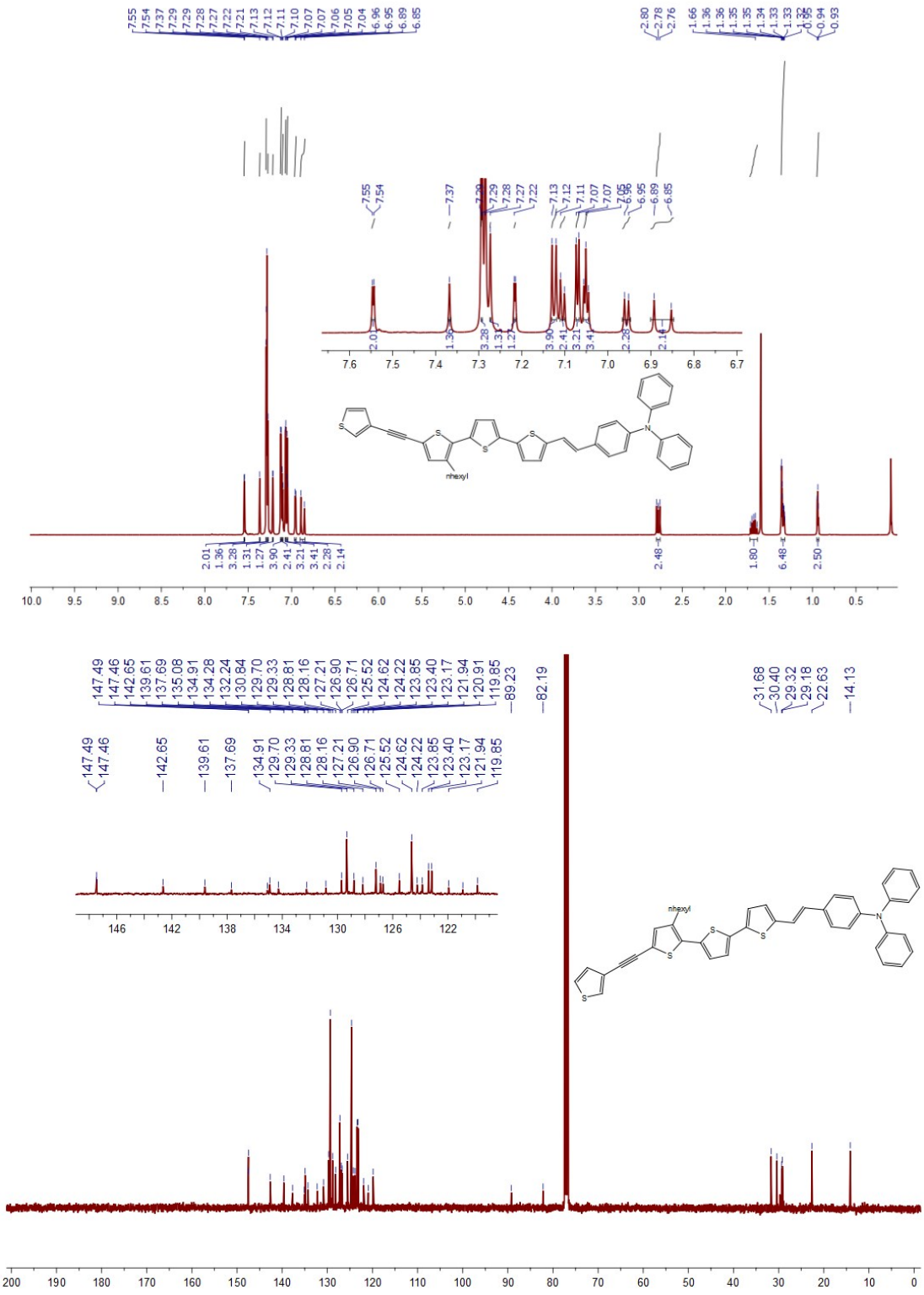




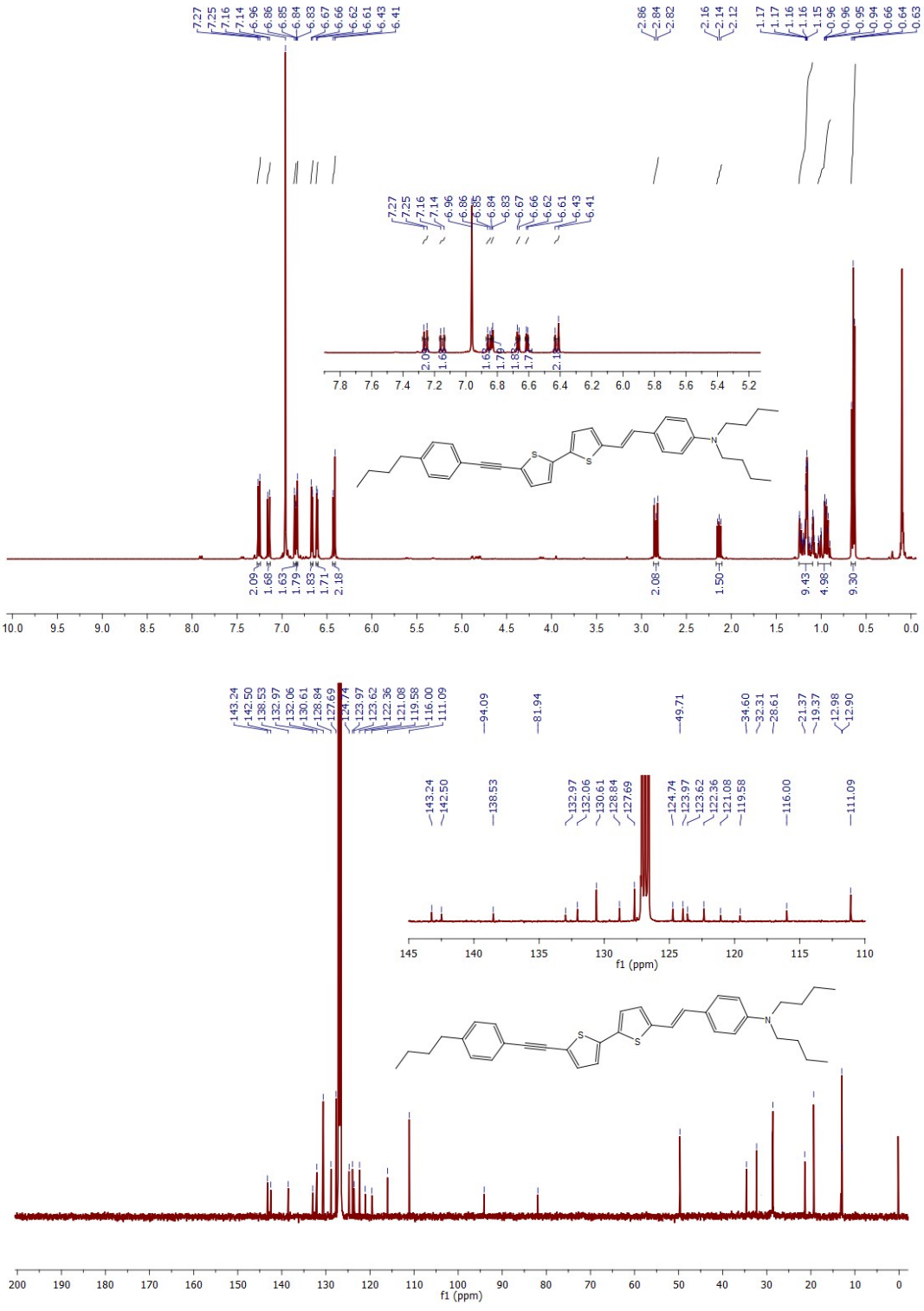
^{1}H NMR & ^{13}C NMR spectrum of compound IX in $CDCl_3$



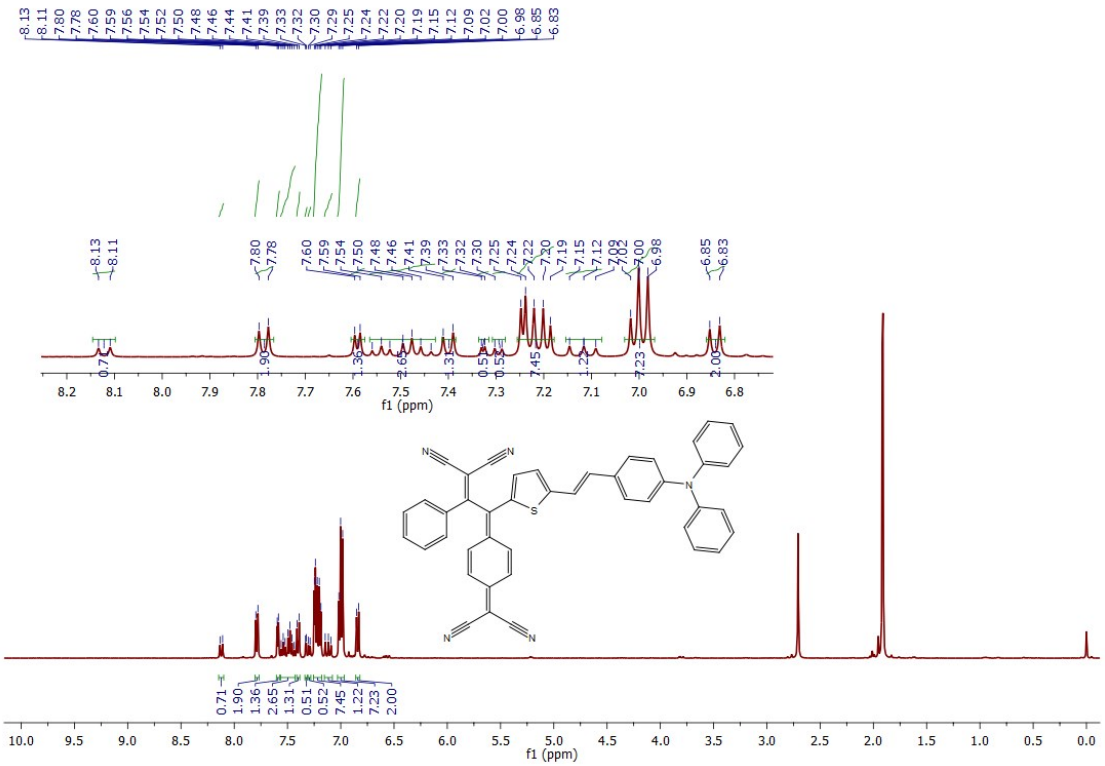
^{1}H NMR & ^{13}C NMR spectrum of compound 1i in $CDCl_3$

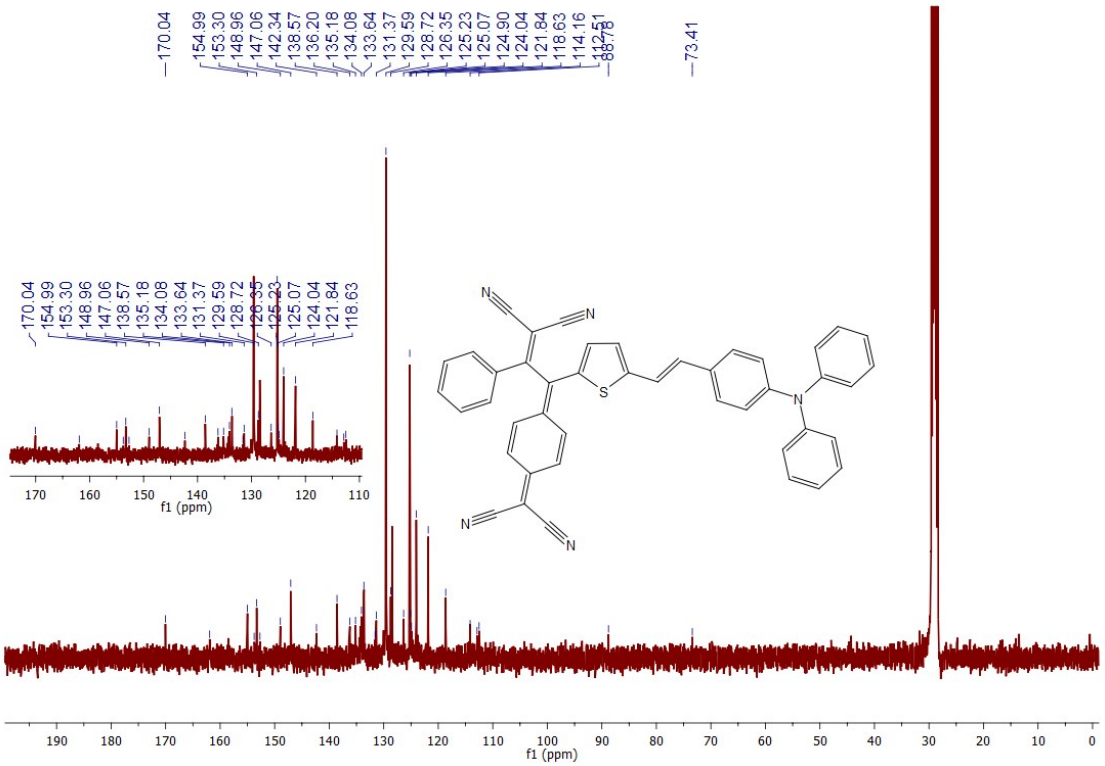


^{1}H NMR & ^{13}C NMR spectrum of compound 1j in C_6D_6

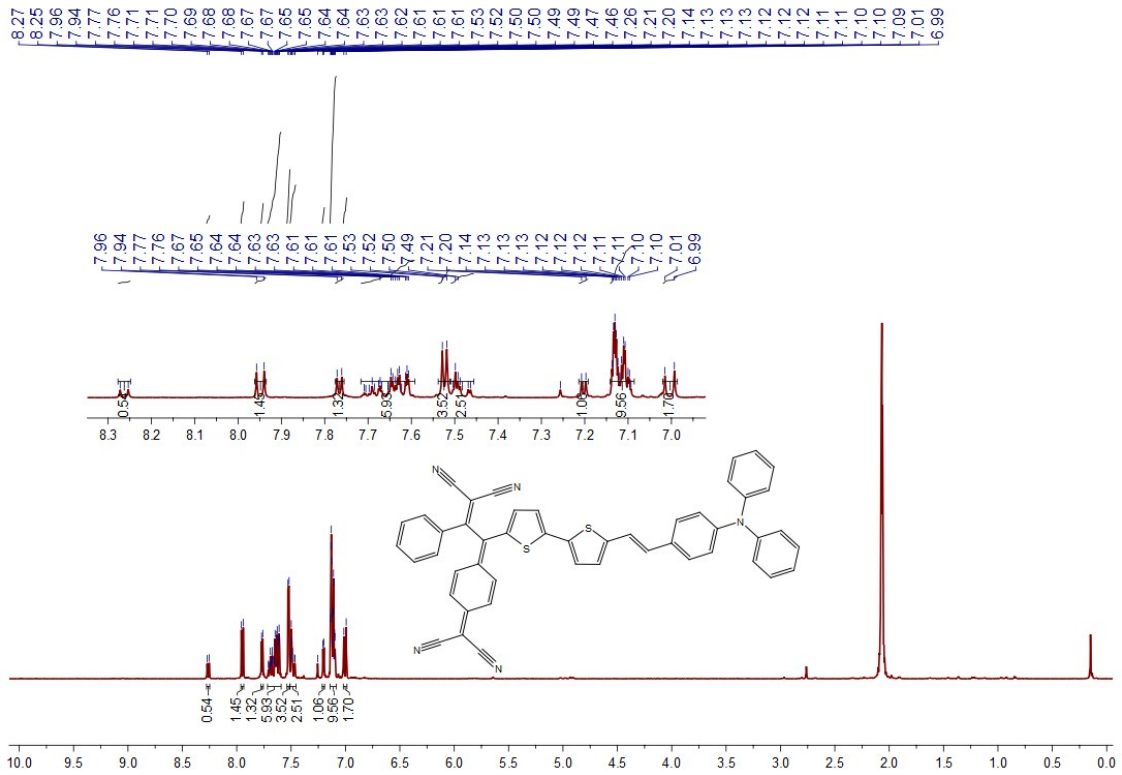


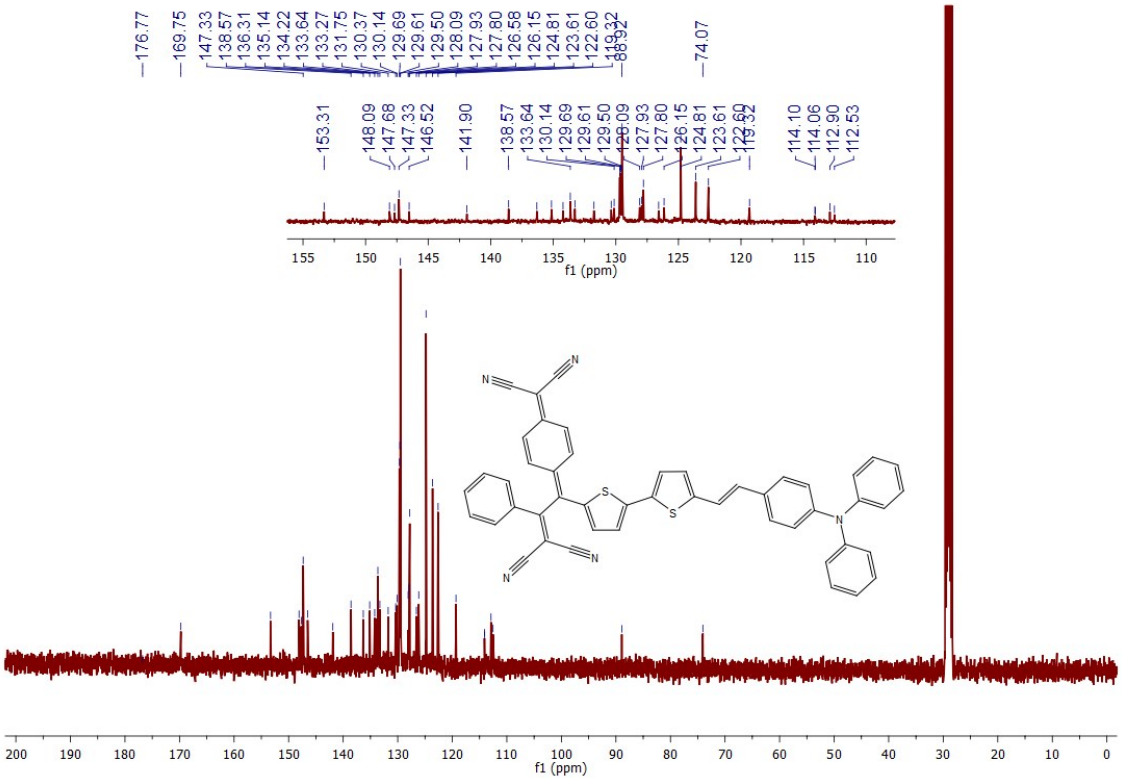
^{1}H NMR & ^{13}C NMR spectrum of compound 2a in Acetone-d_6



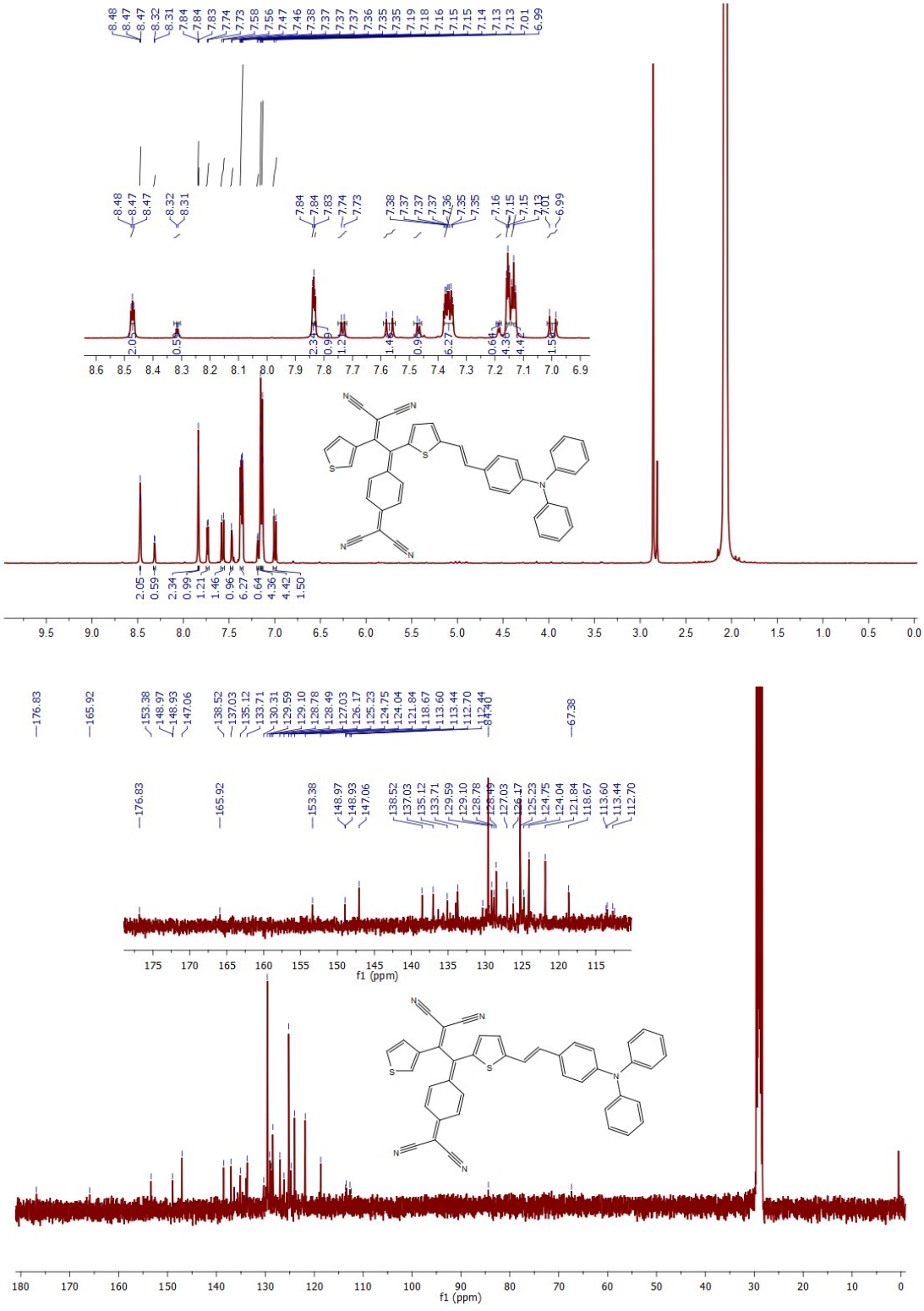


^{1}H NMR & ^{13}C NMR spectrum of compound 2b in Acetone-d_6

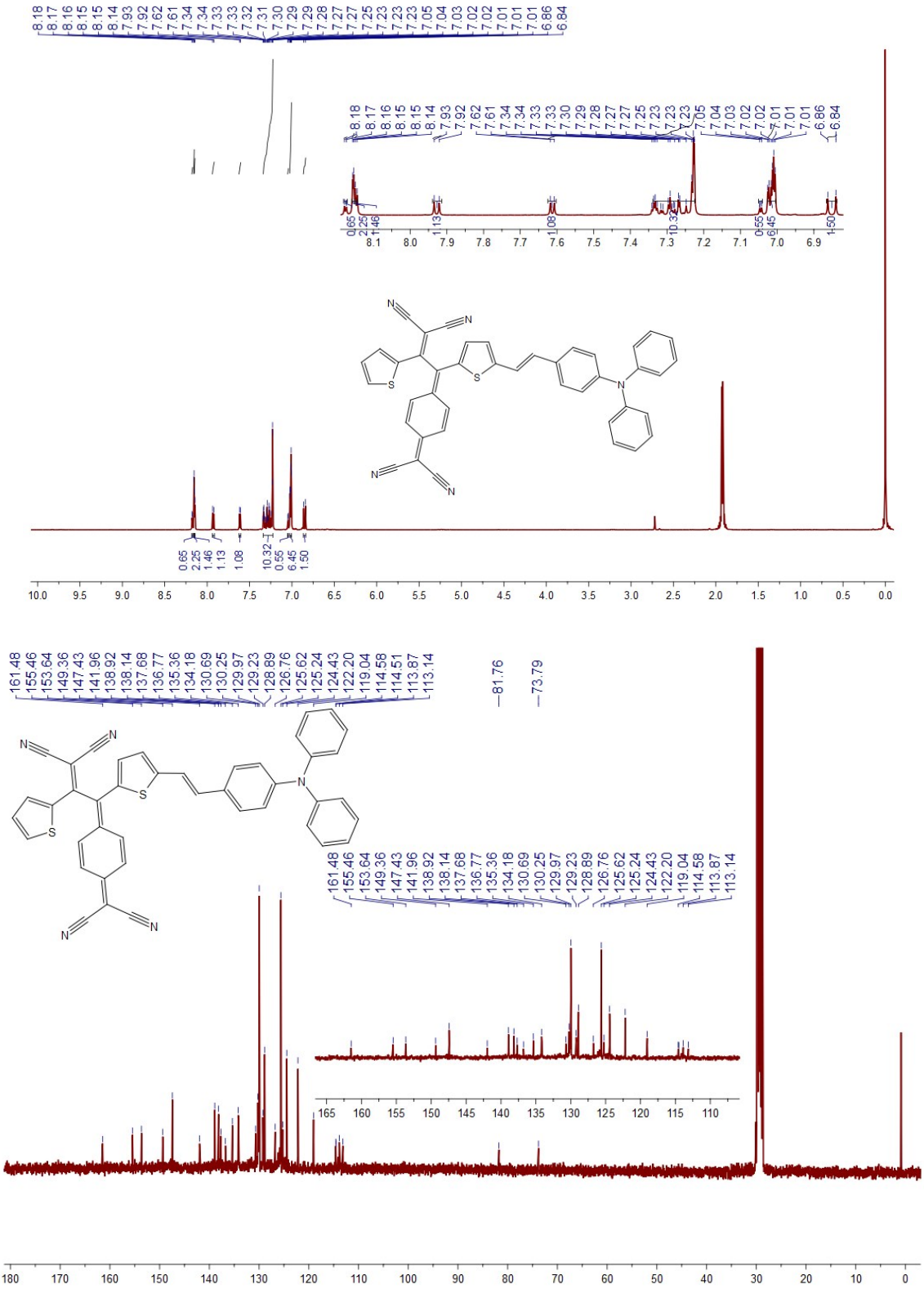




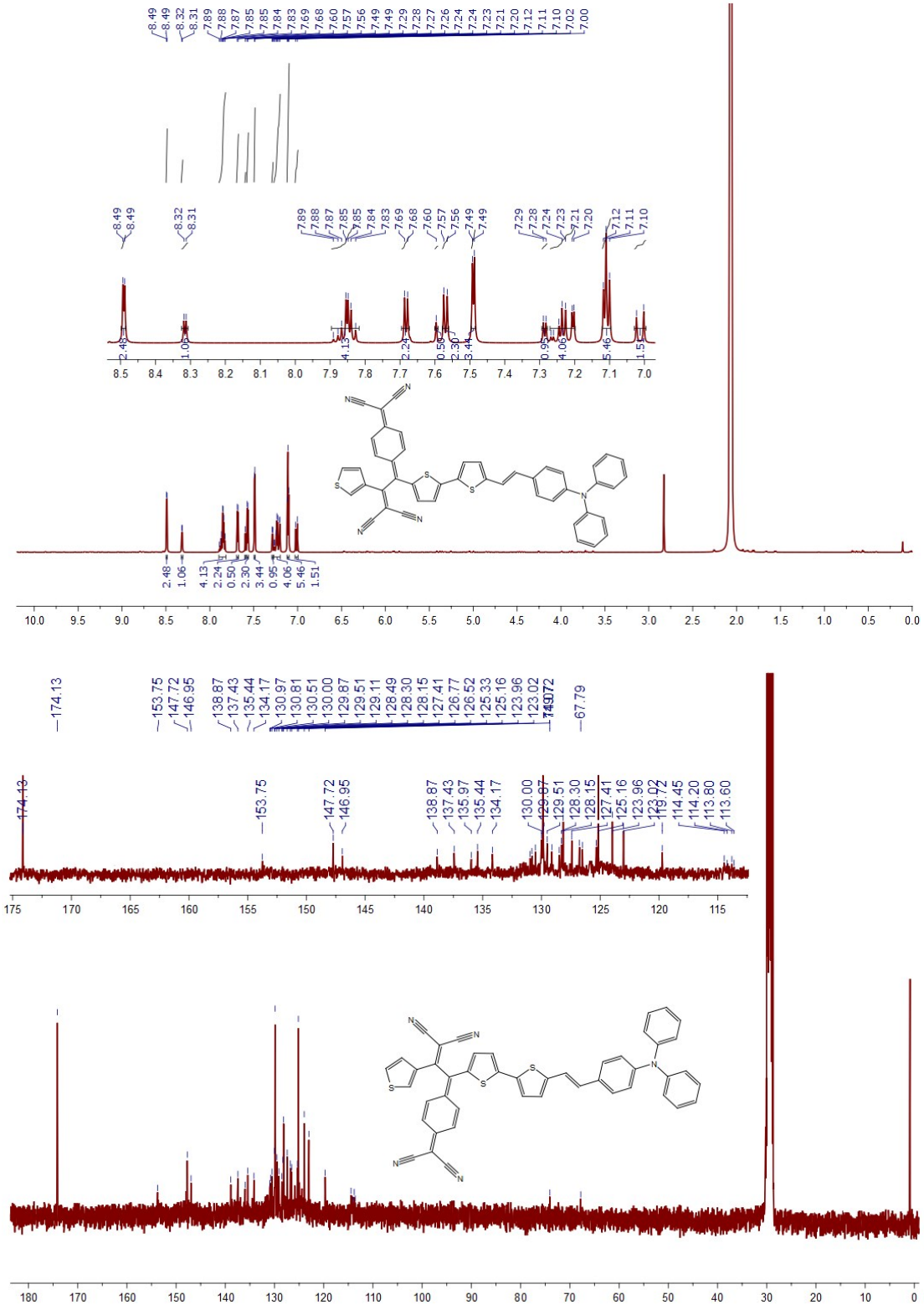
^{1}H NMR & ^{13}C NMR spectrum of compound 2c in Acetone-d_6



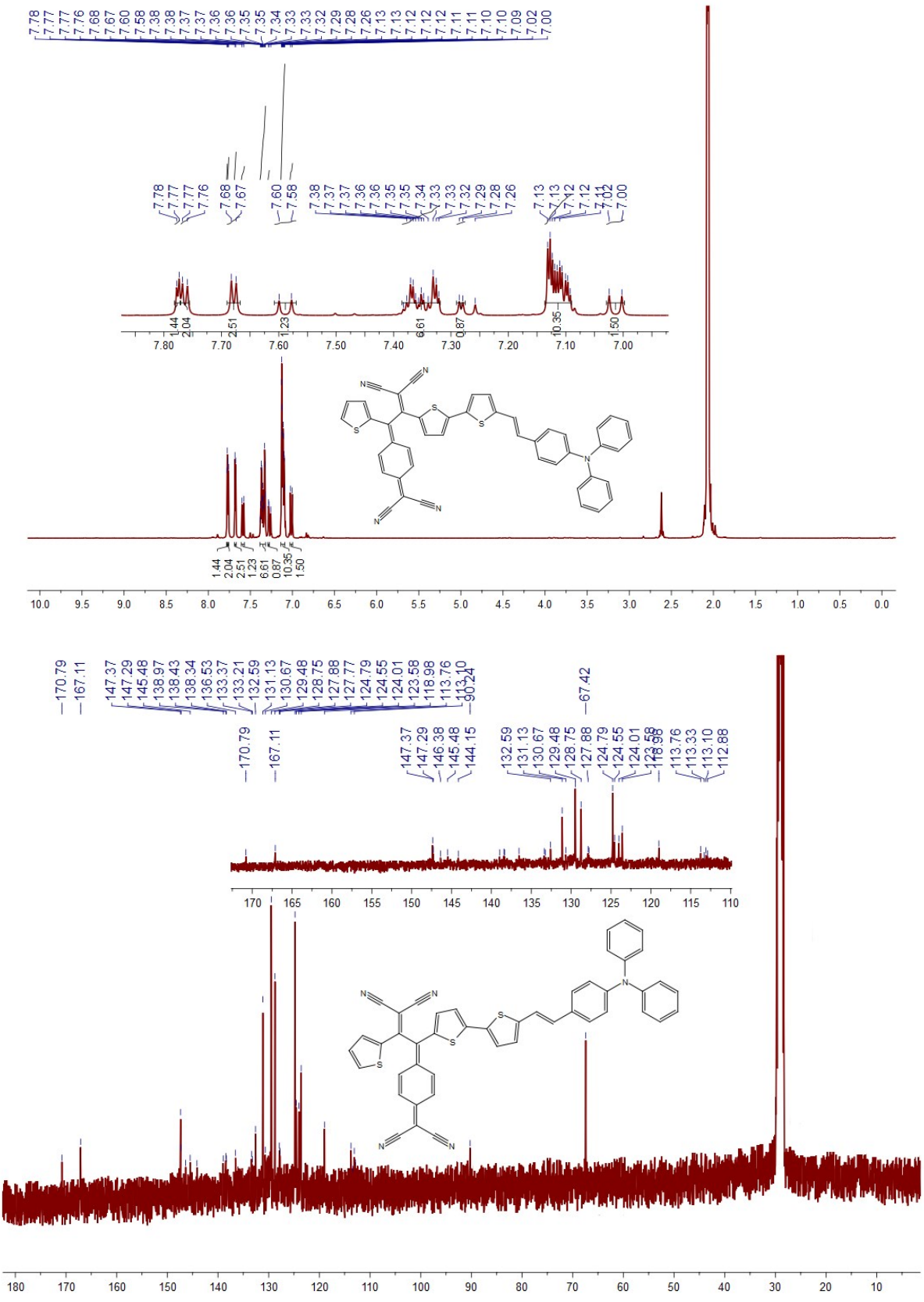
^{1}H NMR & ^{13}C NMR spectrum of compound 2d in Acetone-d_6



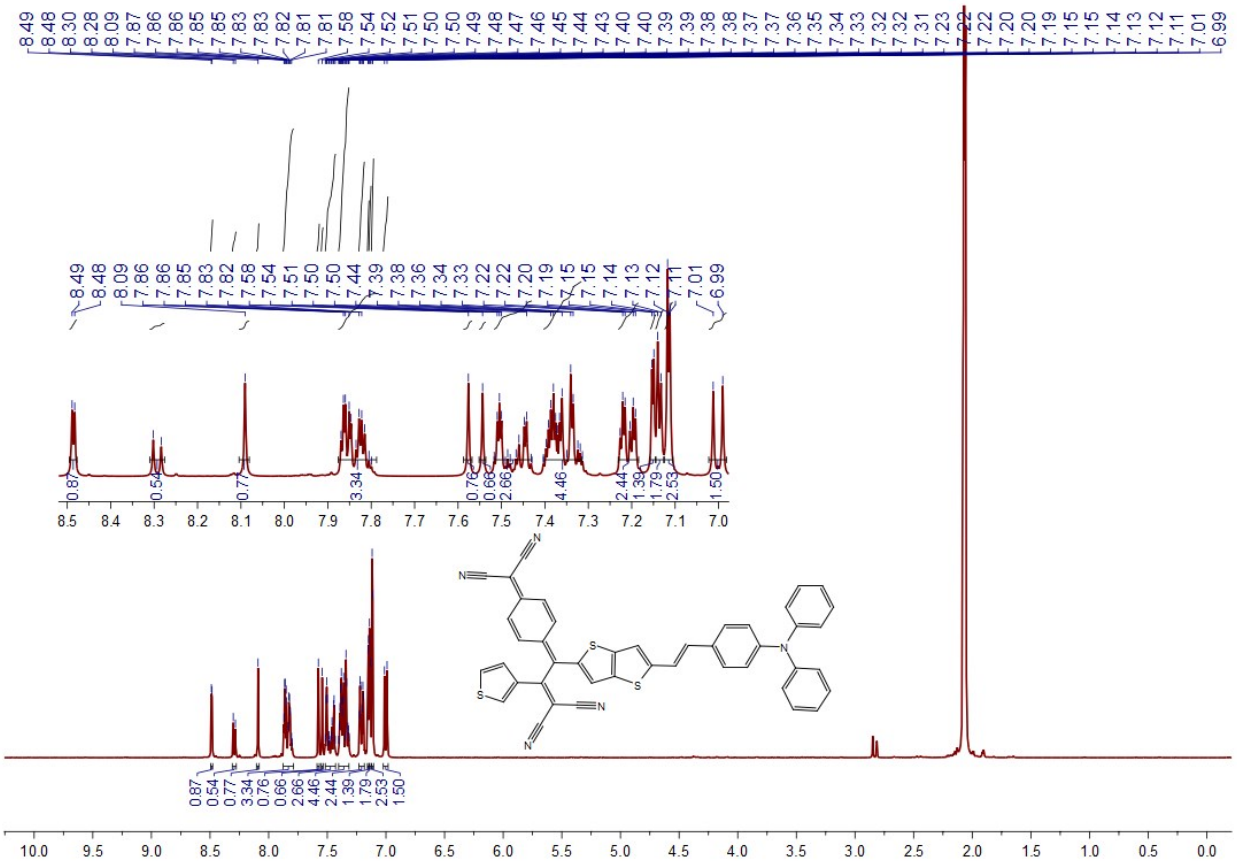
^{1}H NMR & ^{13}C NMR spectrum of compound 2e in Acetone-d_6

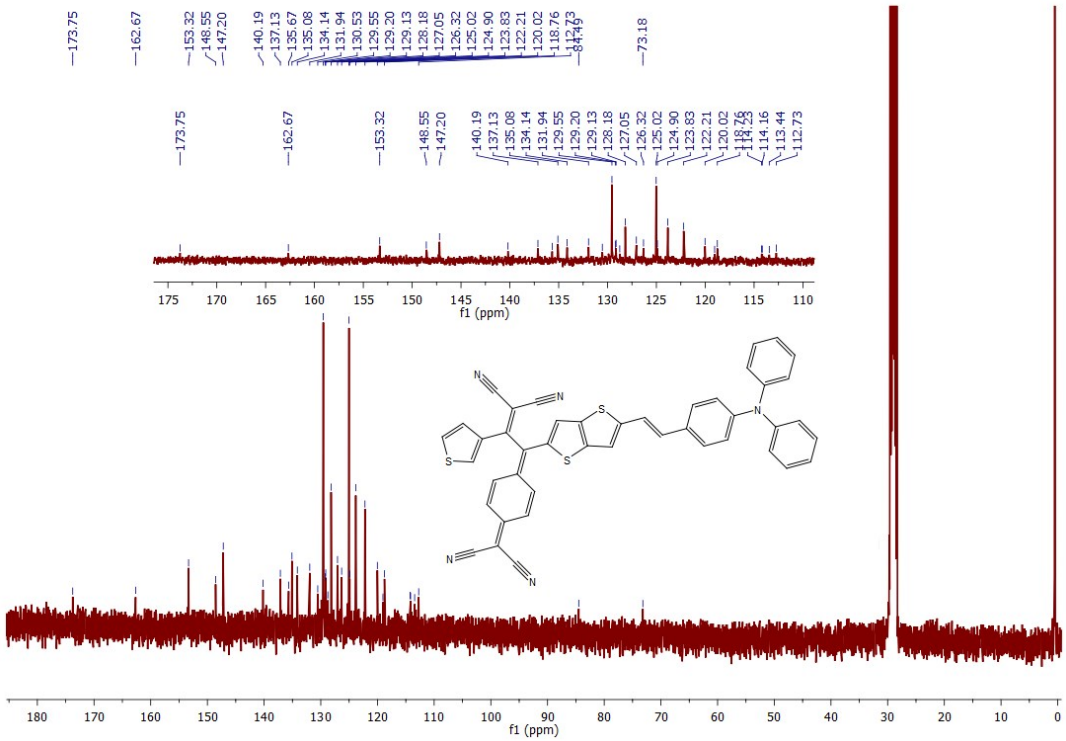


^{1}H NMR & ^{13}C NMR spectrum of compound 2f in Acetone-d_6

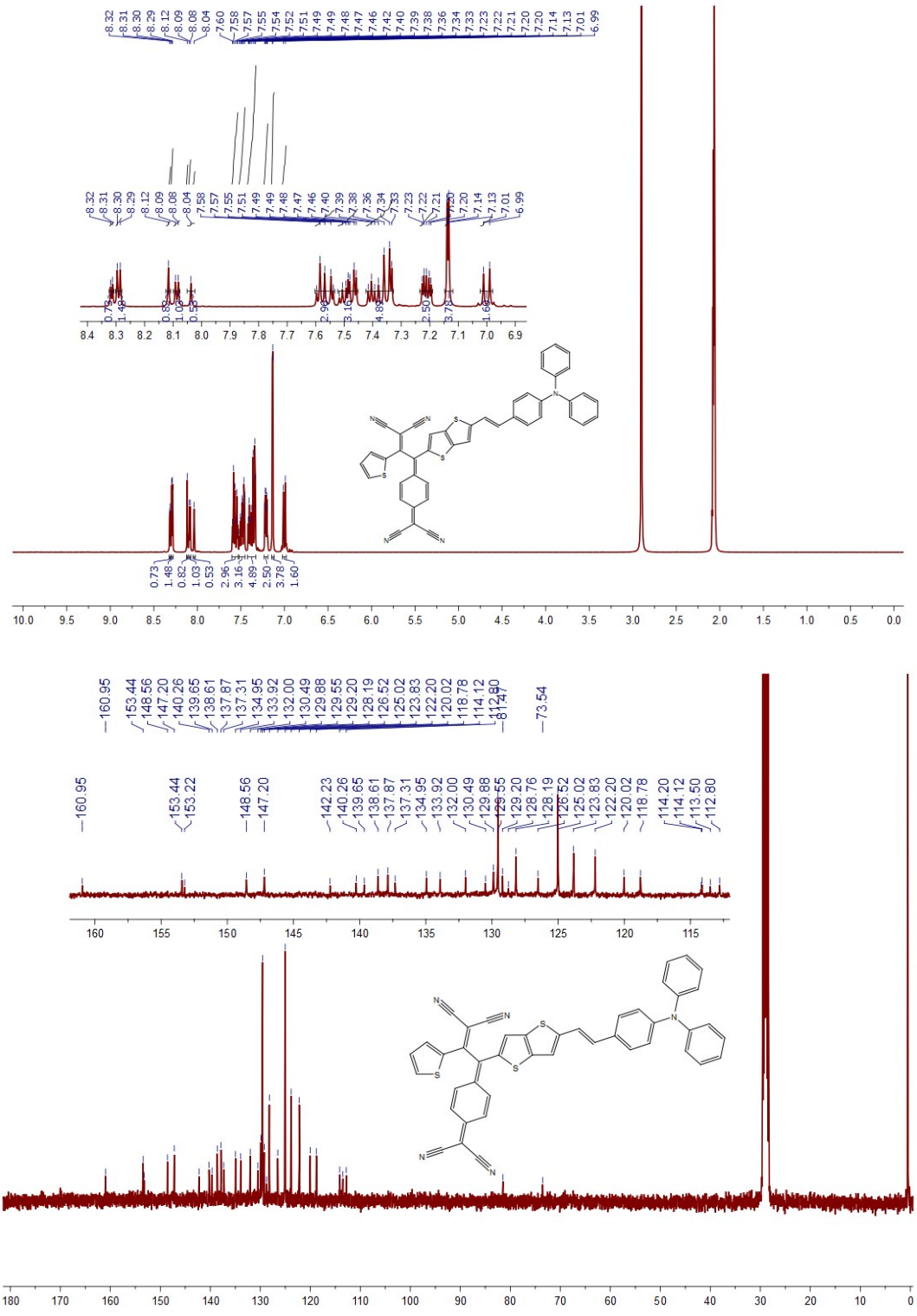


^{1}H NMR & ^{13}C NMR spectrum of compound 2g in Acetone-d_6

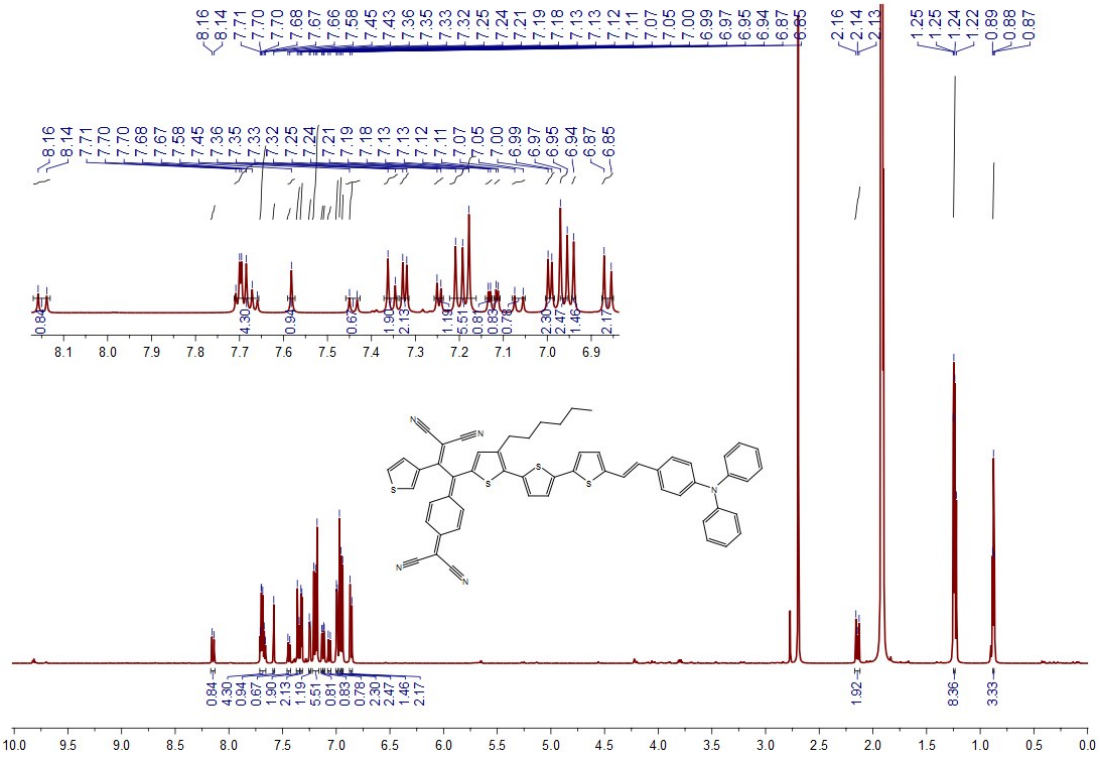


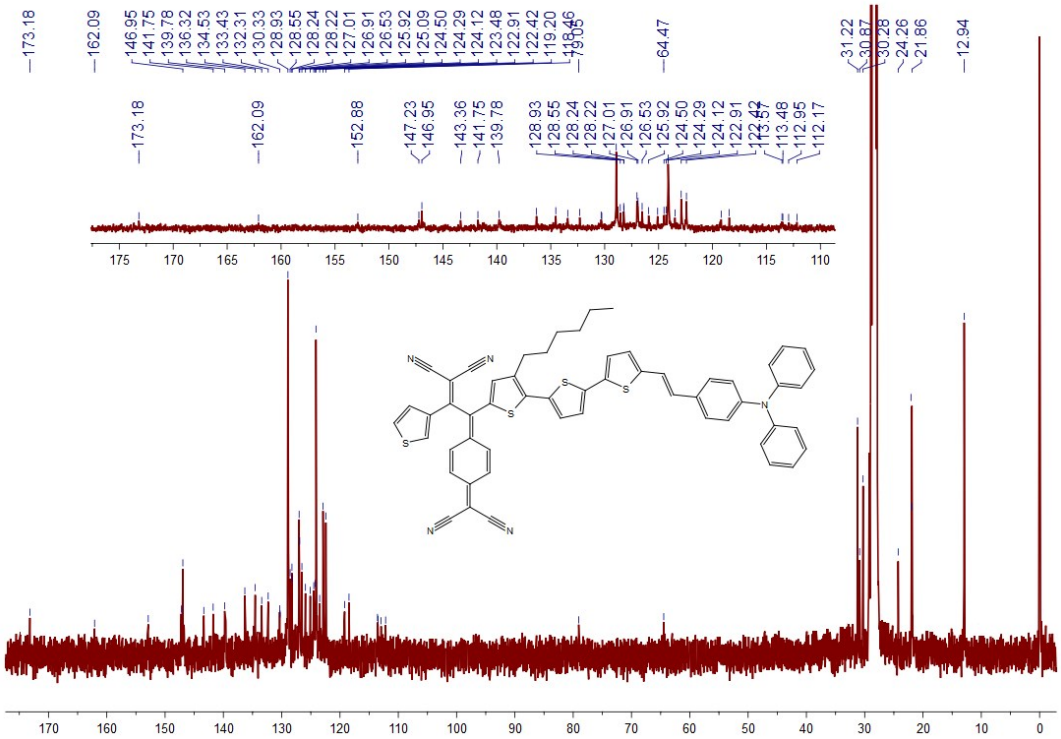


^{1}H NMR & ^{13}C NMR spectrum of compound 2h in Acetone-d_6



^{1}H NMR & ^{13}C NMR spectrum of compound PCR08 2i in Acetone-d_6





^{1}H NMR & ^{13}C NMR spectrum of compound 2j in Acentone-d_6

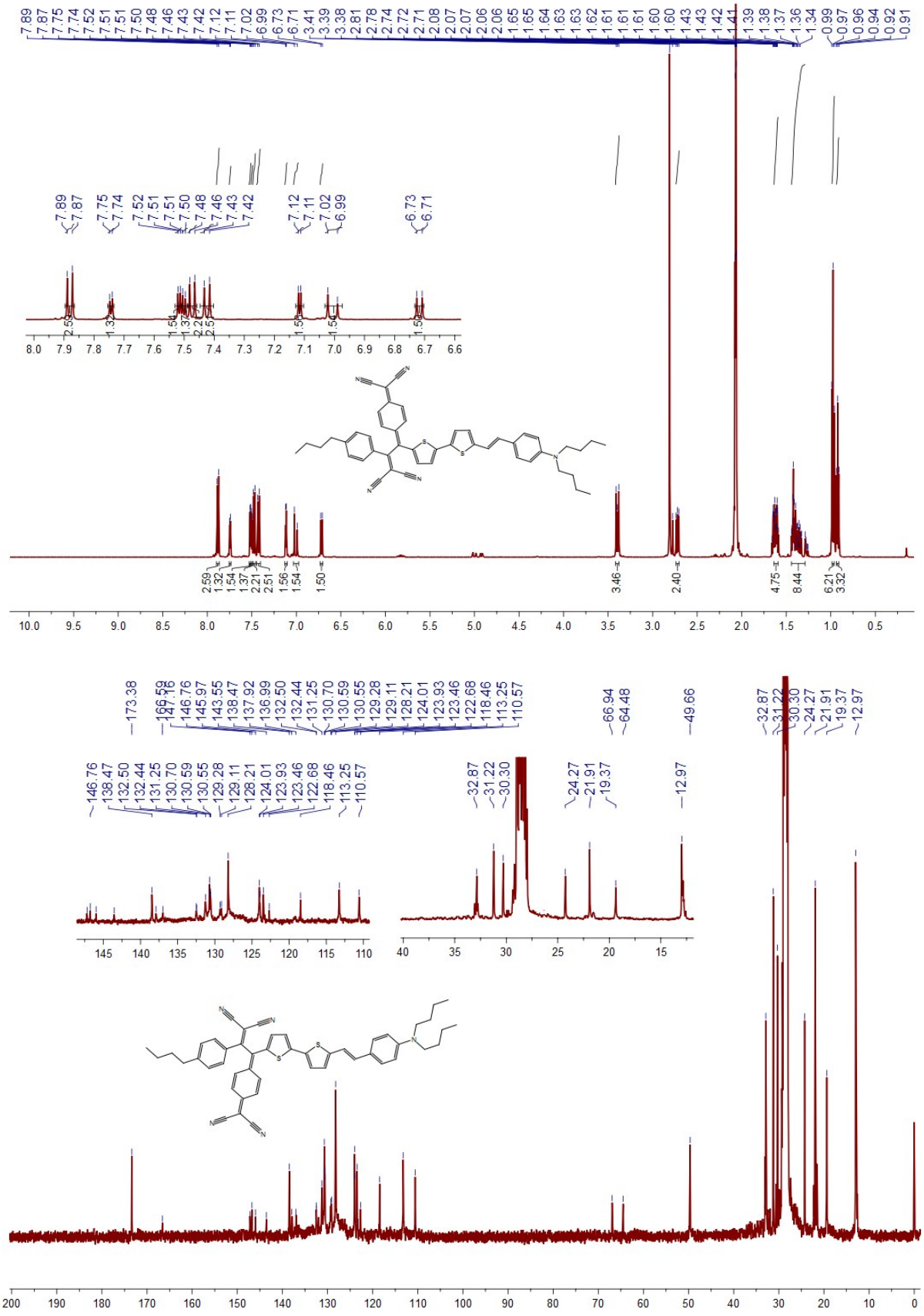
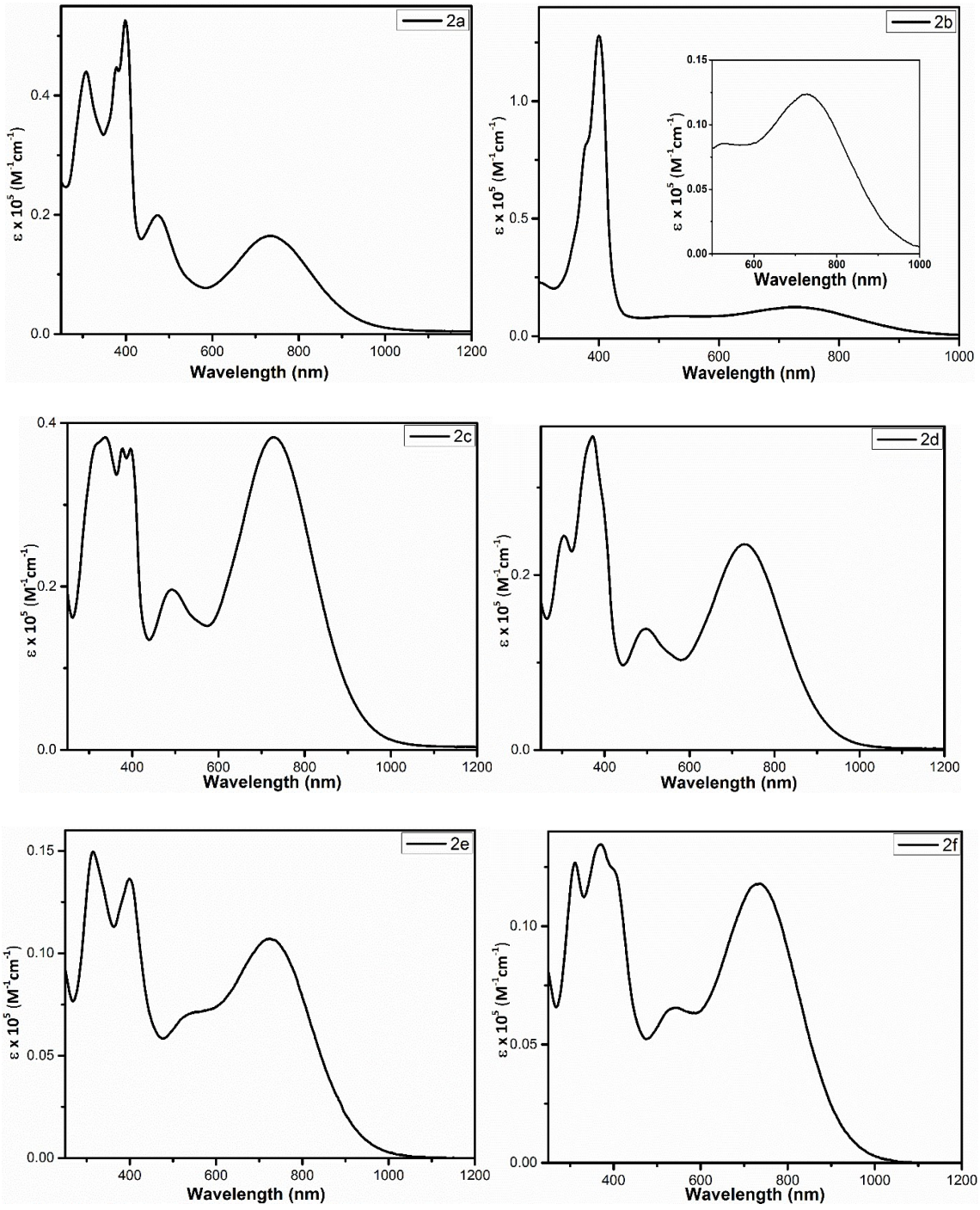
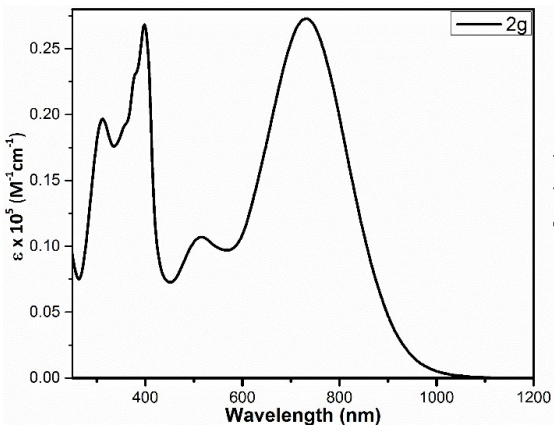
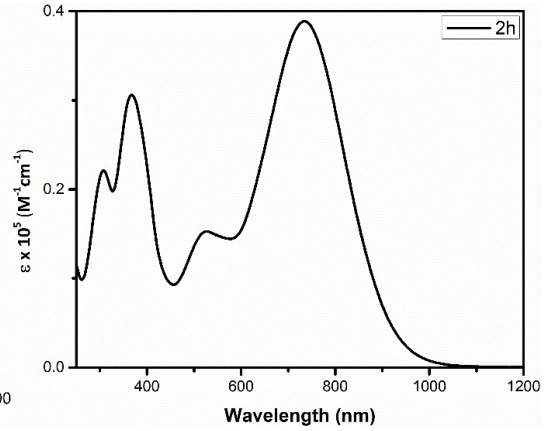
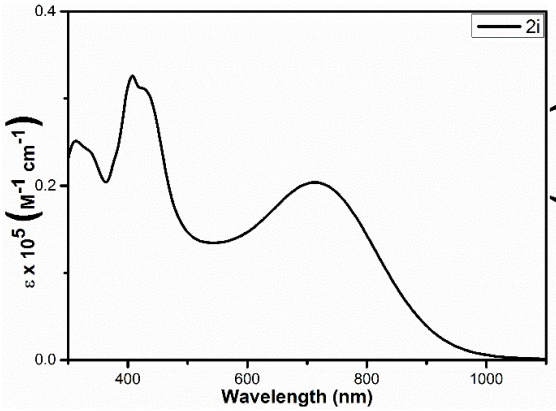


Fig S1: UV-vis individual spectra of compound **2a-j** in chloroform (C = 4.0 X 10^{-5} M)




2g
ε x 10^5 (M^-1cm^-1)
Wavelength (nm)


2h
ε x 10^5 (M^-1cm^-1)
Wavelength (nm)


2i
ε x 10^5 (M^-1 cm^-1)
Wavelength (nm)

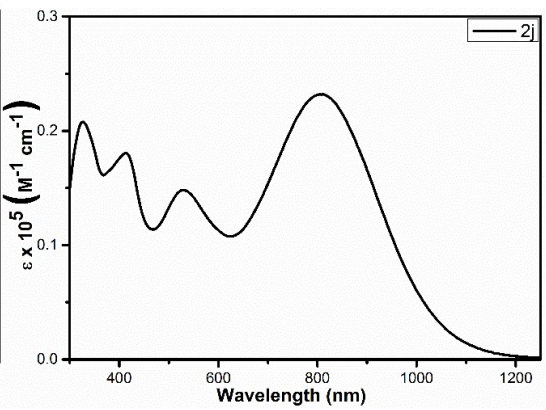
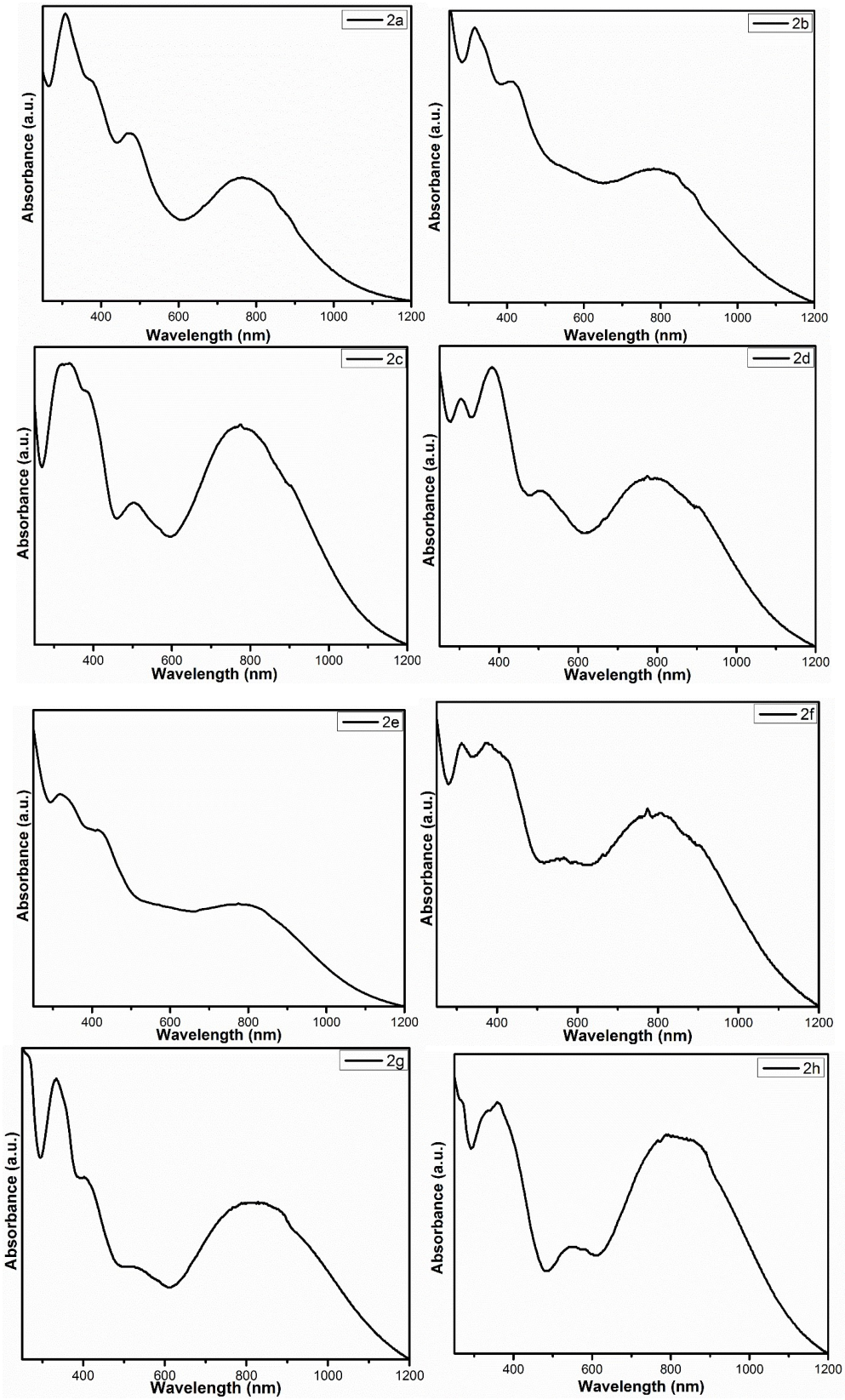

2j
ε x 10^5 (M^-1 cm^-1)
Wavelength (nm)

Fig S2: UV-vis individual spectra of compound **2a-j** as thin solid film



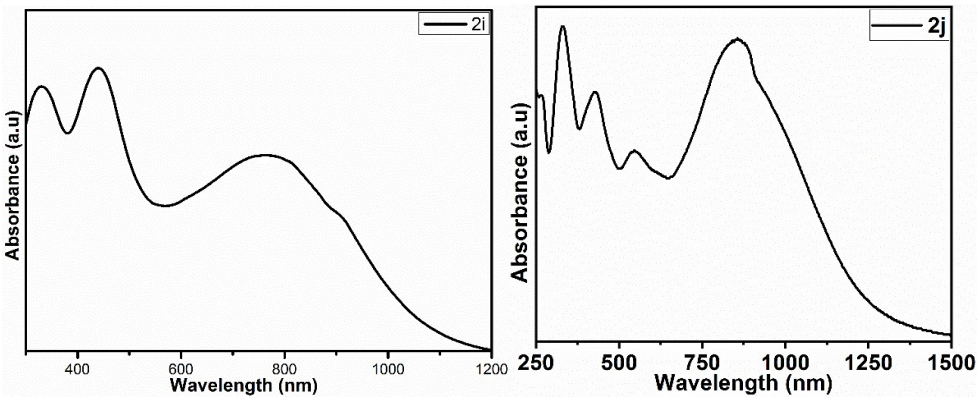

2i
Absorbance (a.u)
400
600
800
1000
1200
Wavelength (nm)
2j
Absorbance (a.u)
250
500
750
1000
1250
1500
Wavelength (nm)

Fig S3: UV-vis spectra of **1i**, **1j** in chloroform (C = 4 x 10^{-5} M)

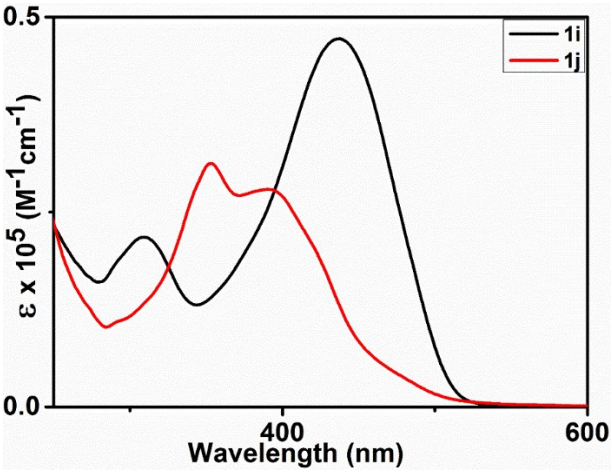


Fig S4: PL spectra of **1i** and **1j** in chloroform (C = 4 x 10^{-5} M)

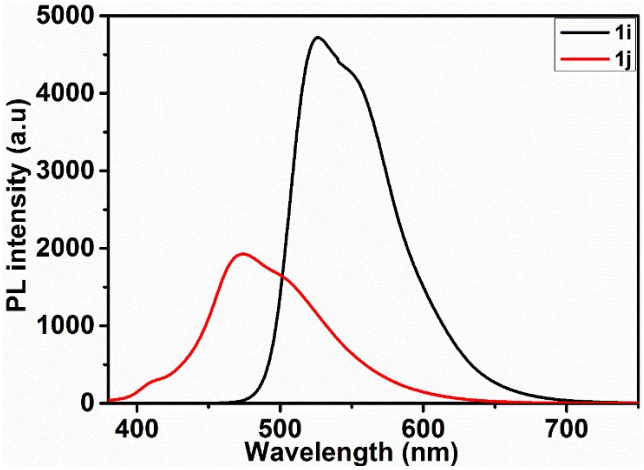
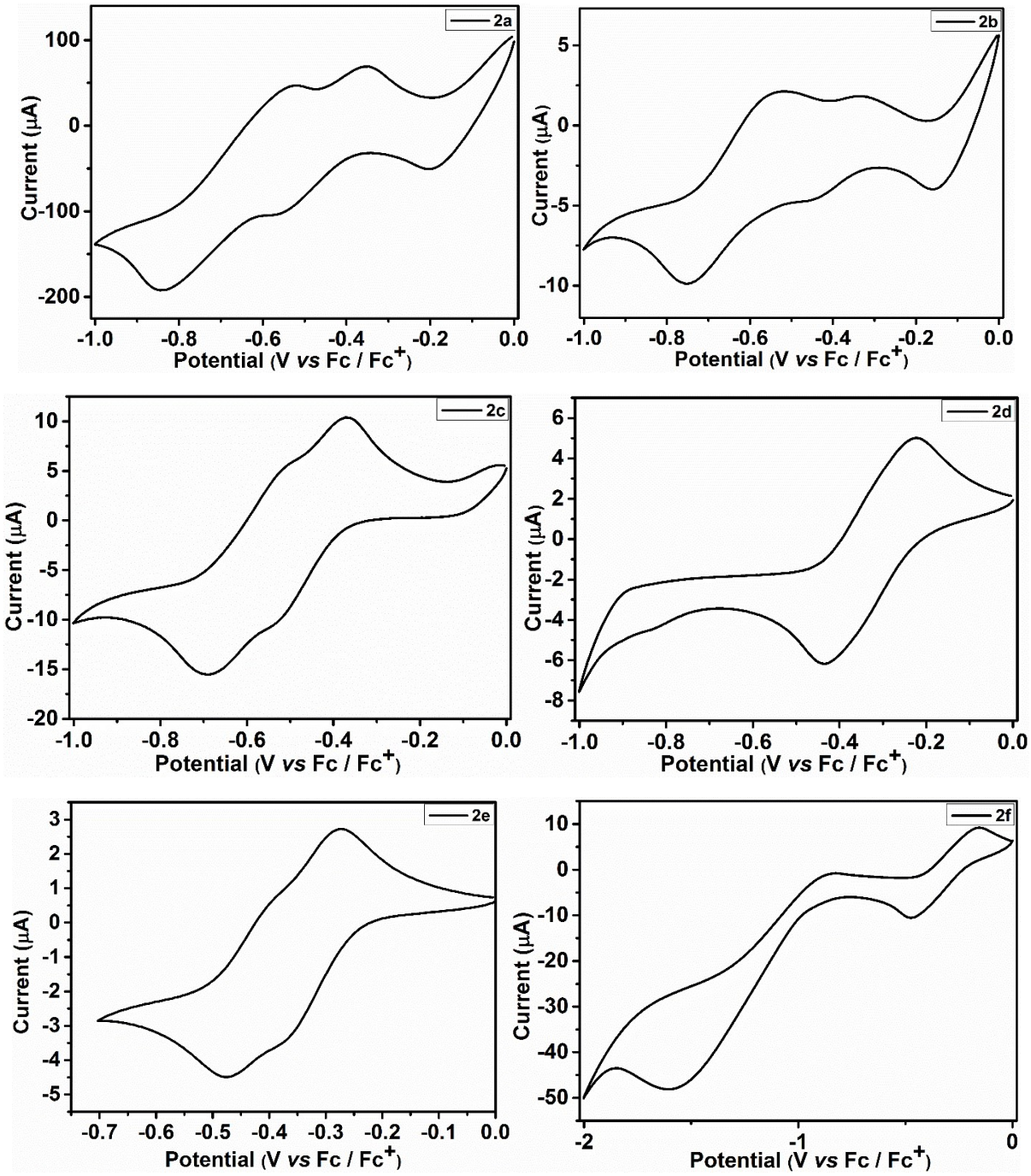


Table S2: Photophysical data of **1i** and **1j**

Intermediates	λ_{max} / λ_{onset} (nm)[a]	ε ($M^{-1}cm^{-1}$)	E_g^{opt} (eV)[b]	λ_{em} (nm)[c]	Φ (%)[d]
1i	436 / 507	47250	2.44	525	23.2
1j	390 / 466	27950	2.66	473	18.7
[a]Absorption in chloroform solution (C = 4.0 × 10^{-5} M); [b]Optical band gap was determined from λ_{onset} in chloroform using Eg^{opt} (eV) = 1240/λ_{onset}; [c]Emission in solution; [d]Quantum yields were measured using quinine sulphate (Φ = 55%) as reference					

Fig S5: Cyclic Voltammagram of **2a-j**



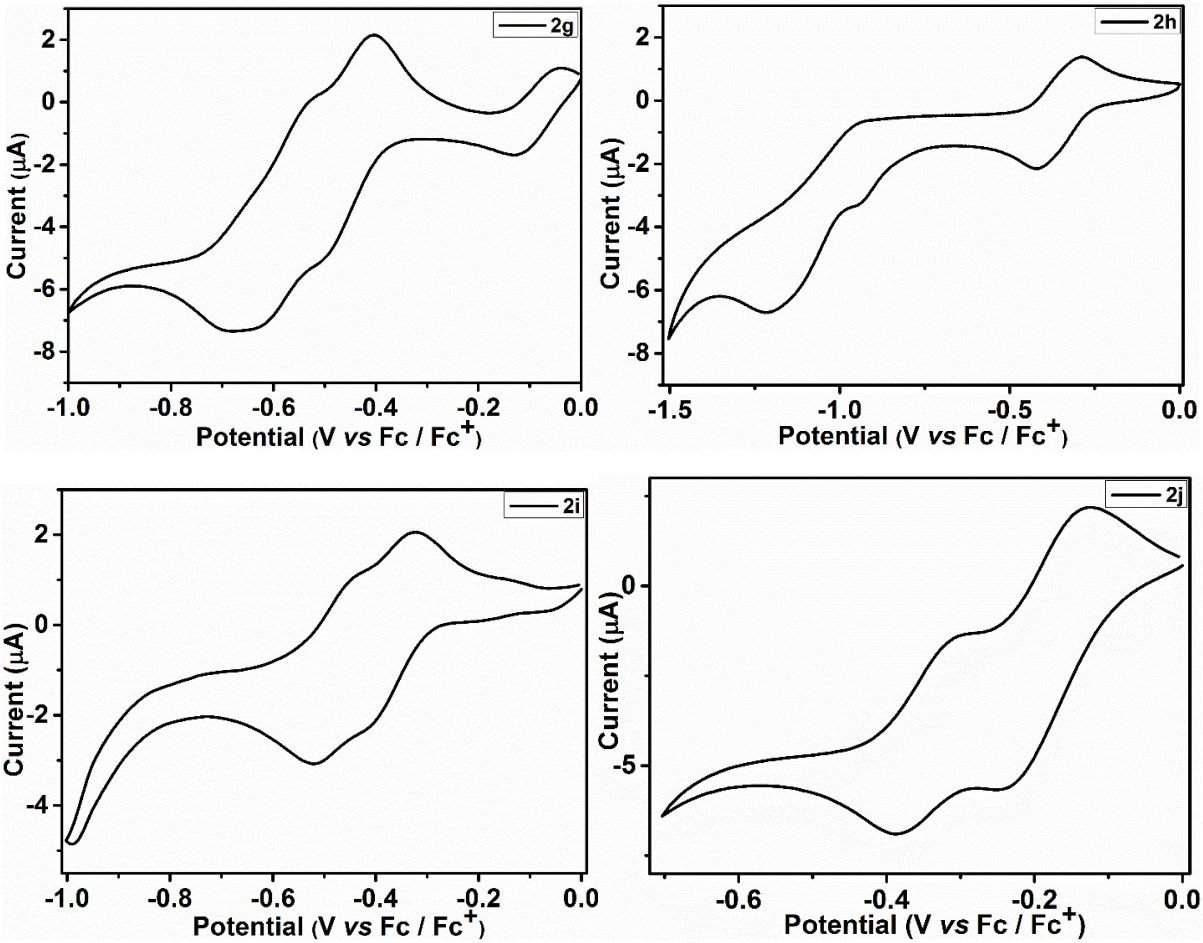
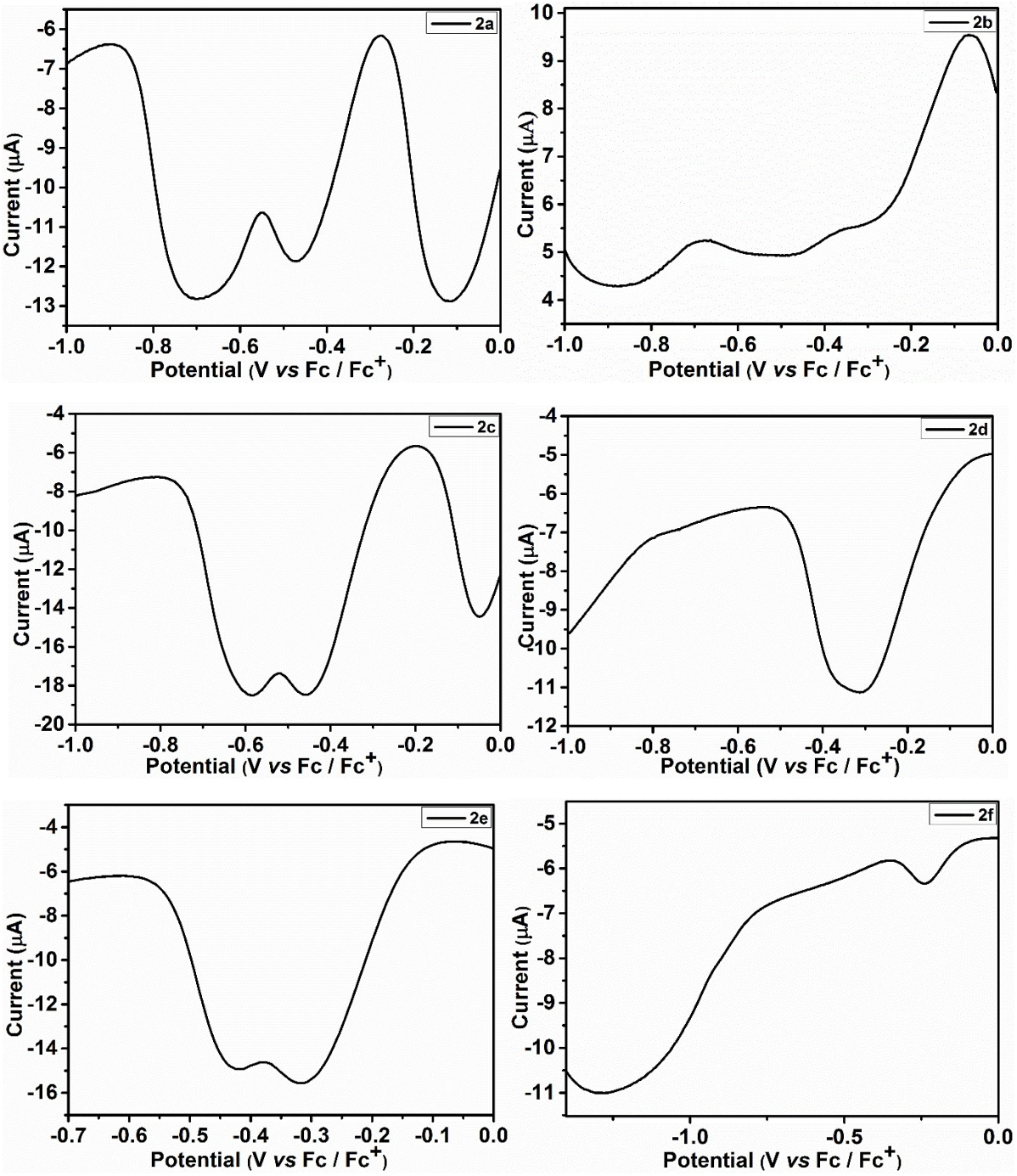

2g
2h
2i
2j
Current (μA)
Potential (V vs Fc / Fc+)

Fig S6: Differential Pulse Voltammagram of **2a-j**



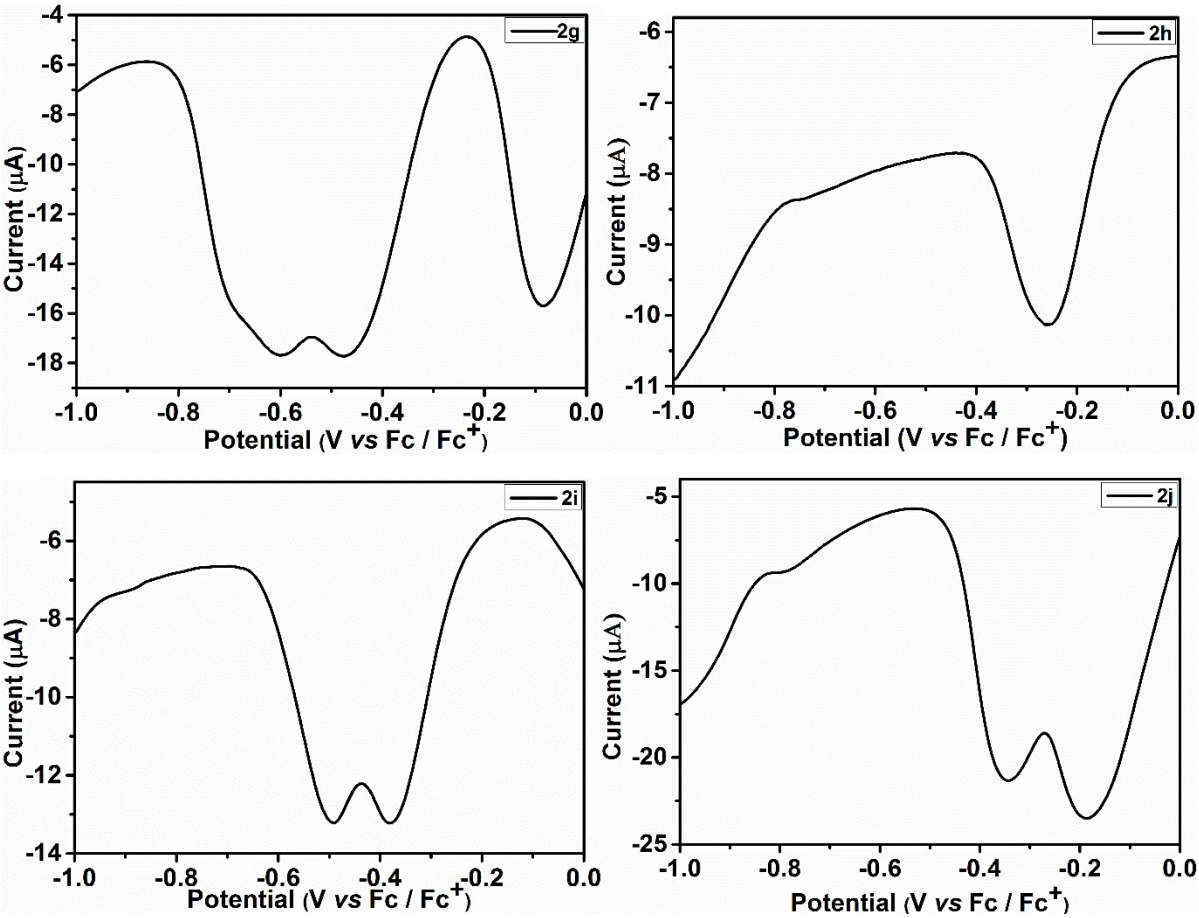
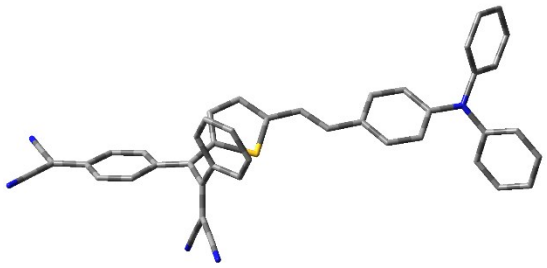
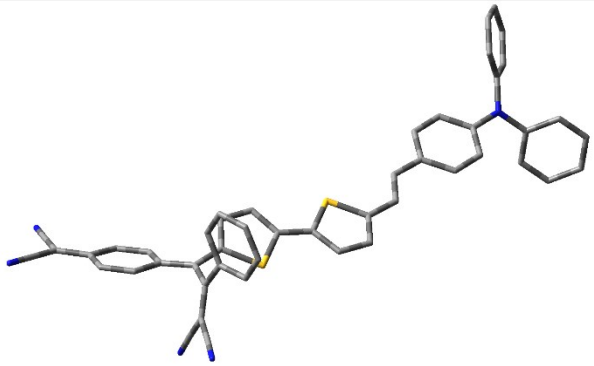
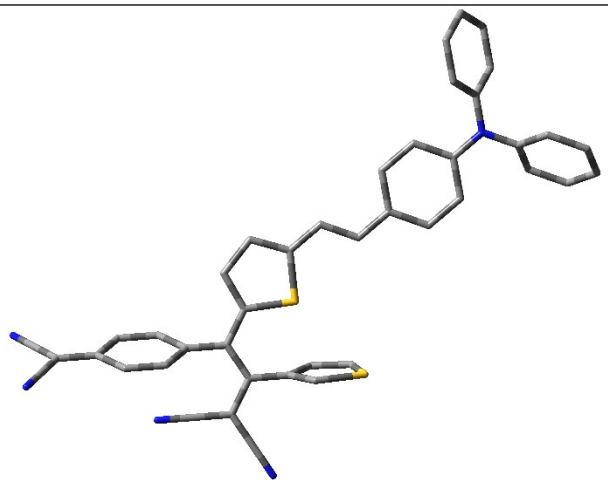
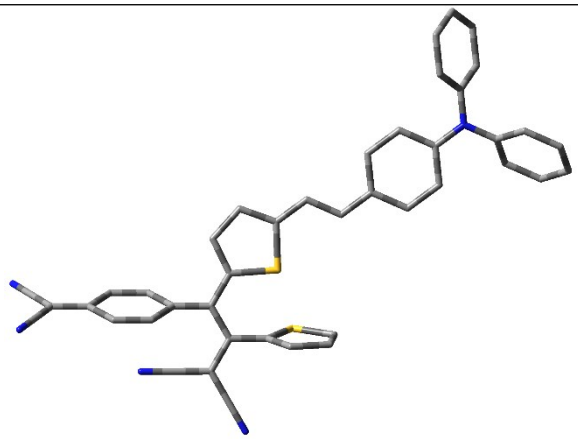
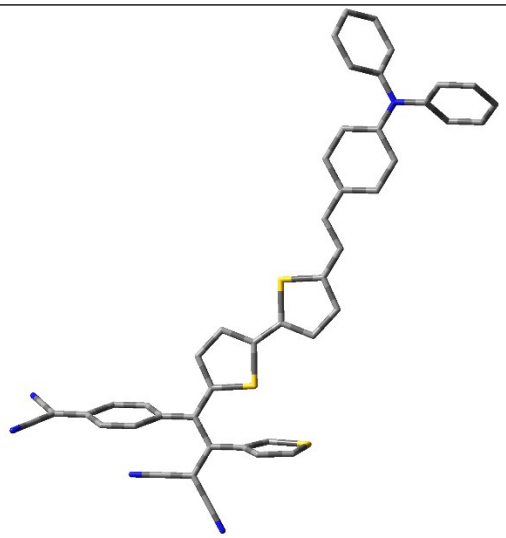
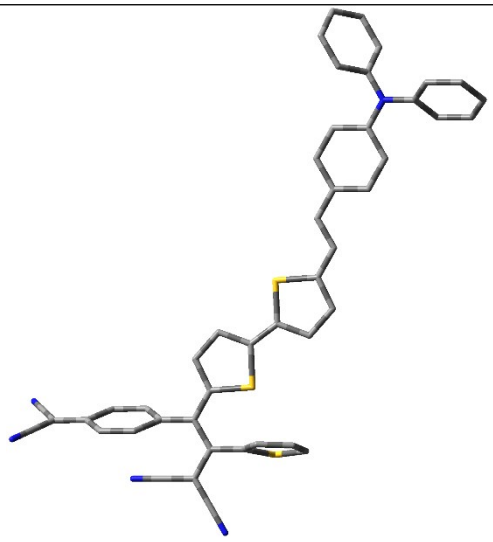
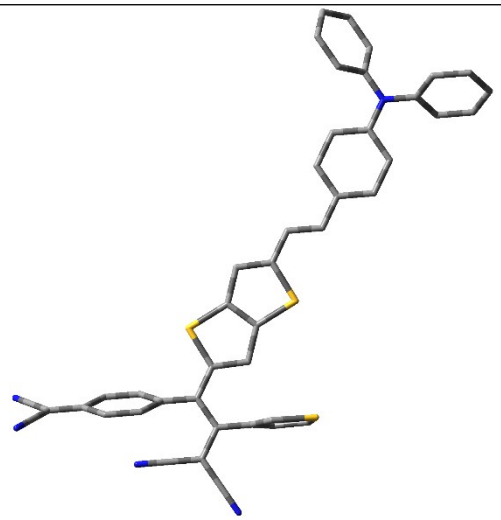
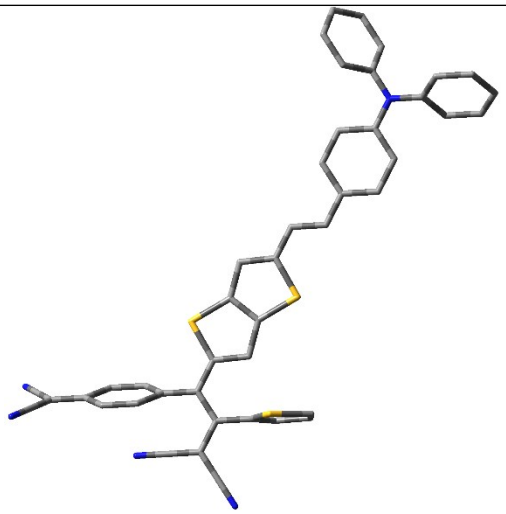
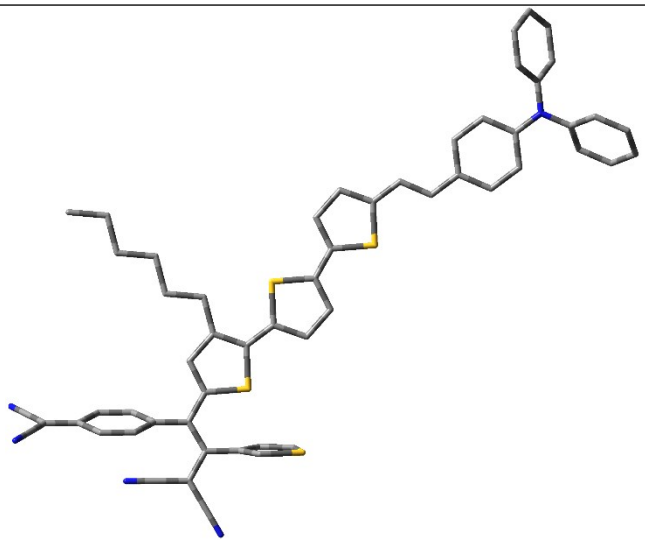

2g
2h
2i
2j
Current (μA)
Potential (V vs Fc / Fc+)

Table S3: Energy minimized structure, selected bond lengths and dihedral angle of the DCNQ moiety of **2a-2j** in gas phase

2a-j	Optimized Geometry*	Bond length (Å)		*Θ*	Conformation
		BL_{SD}	BL_{SA}		
2a		1.4349	1.4363	68.04	*synclinal*
2b		1.4374	1.4368	67.28	*synclinal*
2c		1.4342	1.4342	76.28	*synclinal*

2d		1.4343	1.4335	80.47	*synclinal*
2e		1.4372	1.4348	74.02	*synclinal*
2f		1.4372	1.4337	80.31	*synclinal*

2g		1.4350	1.4337	80.13	*synclinal*
2h		1.4351	1.4345	81.01	*synclinal*
2i		1.4389	1.4340	75.59	*synclinal*

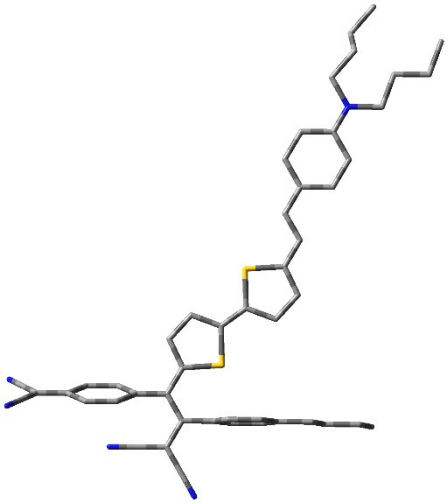
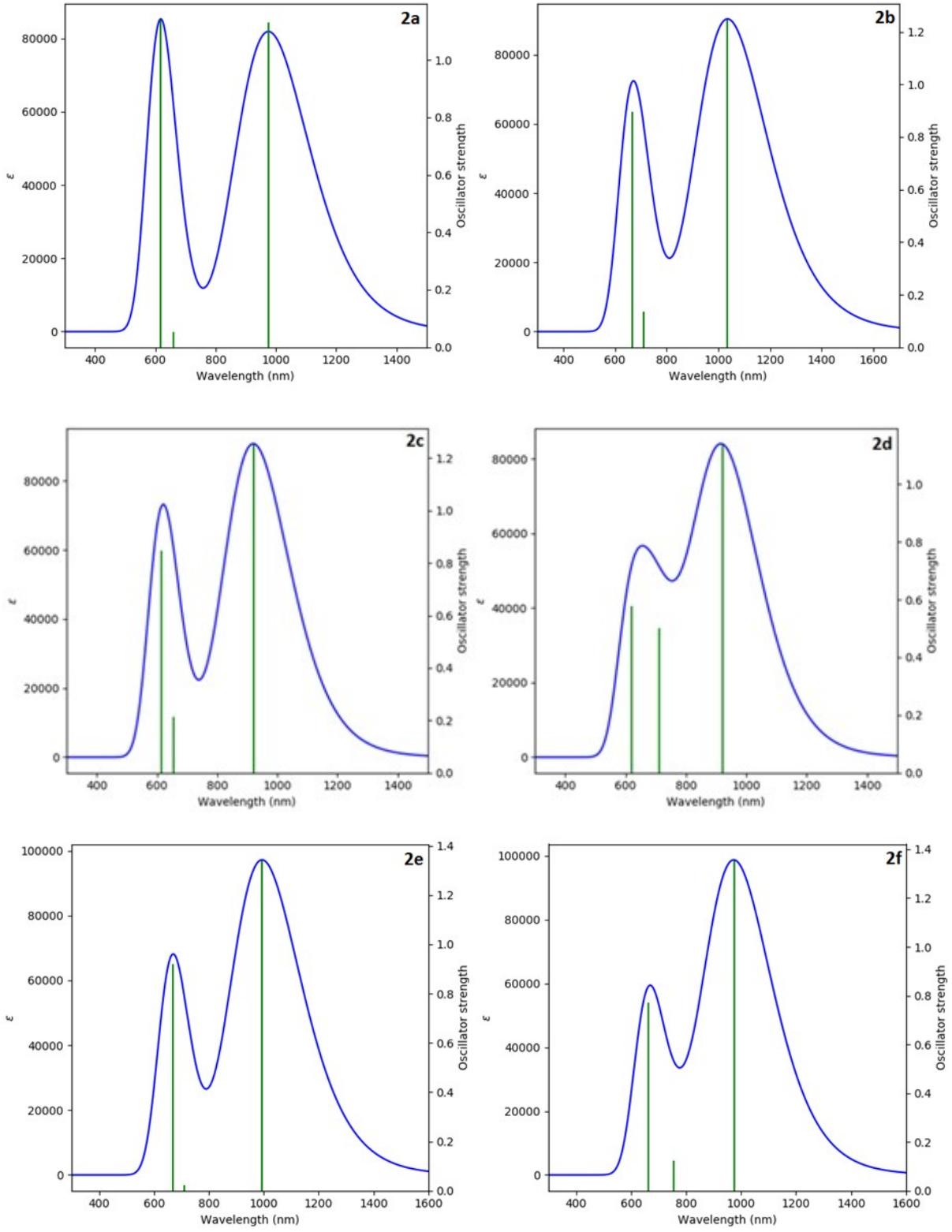
2j		1.4368	1.4354	67.79	*synclinal*
*Ground-state structures showing the orthogonality between $=C(CN)_2$ and DCNQ groups (Hydrogen atoms are omitted for clarity); BL_{SD} = Bond length between spacer and donor; BL_{SA} = Bond length between spacer and acceptor					

Fig S7: Simulated electronic spectra of **2a-2j** in chloroform



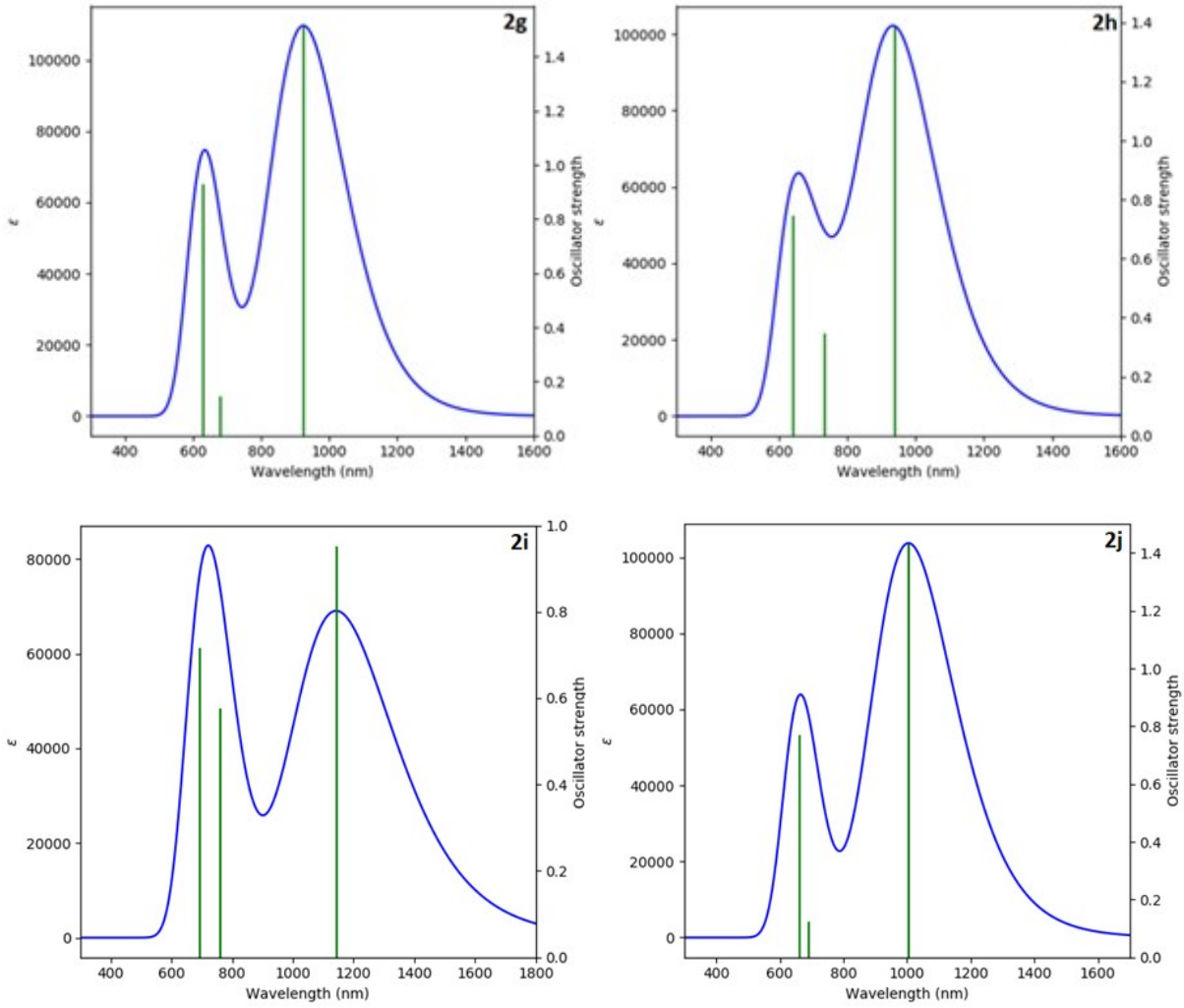
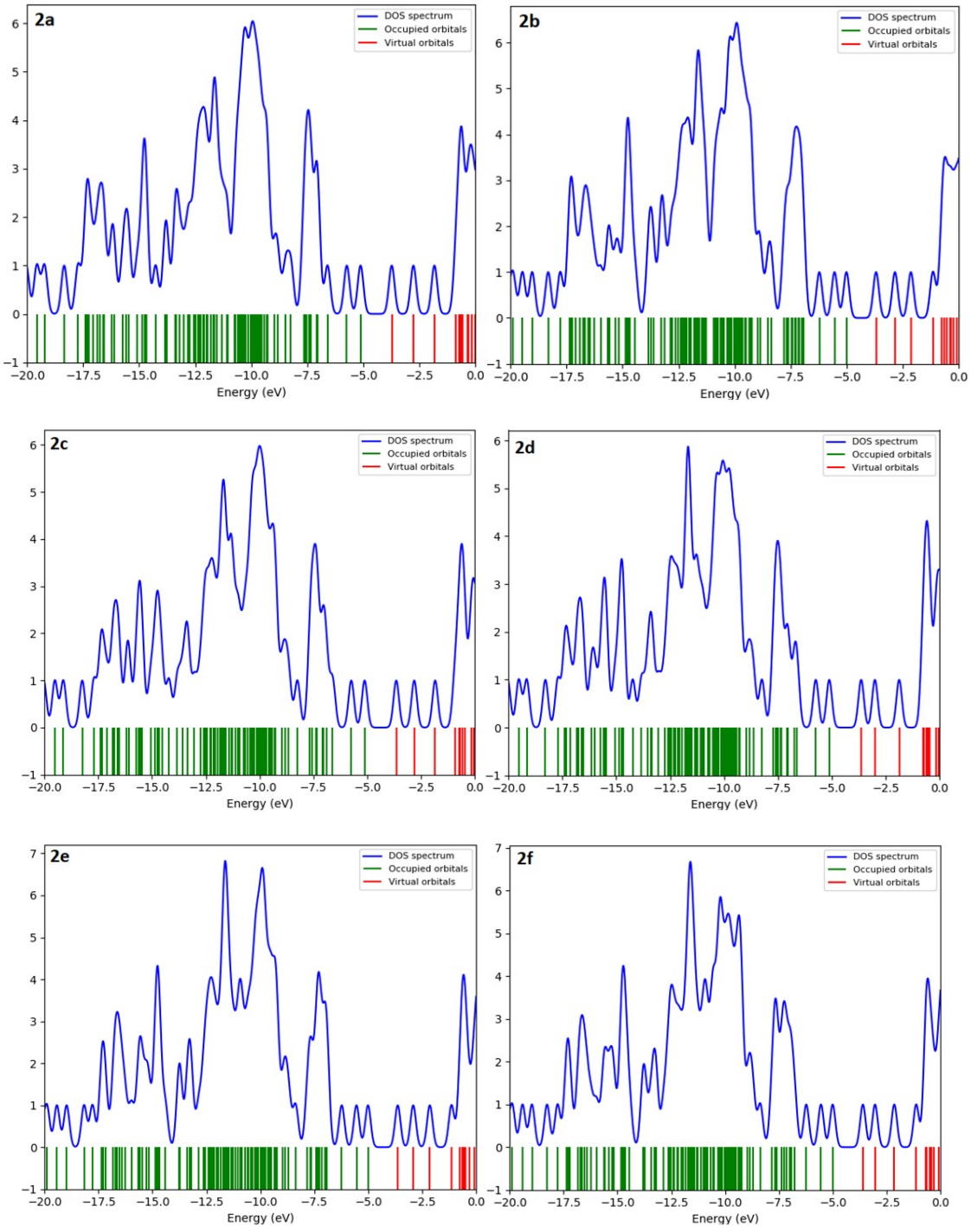

2g
2h
2i
2j
ε
Oscillator strength
Wavelength (nm)

Fig S8: Total density of states (TDOS) of **2a-2j**



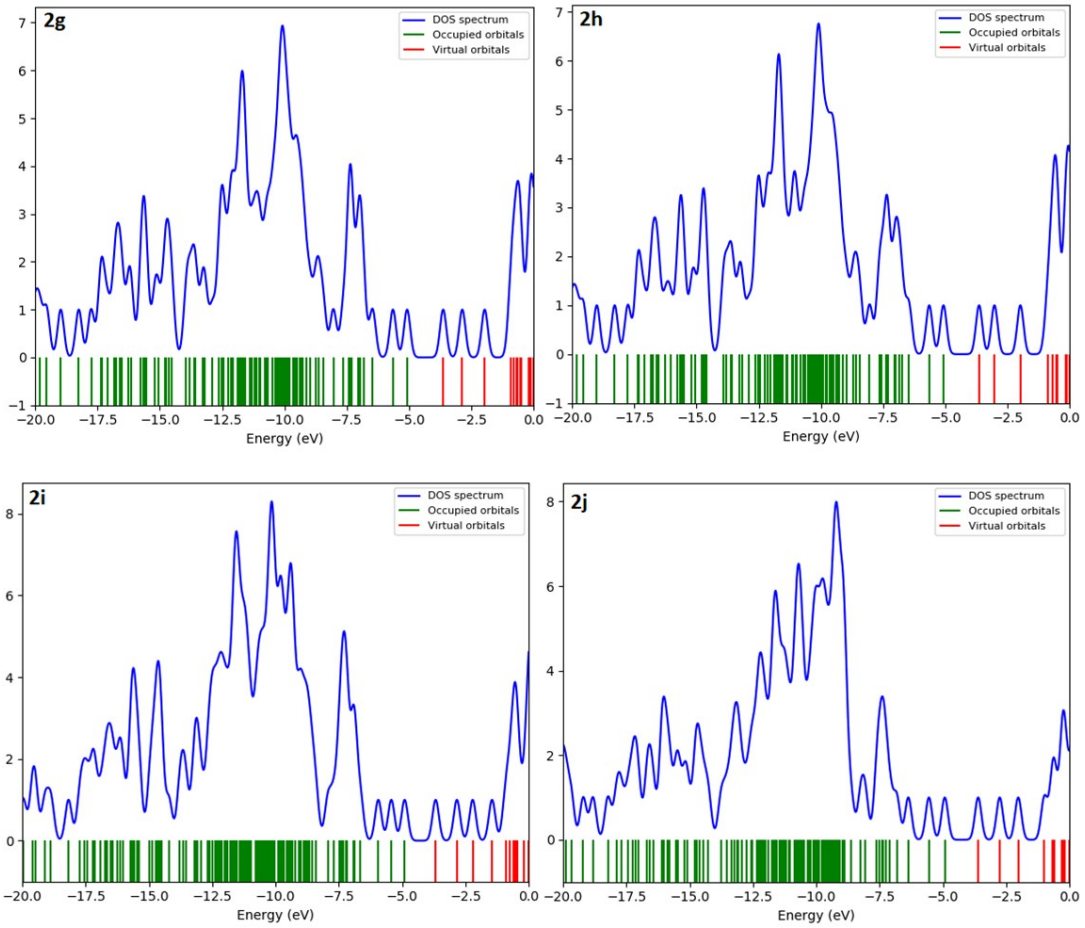

2g
DOS spectrum
Occupied orbitals
Virtual orbitals
Energy (eV)
2h
DOS spectrum
Occupied orbitals
Virtual orbitals
Energy (eV)
2i
DOS spectrum
Occupied orbitals
Virtual orbitals
Energy (eV)
2j
DOS spectrum
Occupied orbitals
Virtual orbitals
Energy (eV)

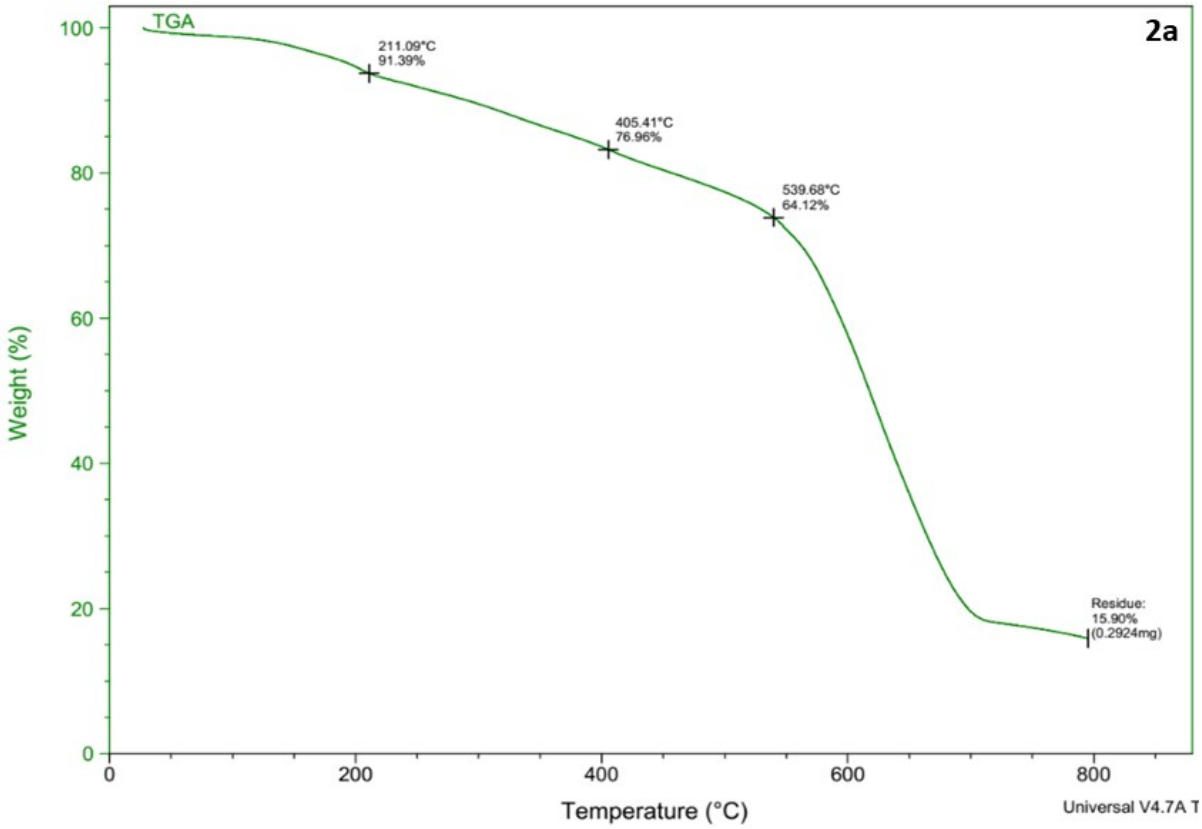
Table S4: Computed absorption spectral data of **2a-2j** obtained on TD-DFT in chloroform

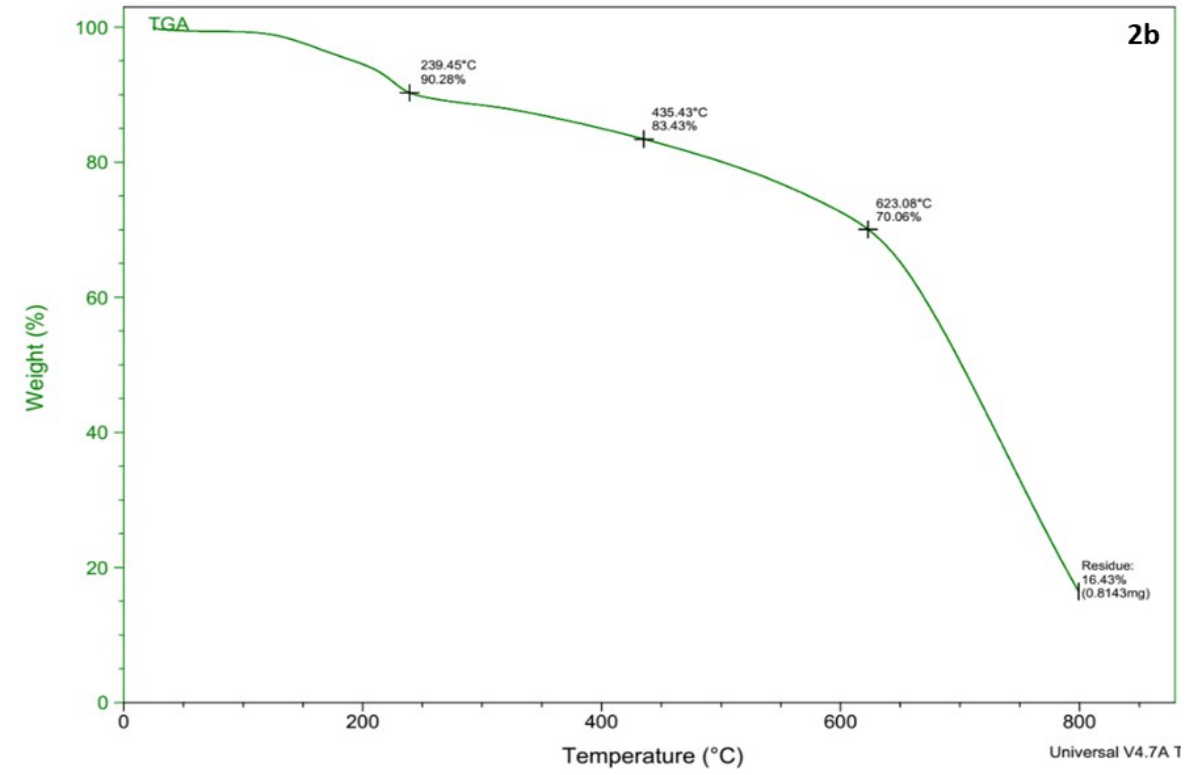
2a-2j	Electronic transition	λ_{max}	eV	*f*	Major contribution	Assignment	LHE
2a	$S_0 \rightarrow S_1$	975	1.27	1.13	HOMO → LUMO (98%)	ICT	0.9258
	$S_0 \rightarrow S_1$	616	2.01	1.13	HOMO → LUMO+1 (79%)	π–π^*	0.9258
2b	$S_0 \rightarrow S_1$	1036	1.19	1.24	HOMO → LUMO (99%)	ICT	0.9424
	$S_0 \rightarrow S_1$	667	1.85	0.89	HOMO → LUMO+1 (78%)	π–π^*	0.8711
2c	$S_0 \rightarrow S_1$	920	1.34	1.25	HOMO → LUMO (98%)	ICT	0.9437
	$S_0 \rightarrow S_1$	614	2.01	0.84	HOMO-1 → LUMO (70%)	π–π^*	0.8554
2d	$S_0 \rightarrow S_1$	921	1.34	1.13	HOMO → LUMO (95%)	ICT	0.9258
	$S_0 \rightarrow S_1$	620	2.00	0.57	HOMO-1 → LUMO (80%)	π–π^*	0.7308
2e	$S_0 \rightarrow S_1$	994	1.24	1.34	HOMO → LUMO (99%)	ICT	0.9542
	$S_0 \rightarrow S_1$	669	1.85	0.92	HOMO-1 → LUMO (67%)	π–π^*	0.8797
2f	$S_0 \rightarrow S_1$	975	1.27	1.35	HOMO → LUMO (99%)	ICT	0.9553
	$S_0 \rightarrow S_1$	664	1.86	6.77	HOMO-1 → LUMO (86%)	π–π^*	0.8301
2g	$S_0 \rightarrow S_1$	924	1.34	1.51	HOMO → LUMO (98%)	ICT	0.9690
	$S_0 \rightarrow S_1$	630	1.96	0.93	HOMO-1 → LUMO (74%)	π–π^*	0.8825
2h	$S_0 \rightarrow S_1$	938	1.32	1.38	HOMO → LUMO (97%)	ICT	0.9583
	$S_0 \rightarrow S_1$	642	1.93	0.74	HOMO-1 → LUMO (79%)	π–π^*	0.8180
2i	$S_0 \rightarrow S_1$	1143	1.08	0.95	HOMO → LUMO (100%)	ICT	0.8877
	$S_0 \rightarrow S_1$	693	1.78	0.71	HOMO → LUMO+1 (92%)	π–π^*	0.8050
2j	$S_0 \rightarrow S_1$	1005	1.23	1.43	HOMO → LUMO (100%)	ICT	0.9628
	$S_0 \rightarrow S_1$	661	1.87	0.76	HOMO-1 → LUMO (58%)	π–π^*	0.8262
LHE = $1\text{-}10^{-f}$							

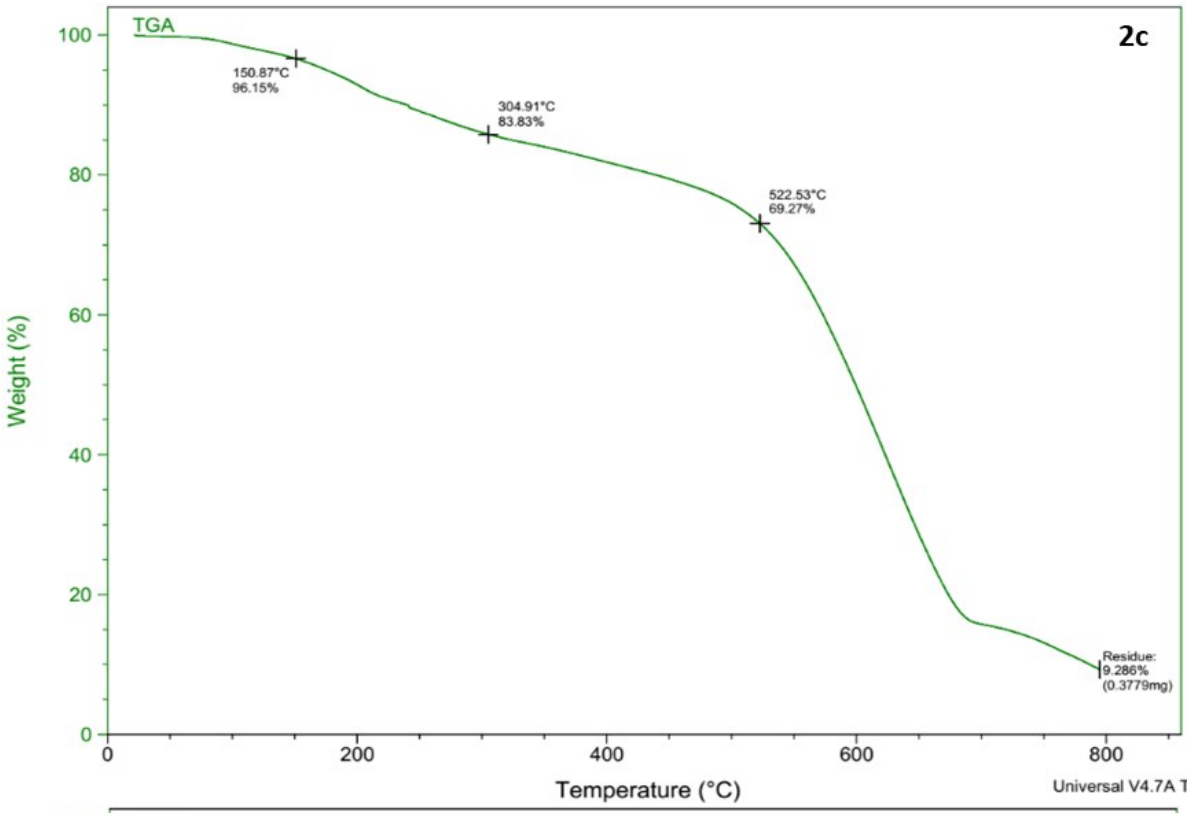
Table S5: and quantum chemical parameters of **2a-2j**

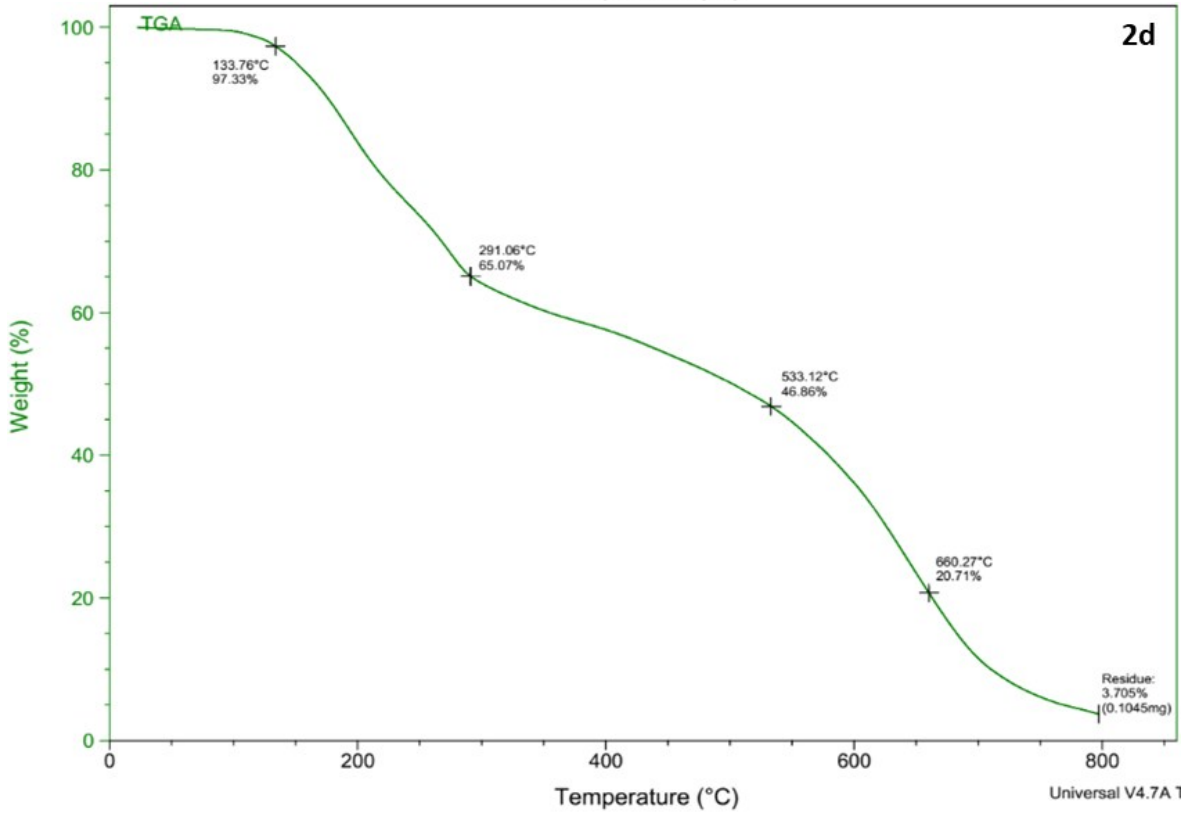
2a-2j	ρ (D)	μ (eV)	η (eV)	σ (eV)	χ (eV)
2a	22.7	-4.42	0.69	1.44	4.42
2b	23.4	-4.34	0.66	1.51	4.34
2c	23.3	-4.38	0.73	1.36	4.38
2d	24.0	-4.37	0.74	1.35	4.37
2e	24.4	-4.32	0.69	1.44	4.32
2f	24.7	-4.30	0.70	1.42	4.30
2g	25.1	-4.35	0.72	1.38	4.35
2h	25.2	-4.35	0.71	1.40	4.35
2i	22.6	-4.28	0.61	1.63	4.28
2j	28.7	-4.26	0.65	1.53	4.26
PCBM	-	-4.92	2.35	0.42	4.92
$\mu = (E_{HOMO} + E_{LUMO})/2$; $\eta = (E_{LUMO} - E_{HOMO})/2$; $\sigma = 1/\eta$; $\chi = -(E_{HOMO} + E_{LUMO})/2$					

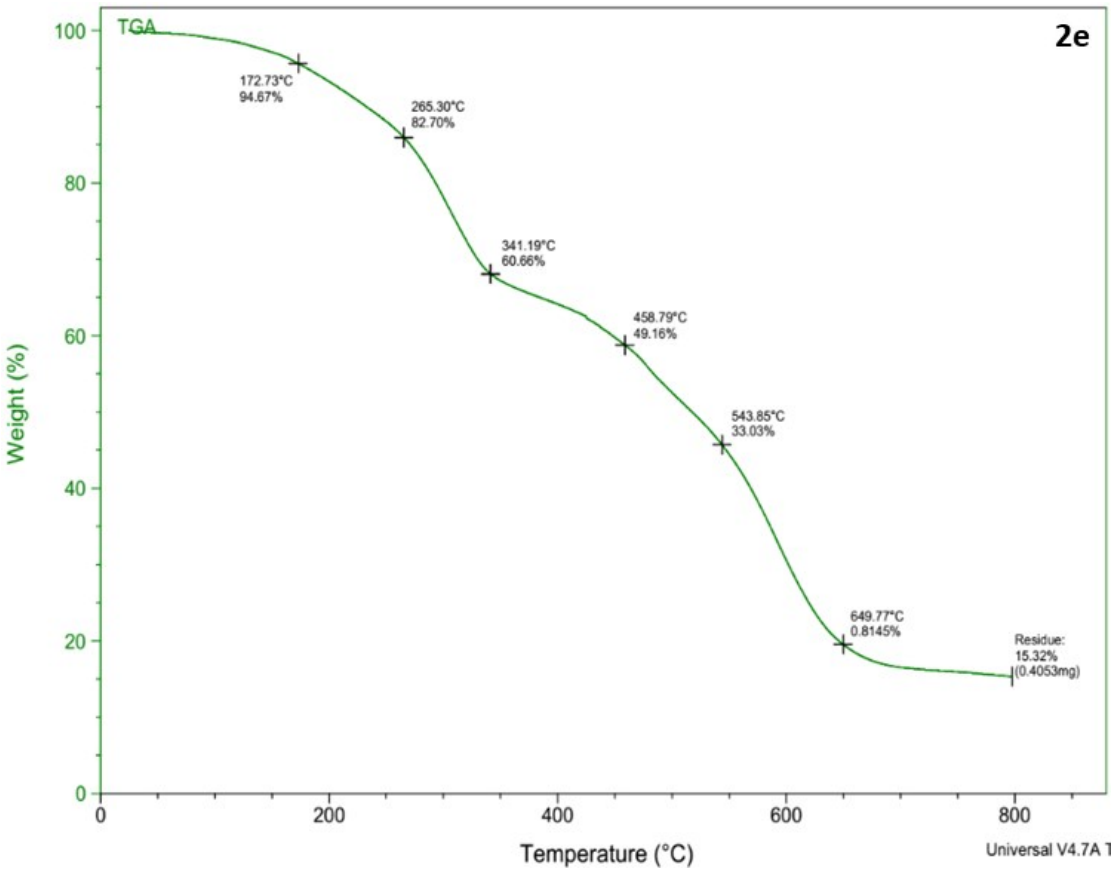
Fig S9: Thermogravimetric analysis of **2a-j**

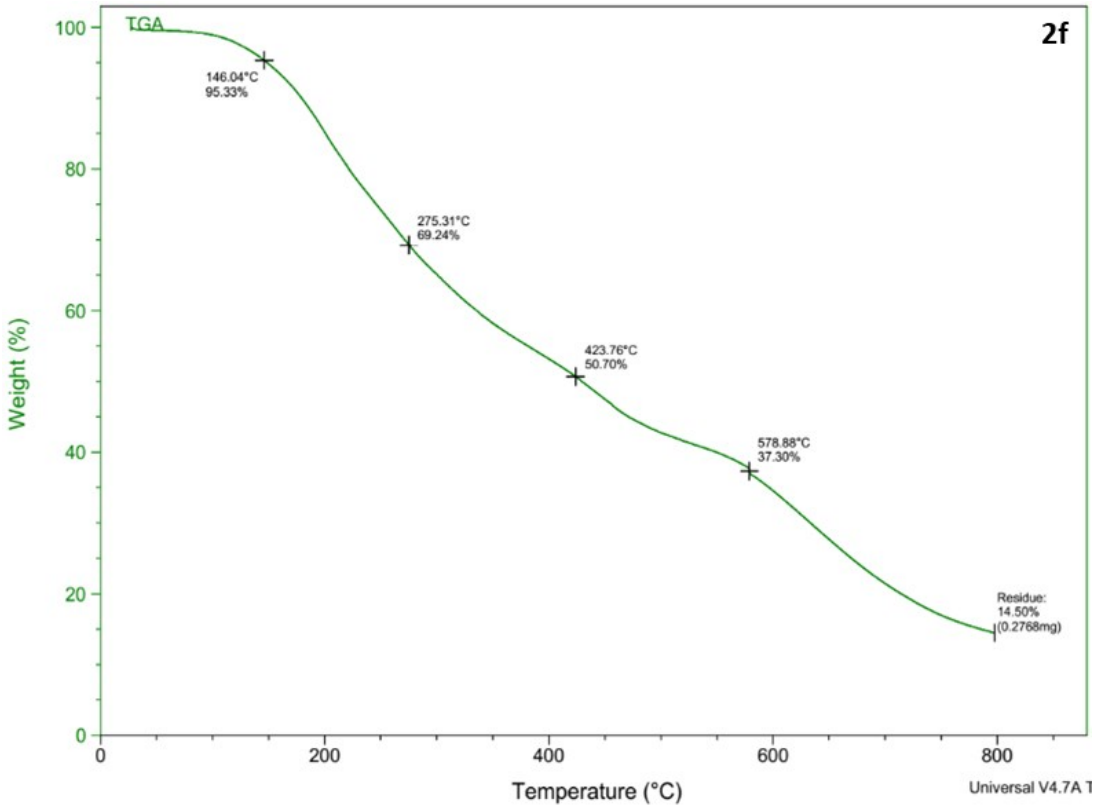


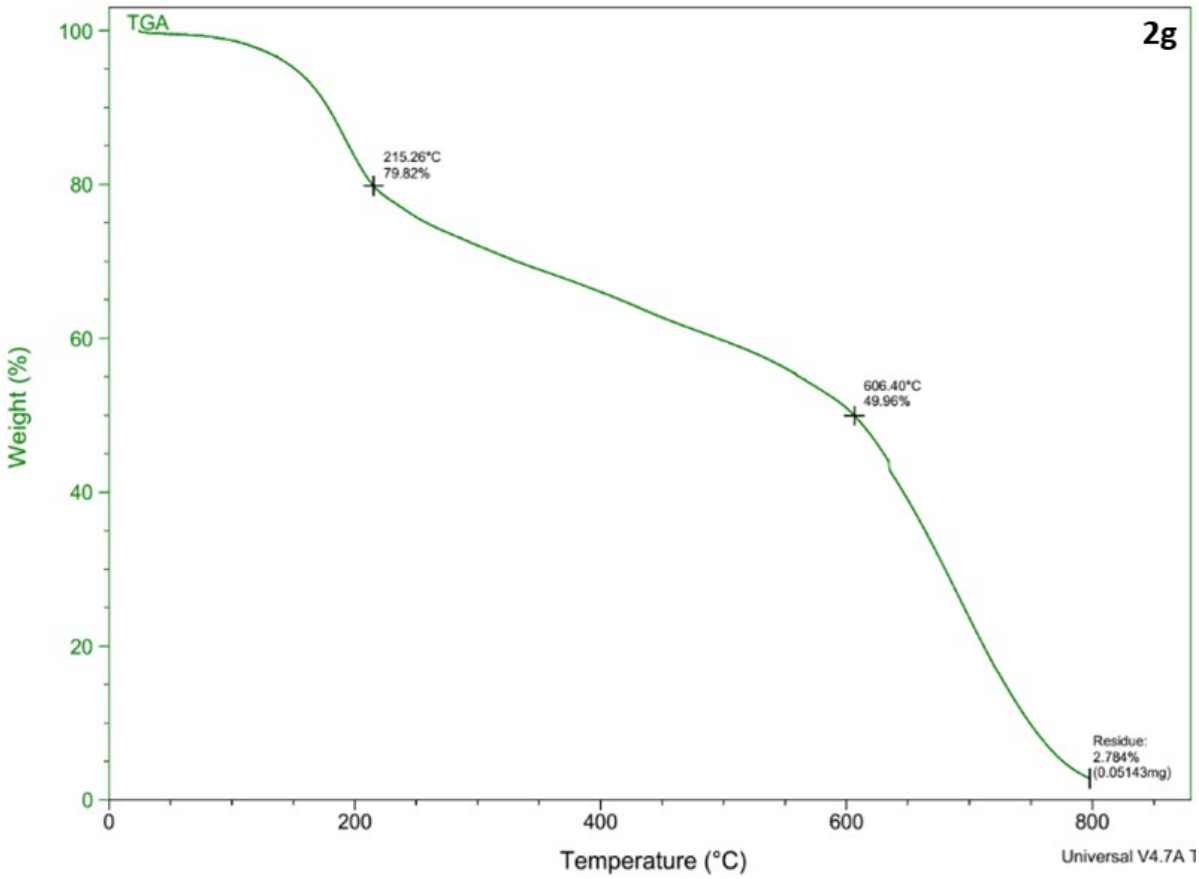


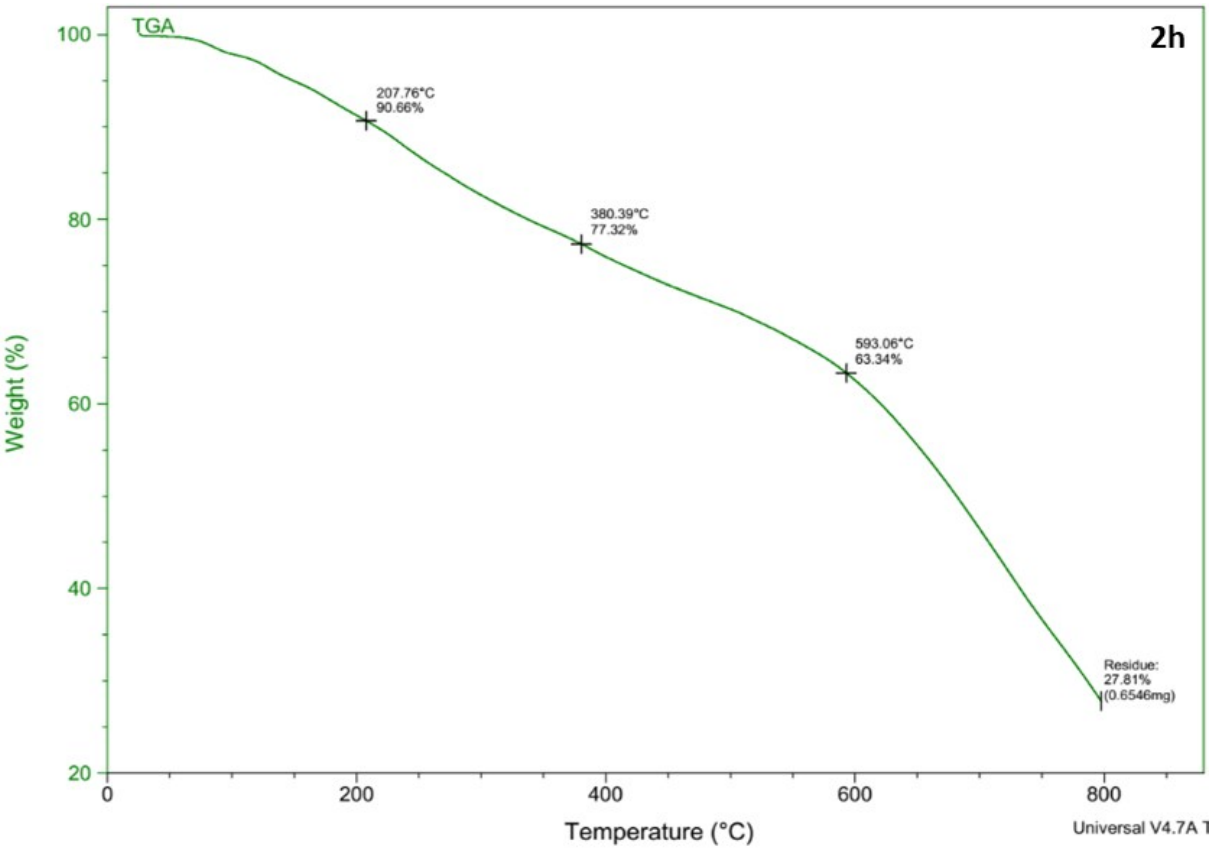

TGA
2c
150.87°C
96.15%
304.91°C
83.83%
522.53°C
69.27%
Residue:
9.286%
(0.3779mg)
Weight (%)
Temperature (°C)
Universal V4.7A T

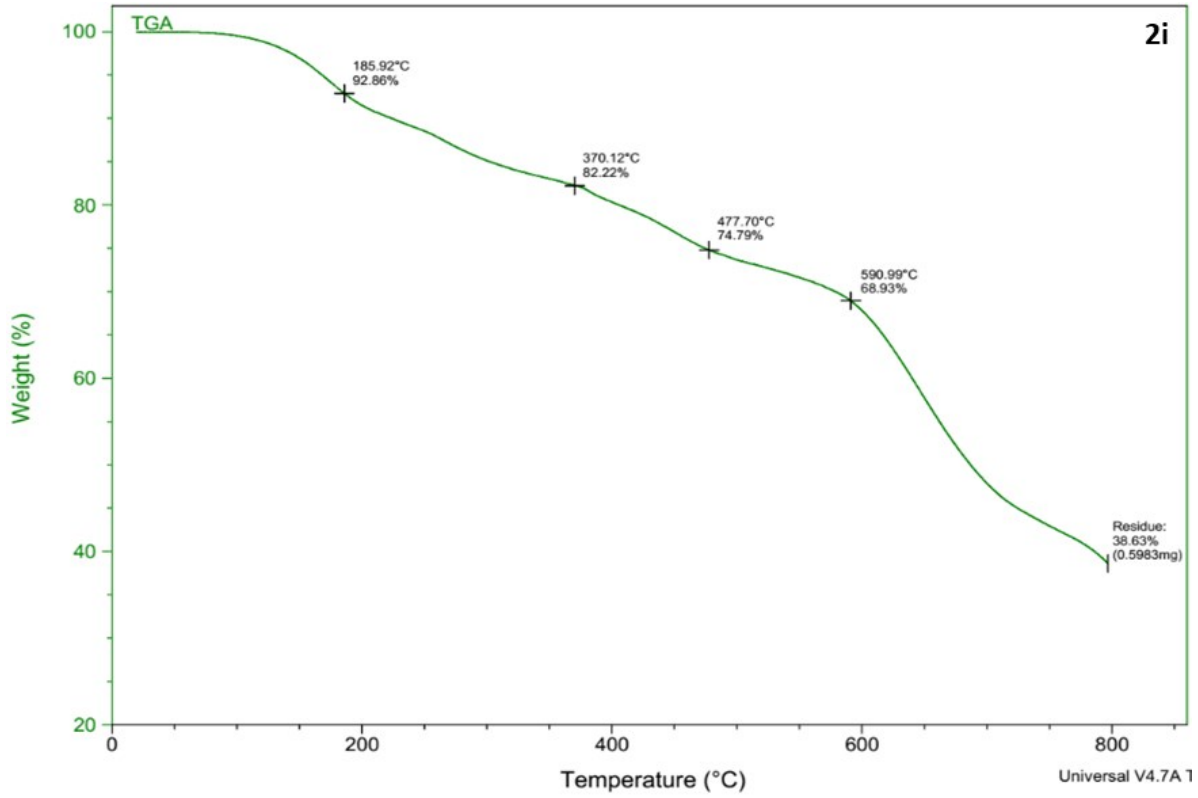

TGA
2d
133.76°C
97.33%
291.06°C
65.07%
533.12°C
46.86%
660.27°C
20.71%
Residue:
3.705%
(0.1045mg)
Weight (%)
Temperature (°C)
Universal V4.7A T


TGA
2e
172.73°C
94.67%
265.30°C
82.70%
341.19°C
60.66%
458.79°C
49.16%
543.85°C
33.03%
649.77°C
0.8145%
Residue:
15.32%
(0.4053mg)
Weight (%)
Temperature (°C)
Universal V4.7A T


TGA
2f
146.04°C
95.33%
275.31°C
69.24%
423.76°C
50.70%
578.88°C
37.30%
Residue:
14.50%
(0.2768mg)
Weight (%)
Temperature (°C)
Universal V4.7A T


TGA
2g
215.26°C
79.82%
606.40°C
49.96%
Residue:
2.784%
(0.05143mg)
Weight (%)
Temperature (°C)
Universal V4.7A T


TGA
2h
207.76°C
90.66%
380.39°C
77.32%
593.06°C
63.34%
Residue:
27.81%
(0.6546mg)
Weight (%)
Temperature (°C)
Universal V4.7A T


TGA
2i
185.92°C
92.86%
370.12°C
82.22%
477.70°C
74.79%
590.99°C
68.93%
Residue:
38.63%
(0.5983mg)
Weight (%)
Temperature (°C)
Universal V4.7A

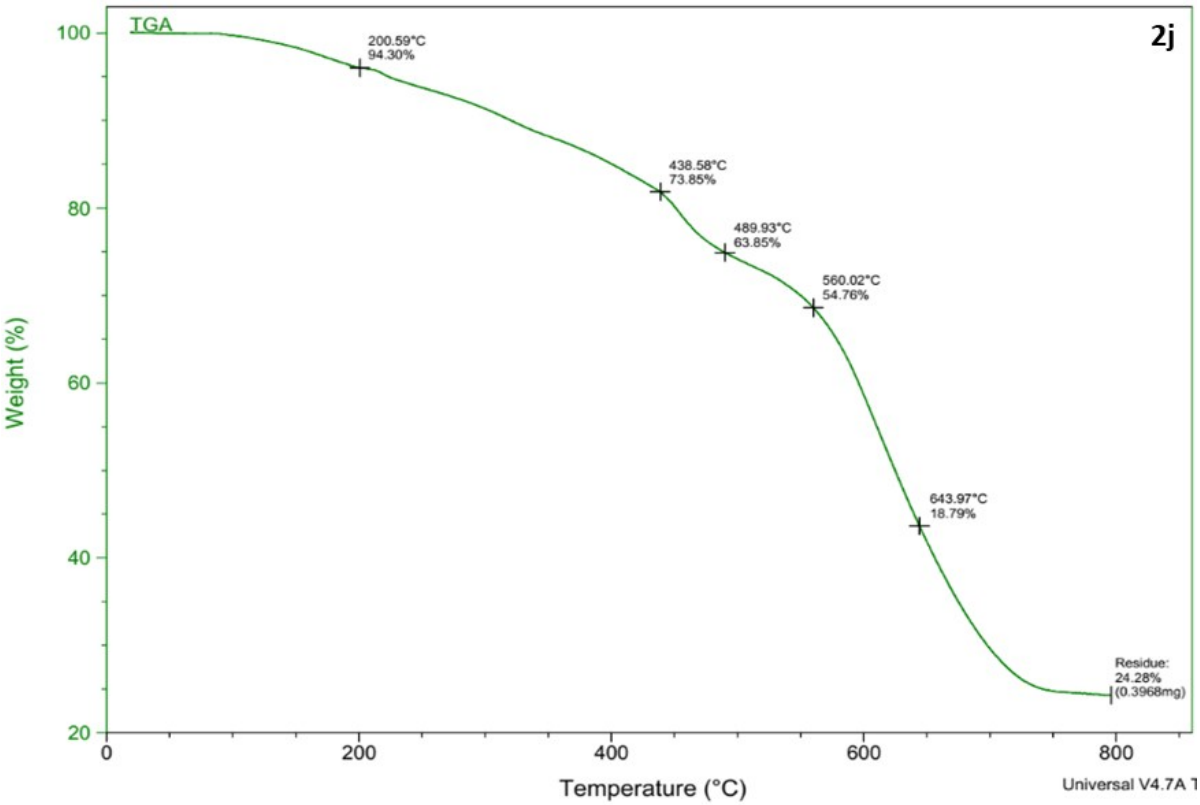
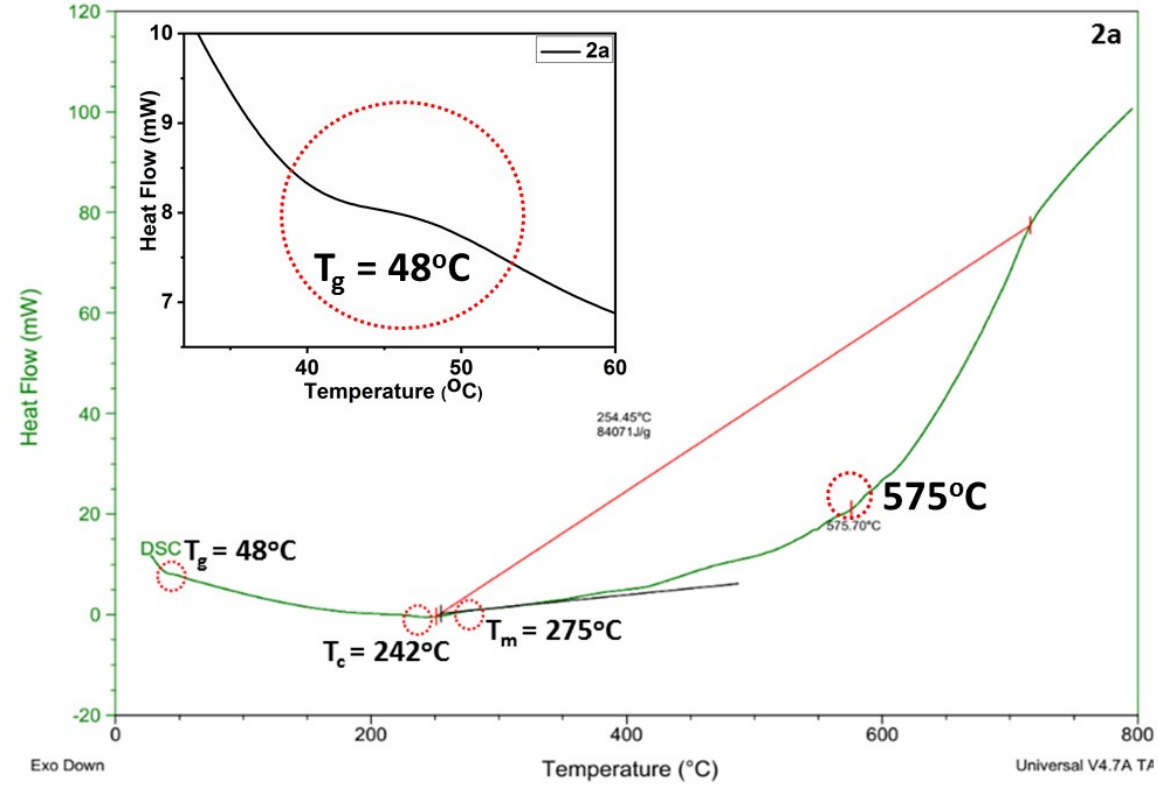
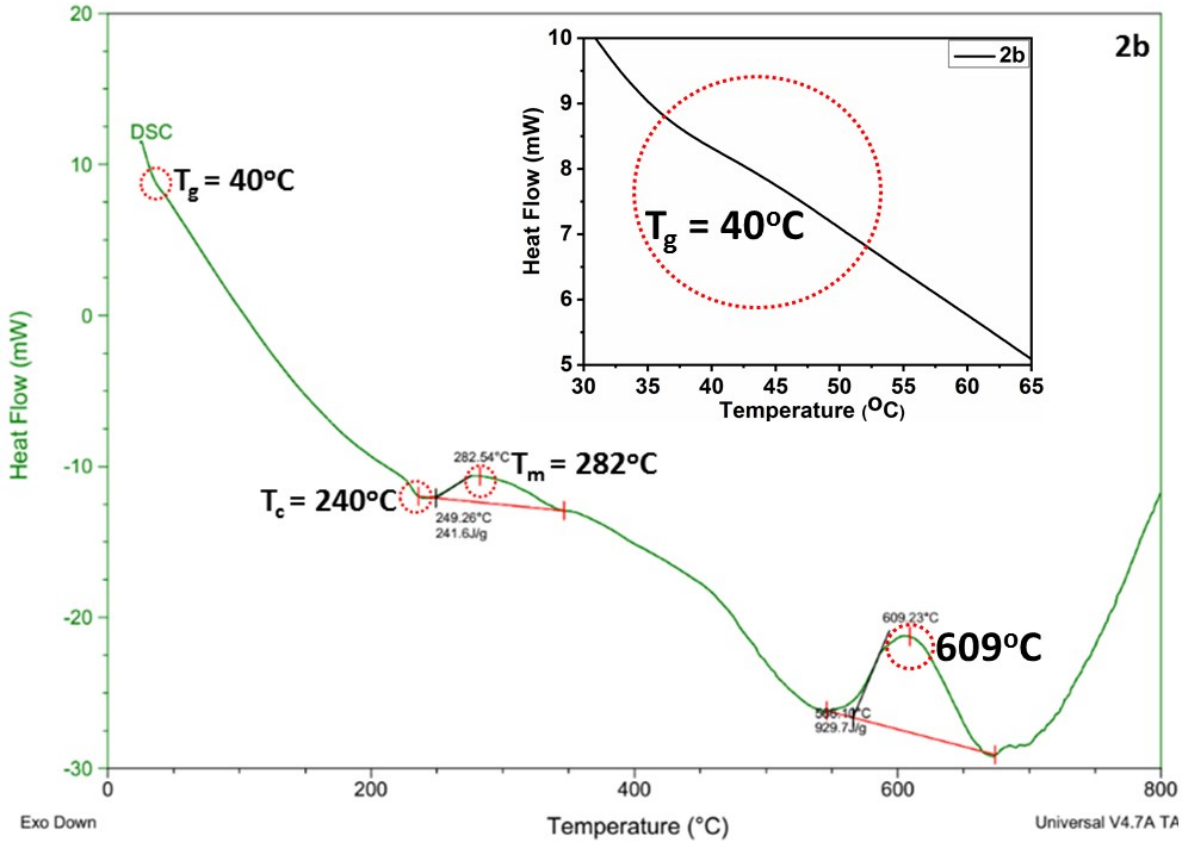
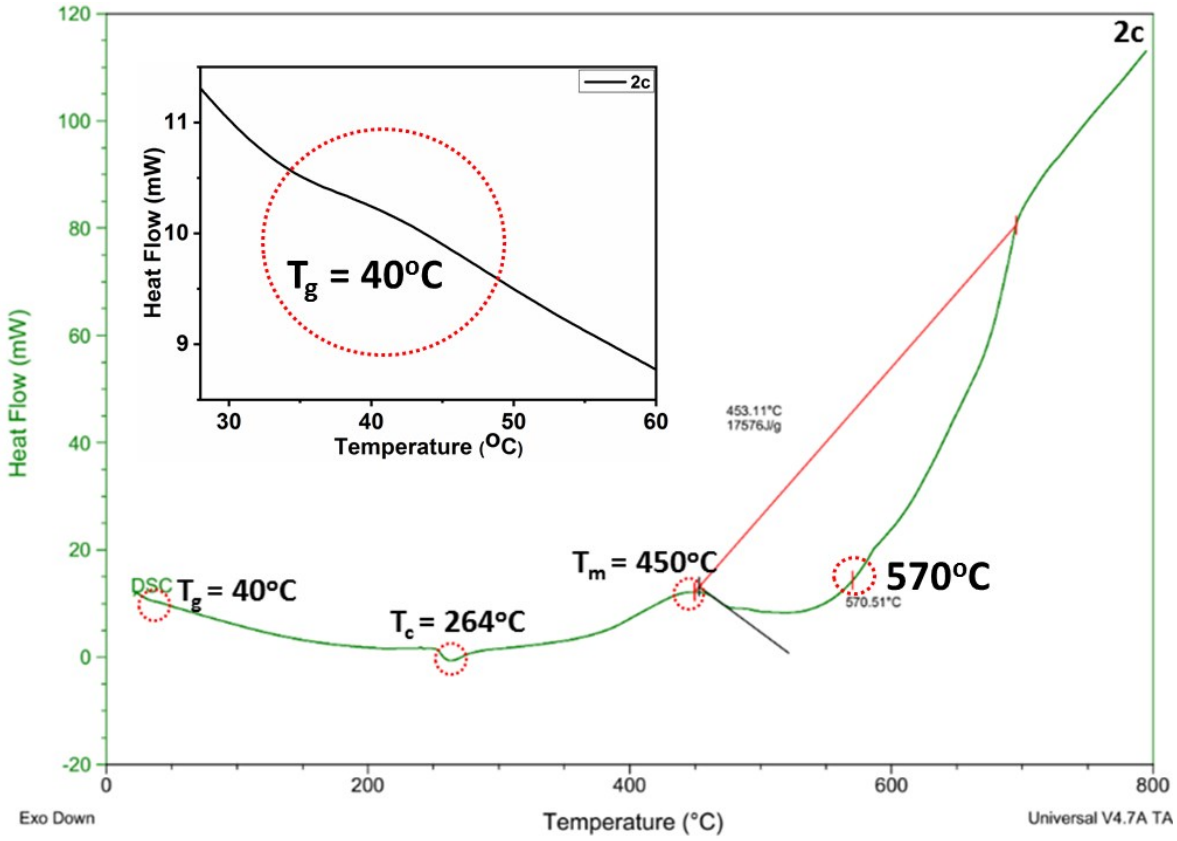
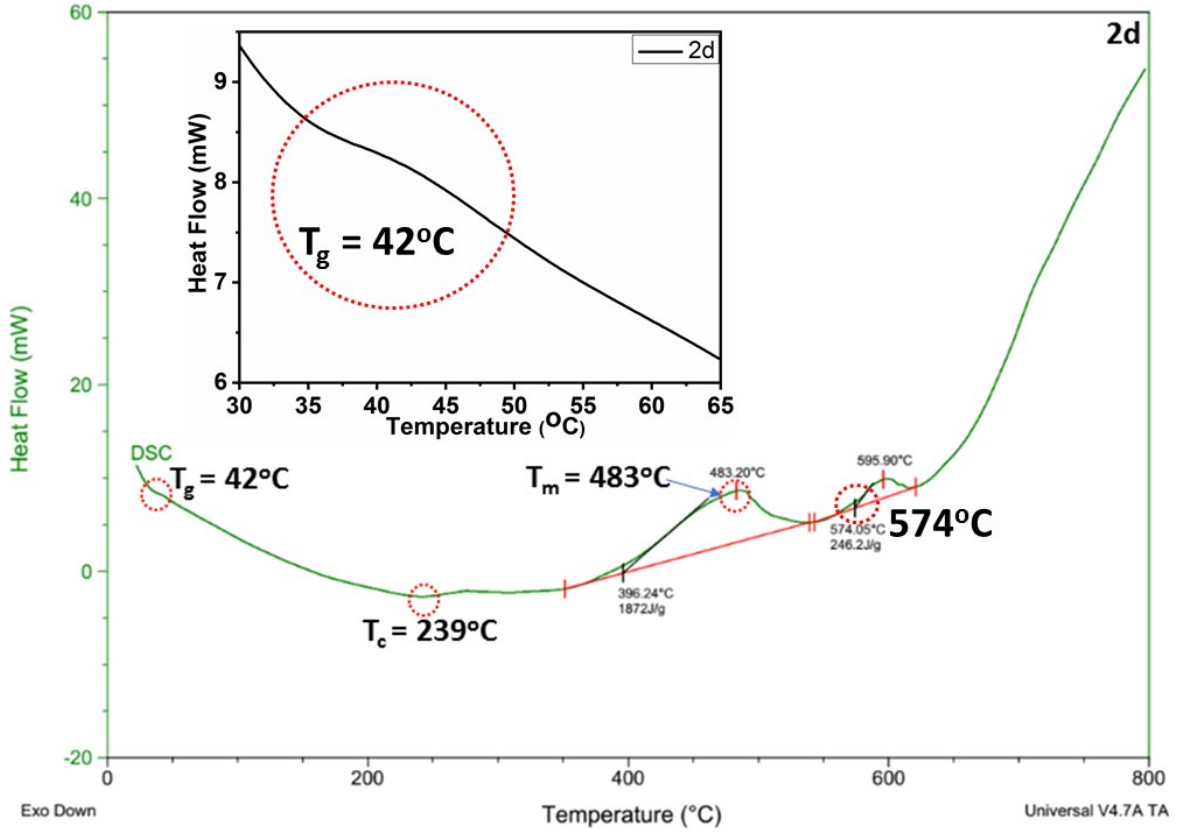

TGA
2j
200.59°C
94.30%
438.58°C
73.85%
489.93°C
63.85%
560.02°C
54.76%
643.97°C
18.79%
Residue:
24.28%
(0.3968mg)
Weight (%)
Temperature (°C)
Universal V4.7A

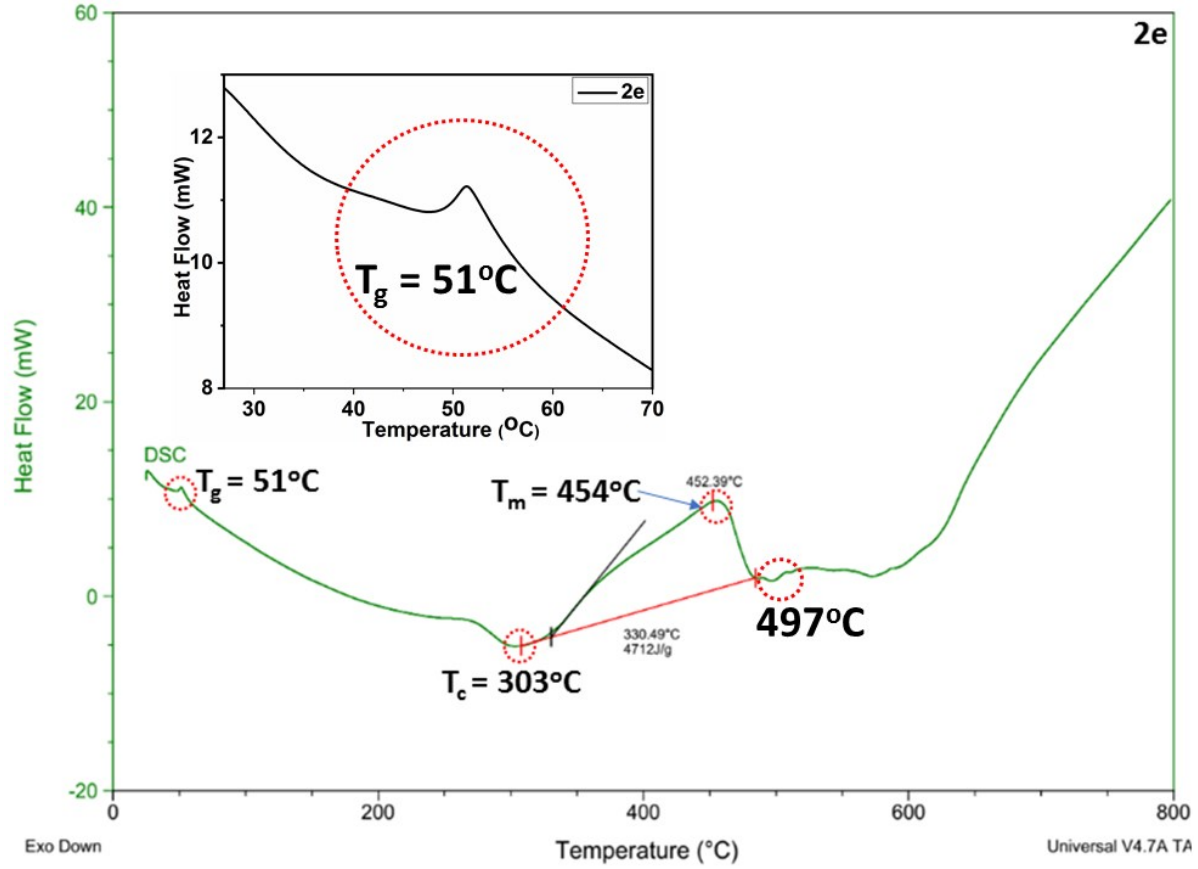
Fig S10: Differential Scanning analysis of **2a-j (**inset showing T_g**)**

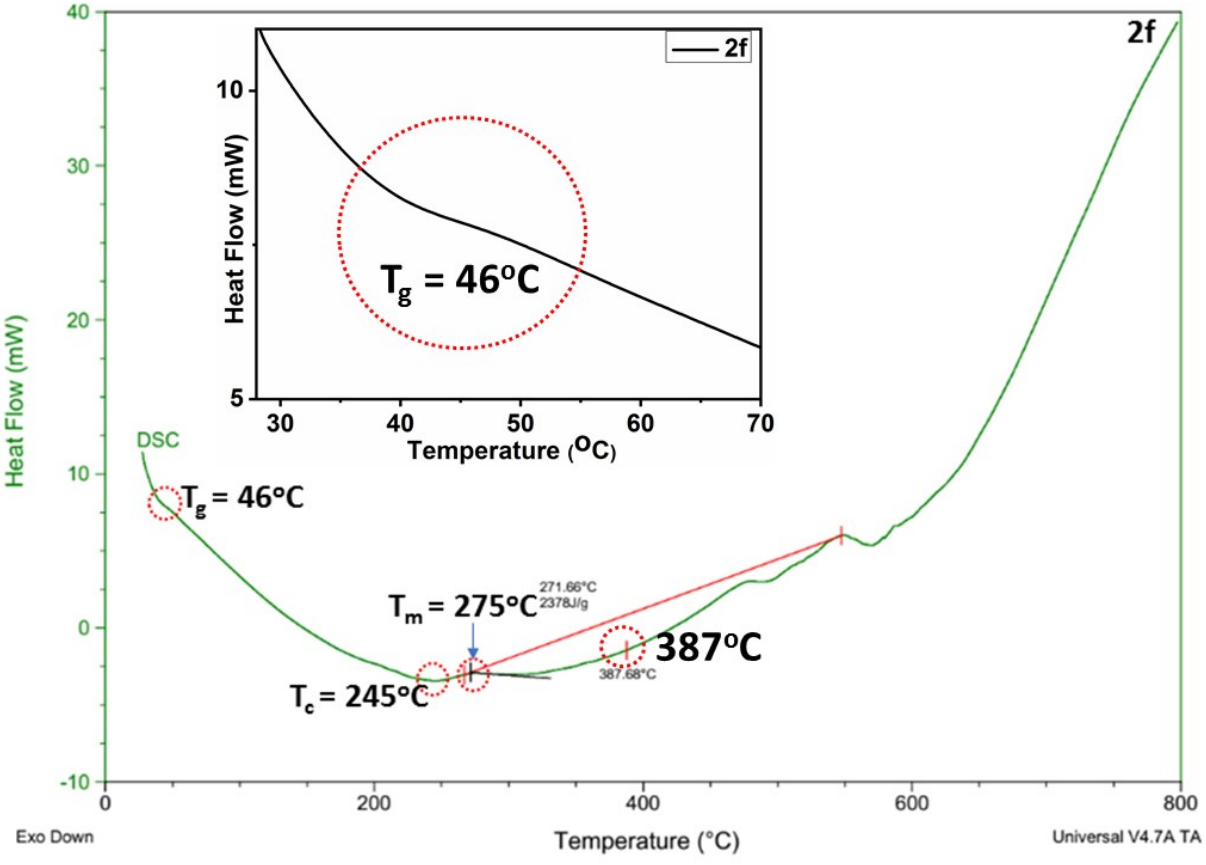


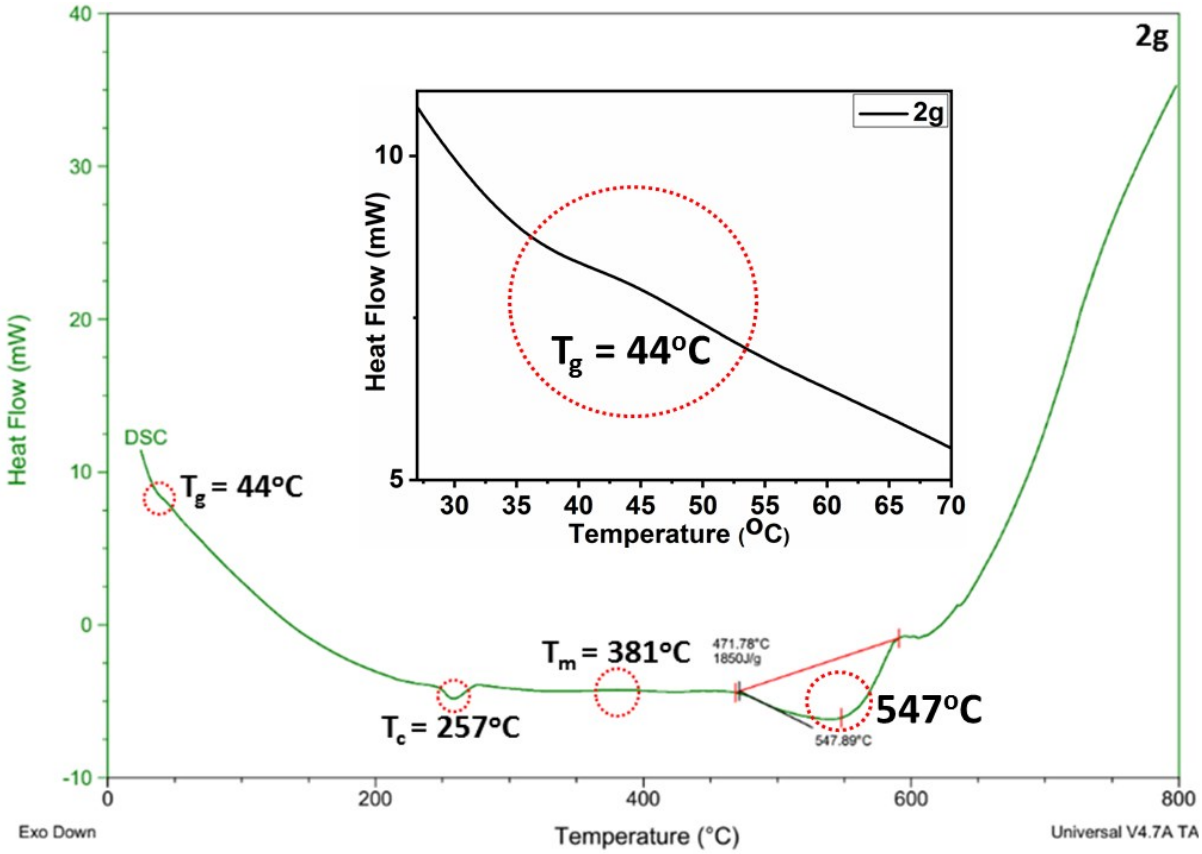


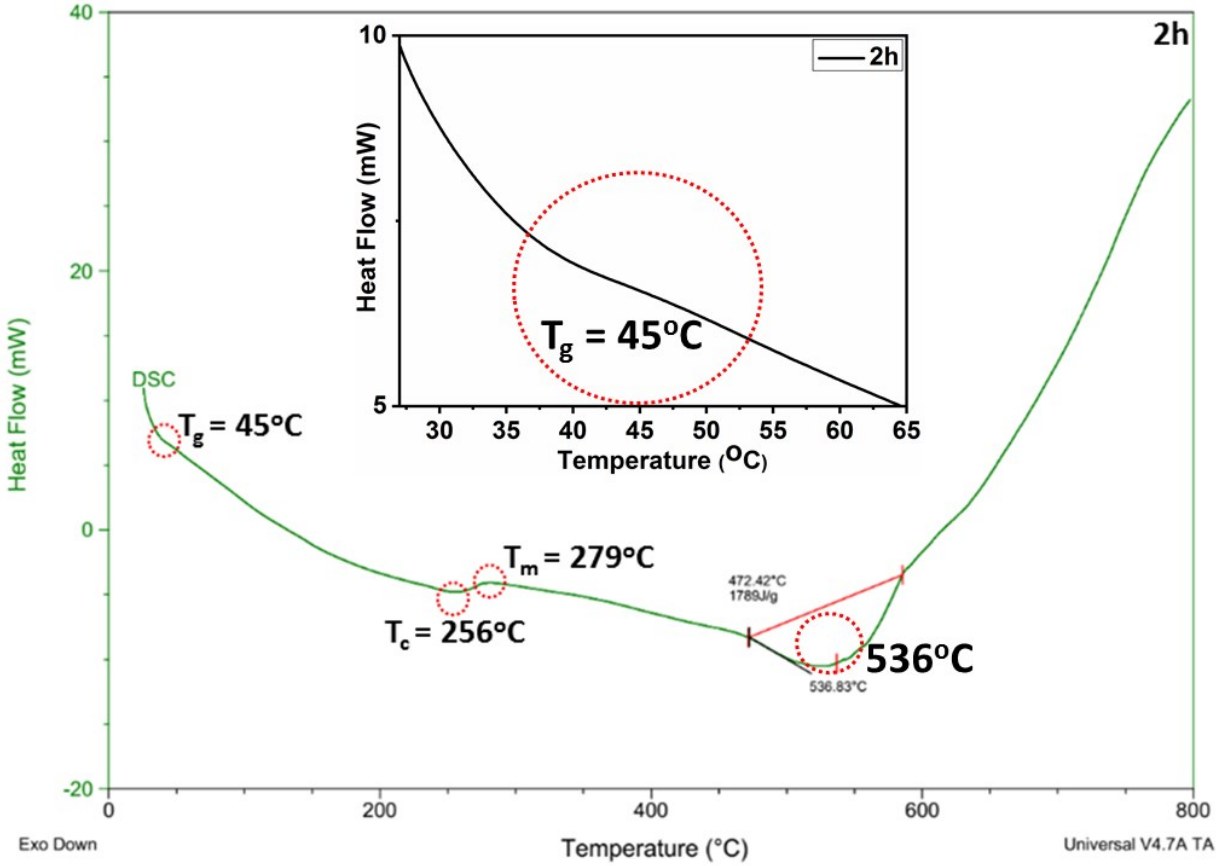

2c
2c
Heat Flow (mW)
Temperature (°C)
T_g = 40°C
DSC
T_g = 40°C
T_c = 264°C
T_m = 450°C
453.11°C
17576J/g
570°C
570.51°C
Exo Down
Universal V4.7A TA

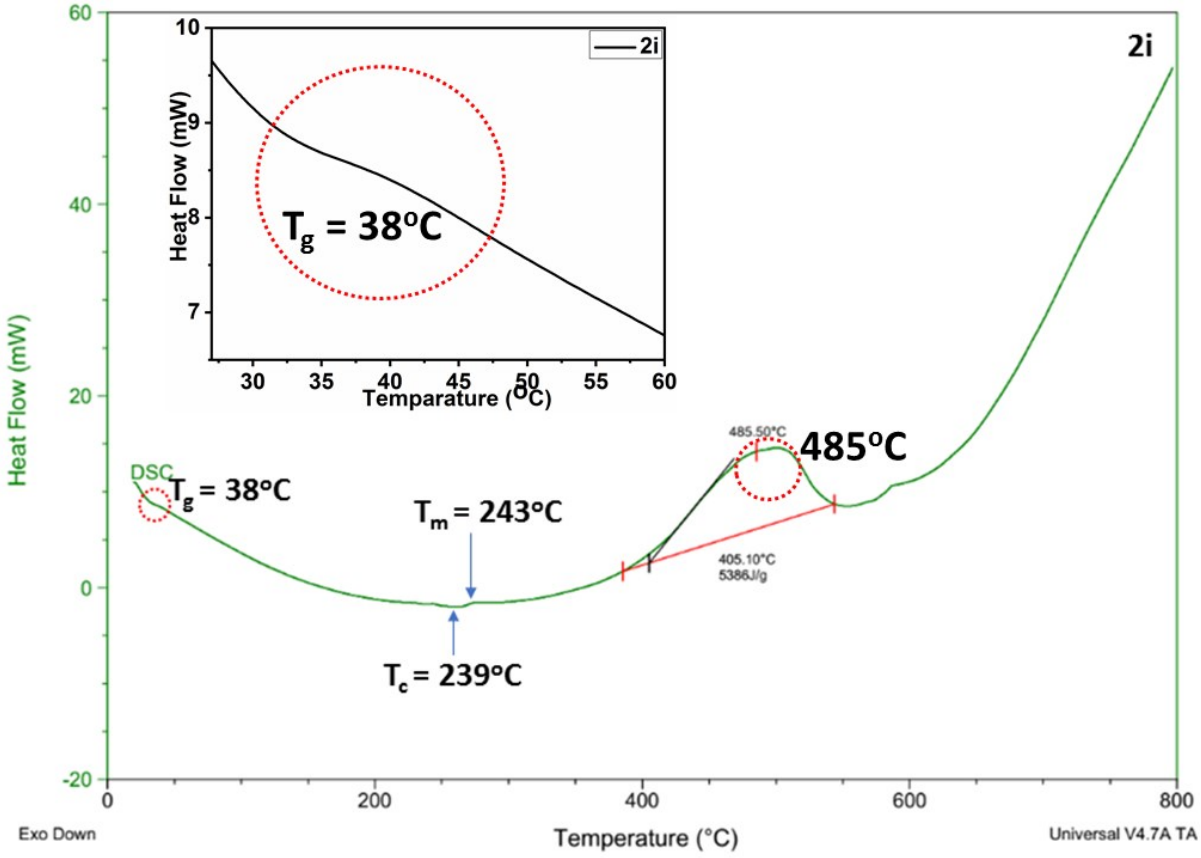

2d
2d
Heat Flow (mW)
Temperature (°C)
T_g = 42°C
DSC
T_g = 42°C
T_m = 483°C
483.20°C
595.90°C
574°C
574.05°C
246.2J/g
396.24°C
1872J/g
T_c = 239°C
Exo Down
Universal V4.7A TA


2e
2e
Heat Flow (mW)
Temperature (°C)
T_g = 51°C
DSC
T_g = 51°C
T_m = 454°C
452.39°C
497°C
330.49°C
4712J/g
T_c = 303°C
Exo Down
Universal V4.7A TA


2f
2f
Heat Flow (mW)
Temperature (°C)
T_g = 46°C
DSC
T_g = 46°C
T_m = 275°C
271.66°C
2378J/g
387°C
387.68°C
T_c = 245°C
Exo Down
Universal V4.7A TA


2g
2g
Heat Flow (mW)
Temperature (°C)
Tg = 44°C
DSC
Tg = 44°C
Tm = 381°C
Tc = 257°C
471.78°C
1850J/g
547°C
547.89°C
Exo Down
Universal V4.7A TA


2h
2h
Heat Flow (mW)
Temperature (°C)
Tg = 45°C
DSC
Tg = 45°C
Tm = 279°C
Tc = 256°C
472.42°C
178J/g
536°C
536.83°C
Exo Down
Universal V4.7A TA


2i
Heat Flow (mW)
Temperature (°C)
Exo Down
Universal V4.7A TA
2i
Heat Flow (mW)
Temparature (°C)
T_g = 38°C
DSC
T_g = 38°C
T_m = 243°C
T_c = 239°C
485.50°C
485°C
405.10°C
5386J/g

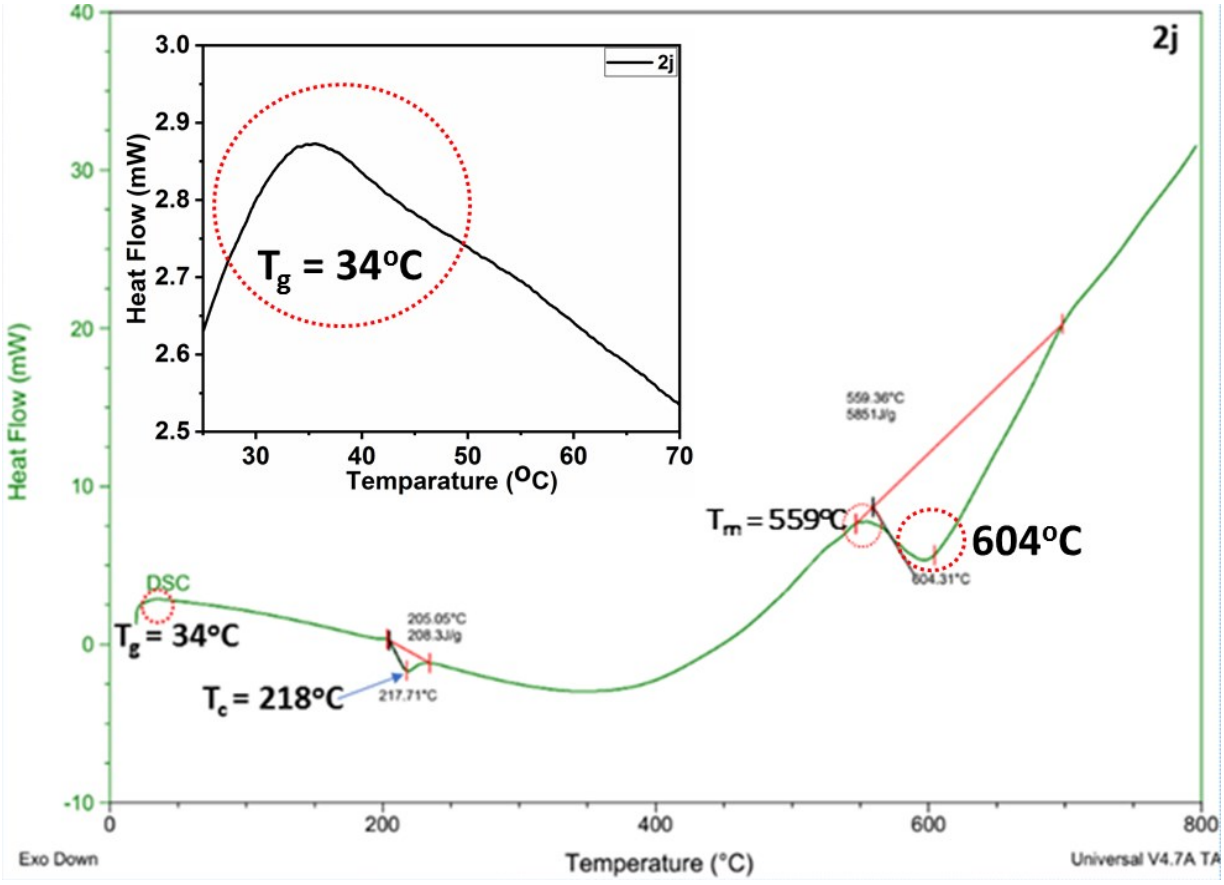

2j
Heat Flow (mW)
Temperature (°C)
Exo Down
Universal V4.7A TA
2j
Heat Flow (mW)
Temparature (°C)
T_g = 34°C
DSC
T_g = 34°C
T_c = 218°C
205.05°C
208.3J/g
217.71°C
559.36°C
5851J/g
T_m = 559°C
604°C
604.31°C

Table S6: TGA and DSC data of **2a-2j**

2a-j	T_d (°C)[a]	T_{dec} (°C)[b]	T_g (°C)[c]	T_c (°C)[d]	T_m (°C)[e]
2a	195	>250	48	242	275
2b	191	>250	40	240	282
2c	174	>250	40	264	450
2d	149	>250	42	239	486
2e	180	>250	51	303	454
2f	149	194-197	46	245	275
2g	152	221-223	44	257	381
2h	149	145-147	45	256	279
2i	168	214-216	38	239	243
2j	222	192-193	34	218	559

[a]First weight loss (5%) temperature (T_d) obtained from TGA; [b]decomposition temperature (T_{dec}) obtained from open-air capillary; [c]Glass transition temperature obtained from DSC; [d]Crystallization temperature obtained from DSC; [e]Melting temperature obtained from DSC.

Fig S11: Current-Voltage curve of **2j** in various blend ratio and additives

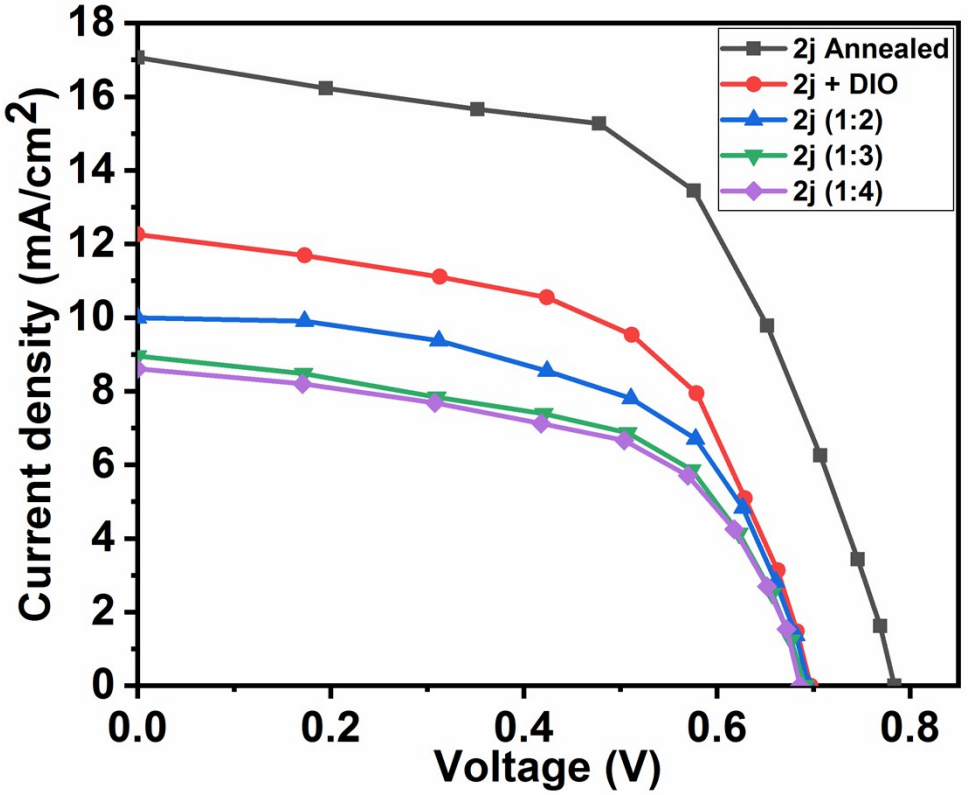


Table S7: photovoltaic results of **2j**:PCBM

2j	V_{OC} (V)[a]	J_{SC} (mA /cm²)[a]	FF (%)	η (%)[b]
2j (1:2)	0.70	10.00	57.4	4.01 (3.98 ± 0.03)
2j (1:3)	0.70	8.96	56.3	3.53 (3.50 ± 0.03)
2j (1:4)	0.69	8.61	56.8	3.37 (3.34 ± 0.03)
2j (Annealed)	0.79	17.07	57.8	7.79 (7.76 ± 0.03)
2j + DIO	0.70	12.26	57.1	4.90 (4.87 ± 0.03)

[a]*J-V* characteristics of photovoltaic devices fabricated from a solution of **2a-j**:PCBM (1:1 blend) in *o*-dichlorobenzene. and thermally annealed at 140 °C for 5 min; [b]Efficiencies of inverted OPVs under AM 1.5 G illumination (100 mW/cm²)

Fig S12: Thin-film UV-visible absorbance of **2j**:PCBM blend at different ratio

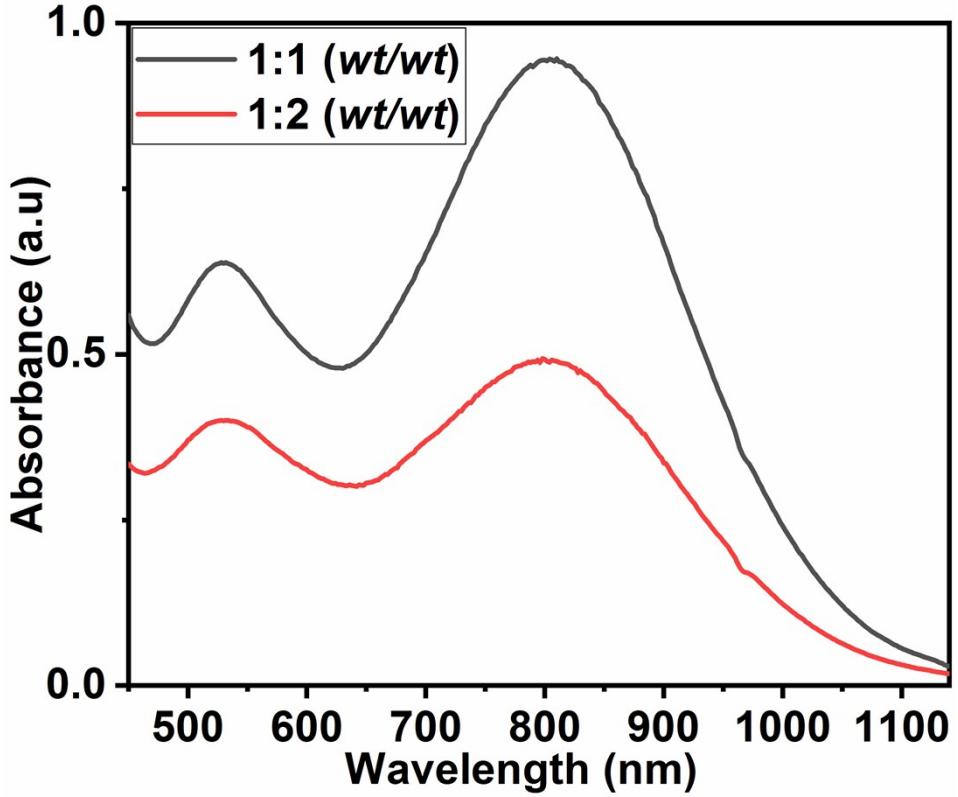
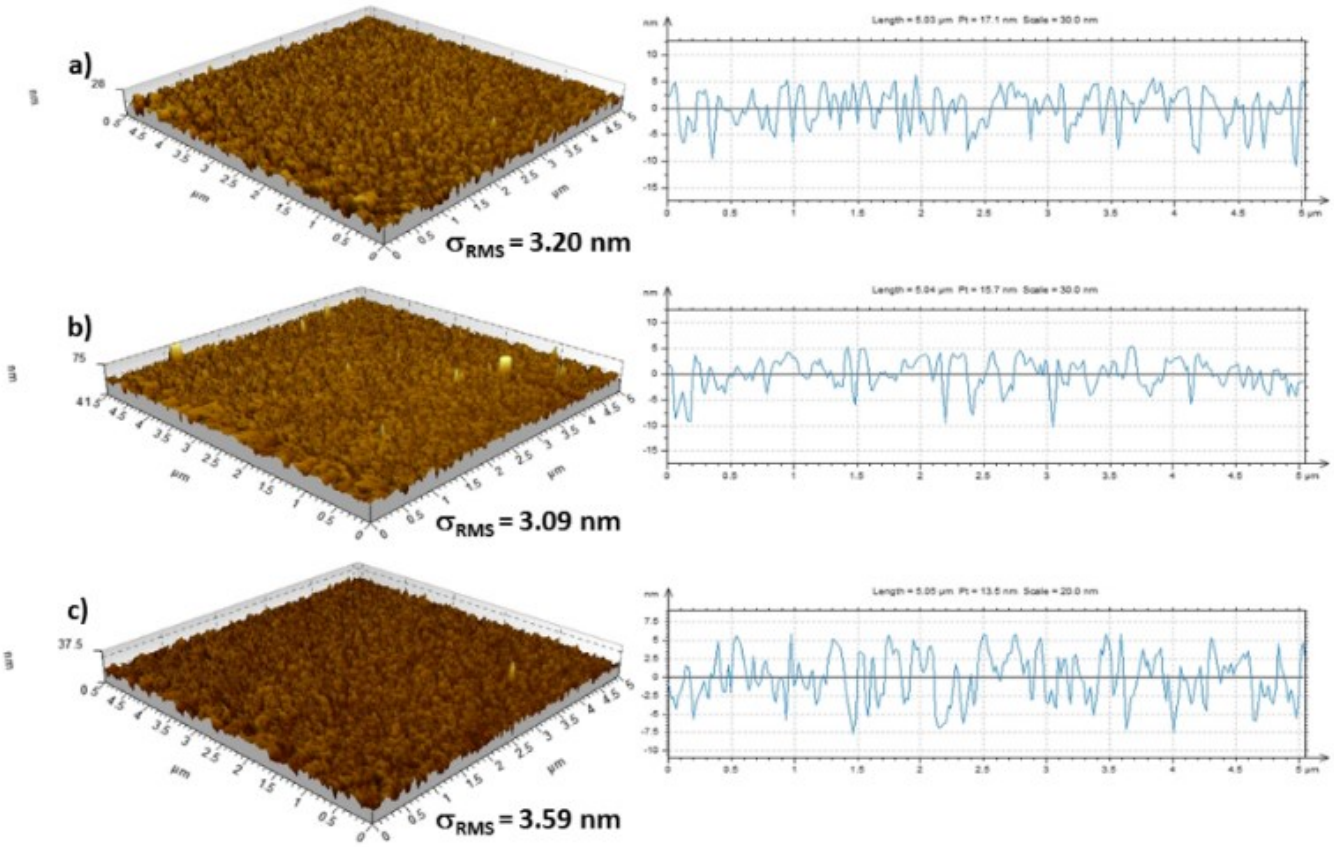


Fig S13: AFM topographic images of **2j**:PCBM blend



Tapping-mode AFM height images (5 μm X 5 μm) of **2j**:PCBM (1:1) (a) as-spun films; (b) annealed film at 120°C for 5 min; (c) as-spun films after 1% DIO treatment

Cartesian coordinates

2a			
Symbol	**X**	**Y**	**Z**
C	7.85311	-0.3531	-0.2542
C	6.65186	0.26895	-0.1071
C	5.39984	-0.4382	-0.2455
C	5.49468	-1.8243	-0.6364
C	6.69348	-2.4447	-0.8084
C	7.93598	-1.7494	-0.5941
C	9.16882	-2.3972	-0.7325
C	4.17287	0.1959	0.00453
C	2.94207	-0.5049	0.24385
C	4.1064	1.69274	0.07436
C	2.7278	-1.7679	0.79729
C	1.37567	-2.1201	0.90487
C	0.49463	-1.1435	0.4453
S	1.38823	0.24563	-0.134
C	3.81724	2.30735	1.38653
C	4.31889	2.41058	-1.0781
C	3.05156	3.48105	1.52053
C	2.81676	4.02986	2.77761
C	3.34216	3.42445	3.92095
C	4.09368	2.25373	3.80351
C	4.3189	1.69229	2.55052
C	-0.9373	-1.2356	0.43117
C	-1.7974	-0.2642	0.02699
C	-3.2448	-0.3273	-0.0169
C	-3.9714	0.81654	-0.4085
C	-5.3558	0.82435	-0.4649
C	-6.0912	-0.3323	-0.1386
C	-5.3757	-1.4881	0.24631
C	-3.9939	-1.4802	0.30707
N	-7.4944	-0.3409	-0.201
C	-8.2604	-1.1663	0.67594
C	-8.1865	0.48473	-1.1388
C	-9.3255	-1.9276	0.17322
C	-10.089	-2.7158	1.03234
C	-9.7931	-2.7682	2.39597
C	-8.7297	-2.0146	2.89689
C	-7.9718	-1.21	2.04822
C	-9.2792	1.25856	-0.7226

C	**-9.9677**	**2.04761**	**-1.6422**
C	**-9.5689**	**2.08772**	**-2.9795**
C	**-8.4776**	**1.32136**	**-3.3939**
C	**-7.7937**	**0.51627**	**-2.485**
C	**10.3987**	**-1.7057**	**-0.5432**
N	**11.3954**	**-1.1232**	**-0.3785**
C	**9.24856**	**-3.7805**	**-1.0592**
N	**9.2913**	**-4.9155**	**-1.3234**
C	**4.38927**	**3.84258**	**-1.1349**
N	**4.46578**	**4.99965**	**-1.2319**
C	**4.49879**	**1.76778**	**-2.3495**
N	**4.63098**	**1.29309**	**-3.4034**
H	**8.77351**	**0.20207**	**-0.1077**
H	**6.63571**	**1.3176**	**0.16827**
H	**4.58347**	**-2.3653**	**-0.8598**
H	**6.72691**	**-3.4766**	**-1.1418**
H	**3.53765**	**-2.3866**	**1.1626**
H	**1.02823**	**-3.056**	**1.32767**
H	**2.61779**	**3.9516**	**0.64669**
H	**2.21713**	**4.93048**	**2.86369**
H	**3.16036**	**3.85907**	**4.89915**
H	**4.50248**	**1.77562**	**4.68813**
H	**4.90267**	**0.78199**	**2.4653**
H	**-1.3244**	**-2.1884**	**0.7854**
H	**-1.3743**	**0.68359**	**-0.3057**
H	**-3.4299**	**1.72519**	**-0.6587**
H	**-5.879**	**1.72772**	**-0.756**
H	**-5.919**	**-2.3954**	**0.48435**
H	**-3.4846**	**-2.3961**	**0.59034**
H	**-9.5493**	**-1.8948**	**-0.8878**
H	**-10.911**	**-3.3006**	**0.63014**
H	**-10.386**	**-3.3877**	**3.06131**
H	**-8.4965**	**-2.0389**	**3.95733**
H	**-7.1574**	**-0.611**	**2.44208**
H	**-9.5832**	**1.23524**	**0.31861**
H	**-10.813**	**2.64228**	**-1.3074**
H	**-10.104**	**2.70802**	**-3.6918**
H	**-8.164**	**1.33688**	**-4.4335**
H	**-6.9557**	**-0.0908**	**-2.8113**

2b			
Symbol	**X**	**Y**	**Z**
C	**3.73179**	**0.95099**	**-0.4301**
C	**4.49052**	**-0.1215**	**0.03959**
S	**3.41459**	**-1.4252**	**0.54784**
C	**1.98575**	**-0.5085**	**0.12065**
C	**2.34758**	**0.73796**	**-0.3844**
C	**0.67101**	**-1.0496**	**0.30398**
C	**0.30248**	**-2.3298**	**0.68729**
C	**-1.0898**	**-2.5175**	**0.76929**
C	**-1.8332**	**-1.3892**	**0.45068**
S	**-0.7617**	**-0.0581**	**0.04599**
C	**-3.267**	**-1.2881**	**0.44196**
C	**-3.9944**	**-0.1886**	**0.12099**
C	**-5.4412**	**-0.0607**	**0.09907**
C	**-6.0163**	**1.17868**	**-0.2481**
C	**-7.3895**	**1.36814**	**-0.2846**
C	**-8.2646**	**0.30824**	**0.01852**
C	**-7.7031**	**-0.9403**	**0.36155**
C	**-6.3304**	**-1.1141**	**0.40371**
N	**-9.6609**	**0.48408**	**-0.0234**
C	**-10.511**	**-0.2353**	**0.86764**
C	**-10.251**	**1.39065**	**-0.9538**
C	**-11.675**	**-0.8533**	**0.38612**
C	**-12.515**	**-1.5412**	**1.25961**
C	**-12.201**	**-1.6363**	**2.6169**
C	**-11.041**	**-1.026**	**3.09684**
C	**-10.204**	**-0.3212**	**2.23398**
C	**-11.243**	**2.28802**	**-0.5321**
C	**-11.832**	**3.15942**	**-1.4458**
C	**-11.433**	**3.16063**	**-2.7835**
C	**-10.441**	**2.27189**	**-3.2037**
C	**-9.8582**	**1.38477**	**-2.301**
C	**5.91722**	**-0.2751**	**0.11317**
C	**6.44146**	**-1.6726**	**-0.0281**
C	**6.25369**	**-2.3489**	**-1.3284**
C	**6.81044**	**0.79646**	**0.26718**
C	**7.06808**	**-2.2478**	**1.05177**
C	**8.21484**	**0.65421**	**-0.0397**
C	**9.07666**	**1.7057**	**0.01701**
C	**8.63524**	**3.01395**	**0.42427**
C	**7.25256**	**3.149**	**0.80255**
C	**6.38935**	**2.10035**	**0.72097**

C	**9.51479**	**4.10138**	**0.47127**
C	**6.00978**	**-3.7314**	**-1.4346**
C	**5.85189**	**-4.3255**	**-2.683**
C	**5.93753**	**-3.5571**	**-3.8458**
C	**6.16784**	**-2.1831**	**-3.7545**
C	**6.31214**	**-1.5814**	**-2.5084**
C	**9.07415**	**5.39685**	**0.86415**
N	**8.69166**	**6.45074**	**1.18489**
C	**10.8874**	**3.96496**	**0.11908**
N	**12.0072**	**3.83454**	**-0.1788**
C	**7.71041**	**-3.5305**	**1.02264**
N	**8.25386**	**-4.5591**	**1.04737**
C	**7.13776**	**-1.5908**	**2.32671**
N	**7.20266**	**-1.1062**	**3.38246**
H	**4.18261**	**1.84079**	**-0.8511**
H	**1.62023**	**1.45928**	**-0.7384**
H	**1.02503**	**-3.1111**	**0.89568**
H	**-1.5564**	**-3.4548**	**1.05003**
H	**-3.774**	**-2.2073**	**0.72732**
H	**-3.4553**	**0.71687**	**-0.1573**
H	**-5.3635**	**2.01636**	**-0.48**
H	**-7.7944**	**2.33978**	**-0.5432**
H	**-8.3582**	**-1.7743**	**0.5861**
H	**-5.9426**	**-2.0946**	**0.66207**
H	**-11.914**	**-0.7888**	**-0.6701**
H	**-13.412**	**-2.0151**	**0.87337**
H	**-12.855**	**-2.1782**	**3.29333**
H	**-10.791**	**-1.084**	**4.15224**
H	**-9.3106**	**0.16598**	**2.61137**
H	**-11.546**	**2.2957**	**0.50953**
H	**-12.599**	**3.84911**	**-1.1057**
H	**-11.89**	**3.84521**	**-3.491**
H	**-10.128**	**2.25635**	**-4.2436**
H	**-9.0994**	**0.68377**	**-2.6326**
H	**8.58603**	**-0.3096**	**-0.3696**
H	**10.1179**	**1.5692**	**-0.255**
H	**6.91055**	**4.10422**	**1.18686**
H	**5.37082**	**2.22672**	**1.06644**
H	**5.91815**	**-4.3387**	**-0.5425**
H	**5.65606**	**-5.3912**	**-2.7465**
H	**5.81799**	**-4.0259**	**-4.8177**
H	**6.23255**	**-1.5789**	**-4.654**
H	**6.49081**	**-0.5134**	**-2.4438**

2c			
Symbol	**X**	**Y**	**Z**
C	**2.89927**	**-0.5527**	**0.13104**
C	**2.68151**	**-1.8431**	**0.61974**
C	**1.32907**	**-2.1933**	**0.71968**
C	**0.44929**	**-1.1883**	**0.32162**
S	**1.34489**	**0.22577**	**-0.1901**
C	**-0.9825**	**-1.2721**	**0.31937**
C	**-1.842**	**-0.2775**	**-0.027**
C	**-3.2899**	**-0.3306**	**-0.0529**
C	**-4.015**	**0.83298**	**-0.3851**
C	**-5.4**	**0.85099**	**-0.4203**
C	**-6.1377**	**-0.3142**	**-0.1313**
C	**-5.4238**	**-1.4894**	**0.19384**
C	**-4.0414**	**-1.492**	**0.23365**
N	**-7.5415**	**-0.3126**	**-0.1713**
C	**-8.2973**	**-1.1719**	**0.68194**
C	**-8.2447**	**0.5544**	**-1.0621**
C	**-9.3691**	**-1.9127**	**0.1631**
C	**-10.121**	**-2.7342**	**1.00012**
C	**-9.8086**	**-2.8401**	**2.35676**
C	**-8.7386**	**-2.107**	**2.87347**
C	**-7.9911**	**-1.2696**	**2.04754**
C	**-9.3323**	**1.30791**	**-0.5977**
C	**-10.033**	**2.13625**	**-1.4721**
C	**-9.6521**	**2.23614**	**-2.8115**
C	**-8.5658**	**1.49033**	**-3.2737**
C	**-7.8696**	**0.64632**	**-2.4106**
C	**4.12898**	**0.15815**	**-0.0676**
C	**4.04662**	**1.66027**	**0.02188**
C	**3.9126**	**2.24596**	**1.35367**
C	**5.37053**	**-0.4462**	**-0.3097**
C	**5.50544**	**-1.8217**	**-0.7256**
C	**6.60149**	**0.2922**	**-0.1502**
C	**7.82034**	**-0.2957**	**-0.2934**
C	**7.9435**	**-1.6847**	**-0.6507**
C	**6.72201**	**-2.4081**	**-0.8917**
C	**4.09832**	**2.36292**	**-1.1606**
C	**9.19442**	**-2.2984**	**-0.7829**
C	**3.50424**	**3.58843**	**1.69658**
C	**3.49491**	**3.81118**	**3.03864**
S	**3.98764**	**2.40436**	**3.93446**

C	4.19518	1.50312	2.49054
C	4.06916	3.79124	-1.2643
N	4.04816	4.9485	-1.387
C	4.18181	1.68986	-2.4255
N	4.23702	1.18691	-3.4733
C	10.4033	-1.5777	-0.5692
N	11.382	-0.9711	-0.3849
C	9.31377	-3.6743	-1.1282
N	9.38867	-4.804	-1.408
H	3.48884	-2.4859	0.94664
H	0.98026	-3.1493	1.09345
H	-1.371	-2.2387	0.632
H	-1.4175	0.68241	-0.3207
H	-3.4715	1.74827	-0.6049
H	-5.9219	1.76868	-0.6652
H	-5.9693	-2.4027	0.40168
H	-3.5339	-2.4218	0.47086
H	-9.6063	-1.8378	-0.8929
H	-10.949	-3.3027	0.58575
H	-10.394	-3.4854	3.0047
H	-8.4918	-2.1732	3.92905
H	-7.1712	-0.6867	2.45407
H	-9.6226	1.23764	0.4453
H	-10.874	2.71449	-1.1001
H	-10.197	2.88682	-3.4885
H	-8.2659	1.55244	-4.3156
H	-7.0361	0.05503	-2.775
H	4.61232	-2.3812	-0.9746
H	6.55414	1.3367	0.13744
H	8.7242	0.28199	-0.1313
H	6.78632	-3.433	-1.2419
H	3.2192	4.34456	0.97986
H	3.22352	4.71797	3.56039
H	4.52421	0.47554	2.53512

2d			
Symbol	X	Y	Z
C	2.89796	-0.6098	0.17499
C	2.67475	-1.9137	0.62526
C	1.32102	-2.2609	0.71548
C	0.44552	-1.2402	0.34853
S	1.34616	0.18562	-0.1181
C	-0.9867	-1.318	0.3423

C	**-1.8407**	**-0.3118**	**0.01628**
C	**-3.2886**	**-0.3566**	**-0.0149**
C	**-4.0057**	**0.81502**	**-0.3363**
C	**-5.3904**	**0.84103**	**-0.3786**
C	**-6.1357**	**-0.3234**	**-0.1073**
C	**-5.4302**	**-1.5061**	**0.20838**
C	**-4.0479**	**-1.5169**	**0.25499**
N	**-7.5394**	**-0.3137**	**-0.1554**
C	**-8.3046**	**-1.1779**	**0.68446**
C	**-8.2327**	**0.56527**	**-1.0422**
C	**-9.3759**	**-1.9093**	**0.15149**
C	**-10.137**	**-2.7358**	**0.97563**
C	**-9.8336**	**-2.8559**	**2.33323**
C	**-8.7641**	**-2.1321**	**2.86398**
C	**-8.0078**	**-1.2899**	**2.05103**
C	**-9.3207**	**1.31822**	**-0.578**
C	**-10.012**	**2.1583**	**-1.4488**
C	**-9.6207**	**2.27062**	**-2.7843**
C	**-8.5339**	**1.52545**	**-3.2462**
C	**-7.8473**	**0.66979**	**-2.3869**
C	**4.13153**	**0.09981**	**0.0019**
C	**4.05321**	**1.60349**	**0.12088**
C	**4.0081**	**2.14051**	**1.46193**
C	**5.3736**	**-0.4971**	**-0.2499**
C	**5.51089**	**-1.8621**	**-0.6983**
C	**6.60299**	**0.24089**	**-0.0777**
C	**7.82275**	**-0.3417**	**-0.2338**
C	**7.94845**	**-1.7233**	**-0.618**
C	**6.72835**	**-2.4432**	**-0.8759**
C	**4.01974**	**2.3206**	**-1.0574**
C	**9.20048**	**-2.3325**	**-0.7606**
C	**4.15453**	**1.38451**	**2.62092**
C	**4.08268**	**2.14084**	**3.81042**
C	**3.87851**	**3.47685**	**3.5658**
S	**3.77623**	**3.83754**	**1.88527**
C	**3.92631**	**3.74545**	**-1.1334**
N	**3.84685**	**4.90319**	**-1.2308**
C	**4.05584**	**1.66111**	**-2.3295**
N	**4.07489**	**1.16553**	**-3.3825**
C	**10.408**	**-1.6145**	**-0.5306**
N	**11.3856**	**-1.0103**	**-0.3327**
C	**9.32251**	**-3.7012**	**-1.1325**
N	**9.39978**	**-4.825**	**-1.4342**
H	**3.47928**	**-2.5697**	**0.93194**

H	**0.96833**	**-3.2269**	**1.05892**
H	**-1.3799**	**-2.2903**	**0.63071**
H	**-1.4107**	**0.65169**	**-0.2568**
H	**-3.456**	**1.72974**	**-0.5427**
H	**-5.906**	**1.76433**	**-0.6154**
H	**-5.9817**	**-2.4186**	**0.40339**
H	**-3.5468**	**-2.452**	**0.48501**
H	**-9.6058**	**-1.8234**	**-0.9052**
H	**-10.964**	**-3.297**	**0.55038**
H	**-10.425**	**-3.5049**	**2.97109**
H	**-8.5246**	**-2.2094**	**3.92048**
H	**-7.1883**	**-0.7142**	**2.46842**
H	**-9.6188**	**1.23844**	**0.46211**
H	**-10.853**	**2.73598**	**-1.077**
H	**-10.158**	**2.93046**	**-3.4585**
H	**-8.2259**	**1.59732**	**-4.2851**
H	**-7.0133**	**0.07921**	**-2.7514**
H	**4.61904**	**-2.417**	**-0.9617**
H	**6.55439**	**1.28015**	**0.22789**
H	**8.72568**	**0.23464**	**-0.0621**
H	**6.79452**	**-3.4602**	**-1.2479**
H	**4.31054**	**0.31386**	**2.59827**
H	**4.17869**	**1.71972**	**4.80363**
H	**3.78518**	**4.27805**	**4.28683**

2e			
Symbol	**X**	**Y**	**Z**
C	**-3.686**	**1.02784**	**0.32653**
C	**-4.4487**	**-0.0584**	**-0.1076**
S	**-3.374**	**-1.3798**	**-0.5765**
C	**-1.9437**	**-0.4497**	**-0.187**
C	**-2.303**	**0.81294**	**0.27992**
C	**-0.6303**	**-0.9978**	**-0.3559**
C	**-0.2652**	**-2.2844**	**-0.7213**
C	**1.12637**	**-2.4797**	**-0.791**
C	**1.87315**	**-1.3511**	**-0.4803**
S	**0.80549**	**-0.0102**	**-0.0989**
C	**3.30725**	**-1.2579**	**-0.4612**
C	**4.03864**	**-0.1594**	**-0.1459**
C	**5.4859**	**-0.0405**	**-0.1122**
C	**6.06588**	**1.19827**	**0.22909**
C	**7.43988**	**1.37906**	**0.27702**
C	**8.31082**	**0.31074**	**-0.0083**

C	**7.7442**	**-0.9371**	**-0.3456**
C	**6.37095**	**-1.1023**	**-0.3992**
N	**9.70765**	**0.47766**	**0.04537**
C	**10.5612**	**-0.2558**	**-0.8311**
C	**10.295**	**1.38855**	**0.97293**
C	**11.7149**	**-0.8789**	**-0.3329**
C	**12.558**	**-1.5806**	**-1.1923**
C	**12.2572**	**-1.6845**	**-2.5518**
C	**11.1064**	**-1.0691**	**-3.0484**
C	**10.2664**	**-0.3507**	**-2.1997**
C	**11.2993**	**2.27319**	**0.55298**
C	**11.8867**	**3.14875**	**1.46422**
C	**11.4728**	**3.16697**	**2.79747**
C	**10.469**	**2.29096**	**3.21572**
C	**9.88821**	**1.39967**	**2.31579**
C	**-5.8735**	**-0.2192**	**-0.1607**
C	**-6.3823**	**-1.629**	**-0.0238**
C	**-6.2932**	**-2.2422**	**1.3018**
C	**-6.7871**	**0.83486**	**-0.2964**
C	**-6.8823**	**-2.2321**	**-1.1561**
C	**-8.1862**	**0.65435**	**0.01376**
C	**-9.0736**	**1.68499**	**-0.0271**
C	**-8.6656**	**3.00841**	**-0.4203**
C	**-7.289**	**3.18054**	**-0.8064**
C	**-6.4005**	**2.15209**	**-0.7423**
C	**-9.5711**	**4.07501**	**-0.4492**
C	**-6.1048**	**-1.4525**	**2.49572**
C	**-6.0553**	**-2.1989**	**3.63189**
S	**-6.2213**	**-3.893**	**3.28592**
C	**-6.3719**	**-3.5939**	**1.60301**
C	**-9.1639**	**5.38514**	**-0.8292**
N	**-8.8083**	**6.45144**	**-1.1399**
C	**-10.938**	**3.90119**	**-0.0909**
N	**-12.053**	**3.73962**	**0.21134**
C	**-7.4272**	**-3.5555**	**-1.188**
N	**-7.867**	**-4.6322**	**-1.2382**
C	**-6.8752**	**-1.5684**	**-2.4279**
N	**-6.8791**	**-1.0751**	**-3.4818**
H	**-4.1327**	**1.93076**	**0.72298**
H	**-1.5738**	**1.54617**	**0.60445**
H	**-0.9898**	**-3.0645**	**-0.9269**
H	**1.59039**	**-3.4224**	**-1.0575**
H	**3.8111**	**-2.1833**	**-0.7319**
H	**3.50279**	**0.75231**	**0.11799**

H	**5.41648**	**2.04225**	**0.4473**
H	**7.84877**	**2.3503**	**0.53082**
H	**8.39592**	**-1.7773**	**-0.5566**
H	**5.97917**	**-2.0825**	**-0.6526**
H	**11.9441**	**-0.8076**	**0.72509**
H	**13.448**	**-2.0583**	**-0.7933**
H	**12.9132**	**-2.237**	**-3.2172**
H	**10.8667**	**-1.1339**	**-4.1057**
H	**9.38112**	**0.14046**	**-2.5899**
H	**11.6139**	**2.26778**	**-0.4853**
H	**12.6631**	**3.82837**	**1.12554**
H	**11.9283**	**3.85477**	**3.503**
H	**10.1449**	**2.28858**	**4.25234**
H	**9.11995**	**0.70855**	**2.64633**
H	**-8.5325**	**-0.3227**	**0.33217**
H	**-10.11**	**1.51995**	**0.24634**
H	**-6.9728**	**4.14761**	**-1.1831**
H	**-5.389**	**2.30604**	**-1.097**
H	**-6.0265**	**-0.3733**	**2.48924**
H	**-5.936**	**-1.8606**	**4.6512**
H	**-6.4936**	**-4.4262**	**0.9276**

2f			
Symbol	**X**	**Y**	**Z**
C	**-3.6581**	**1.06084**	**0.31702**
C	**-4.4241**	**-0.0449**	**-0.0604**
S	**-3.3527**	**-1.3945**	**-0.4513**
C	**-1.9201**	**-0.4479**	**-0.1125**
C	**-2.2758**	**0.83944**	**0.28474**
C	**-0.6086**	**-1.0076**	**-0.253**
C	**-0.2475**	**-2.3105**	**-0.5606**
C	**1.1433**	**-2.5131**	**-0.621**
C	**1.89375**	**-1.3742**	**-0.3609**
S	**0.83052**	**-0.0143**	**-0.0391**
C	**3.32808**	**-1.2842**	**-0.349**
C	**4.06305**	**-0.1751**	**-0.0832**
C	**5.51067**	**-0.0575**	**-0.0626**
C	**6.09447**	**1.19174**	**0.23054**
C	**7.46899**	**1.37246**	**0.26141**
C	**8.3366**	**0.29385**	**0.00649**
C	**7.7662**	**-0.9645**	**-0.2819**
C	**6.39242**	**-1.1299**	**-0.3188**

N	**9.7341**	**0.46088**	**0.0414**
C	**10.5782**	**-0.3015**	**-0.8194**
C	**10.3308**	**1.40366**	**0.93016**
C	**11.7365**	**-0.9094**	**-0.3131**
C	**12.5702**	**-1.6393**	**-1.1581**
C	**12.2554**	**-1.7867**	**-2.5104**
C	**11.1**	**-1.1866**	**-3.0147**
C	**10.2693**	**-0.4402**	**-2.1811**
C	**11.3311**	**2.27239**	**0.46961**
C	**11.9271**	**3.17968**	**1.34348**
C	**11.5258**	**3.24556**	**2.67905**
C	**10.5259**	**2.38537**	**3.13756**
C	**9.93659**	**1.46281**	**2.27551**
C	**-5.8487**	**-0.2016**	**-0.1013**
C	**-6.3662**	**-1.6093**	**0.07659**
C	**-6.4136**	**-2.1103**	**1.43136**
C	**-6.7652**	**0.84268**	**-0.2782**
C	**-6.7323**	**-2.2873**	**-1.0682**
C	**-8.1662**	**0.66358**	**0.02334**
C	**-9.0601**	**1.68553**	**-0.0653**
C	**-8.657**	**2.99662**	**-0.5025**
C	**-7.2785**	**3.16308**	**-0.8841**
C	**-6.3841**	**2.14364**	**-0.7743**
C	**-9.5691**	**4.05539**	**-0.5779**
C	**-6.1271**	**-1.3542**	**2.56394**
C	**-6.256**	**-2.0668**	**3.77541**
C	**-6.6396**	**-3.3701**	**3.57384**
S	**-6.8551**	**-3.7506**	**1.90851**
C	**-9.1668**	**5.35352**	**-1.0018**
N	**-8.8155**	**6.41016**	**-1.3482**
C	**-10.938**	**3.88532**	**-0.2253**
N	**-12.054**	**3.72695**	**0.07309**
C	**-7.2231**	**-3.6302**	**-1.0896**
N	**-7.6223**	**-4.7229**	**-1.1424**
C	**-6.6218**	**-1.6765**	**-2.3602**
N	**-6.5401**	**-1.2209**	**-3.4281**
H	**-4.1019**	**1.98515**	**0.66398**
H	**-1.5449**	**1.58784**	**0.56815**
H	**-0.9747**	**-3.0963**	**-0.7332**
H	**1.60423**	**-3.4681**	**-0.8461**
H	**3.82889**	**-2.2215**	**-0.5815**
H	**3.53017**	**0.74795**	**0.14508**
H	**5.44761**	**2.0437**	**0.42378**
H	**7.88067**	**2.35163**	**0.4775**

H	8.41553	-1.8122	-0.4689
H	5.99776	-2.1177	-0.5354
H	11.9766	-0.8044	0.73964
H	13.4639	-2.1049	-0.753
H	12.9041	-2.3612	-3.1642
H	10.8493	-1.2855	-4.0668
H	9.38038	0.03898	-2.5779
H	11.636	2.2298	-0.5707
H	12.7004	3.84643	0.9734
H	11.9879	3.95787	3.35536
H	10.2115	2.42015	4.17659
H	9.17118	0.78441	2.63751
H	-8.5095	-0.3039	0.37243
H	-10.099	1.52303	0.20214
H	-6.9654	4.11709	-1.2951
H	-5.3718	2.29067	-1.1296
H	-5.8335	-0.3141	2.50736
H	-6.0756	-1.638	4.75344
H	-6.8126	-4.135	4.31921

2g			
Symbol	X	Y	Z
C	-2.7269	-1.1154	-0.4477
C	-3.7313	-0.1571	-0.2676
S	-3.0097	1.43498	0.10478
C	-1.4032	0.78181	-0.008
C	-1.4388	-0.5868	-0.3129
C	-5.1409	-0.4195	-0.2678
C	-5.4929	-1.875	-0.0692
C	-5.4251	-2.4015	1.29131
C	-6.1865	0.50748	-0.3942
C	-5.8424	-2.5891	-1.1928
C	-5.9964	1.86597	-0.8428
C	-7.0237	2.75609	-0.9099
C	-8.3618	2.39105	-0.526
C	-8.5735	1.02642	-0.1223
C	-7.546	0.13542	-0.0755
C	-9.4109	3.31702	-0.5617
C	-5.4553	-3.7837	1.71203
C	-5.3773	-3.9272	3.06275
S	-5.2716	-2.3926	3.87401
C	-5.3208	-1.5501	2.38226
C	-0.1069	1.3132	0.12581

C	**0.87825**	**0.35421**	**-0.0744**
S	**0.17921**	**-1.2374**	**-0.437**
C	**2.29325**	**0.5828**	**-0.0047**
C	**3.26734**	**-0.3395**	**-0.2182**
C	**4.70233**	**-0.1362**	**-0.1587**
C	**5.56271**	**-1.2239**	**-0.4147**
C	**6.94221**	**-1.0964**	**-0.371**
C	**7.53588**	**0.1455**	**-0.0728**
C	**6.68617**	**1.24453**	**0.18152**
C	**5.31064**	**1.10246**	**0.14193**
N	**8.93322**	**0.29116**	**-0.0323**
C	**9.54254**	**1.23427**	**0.84851**
C	**9.77289**	**-0.505**	**-0.8687**
C	**10.9035**	**-1.1382**	**-0.3329**
C	**11.7346**	**-1.8975**	**-1.1544**
C	**11.4435**	**-2.048**	**-2.5115**
C	**10.315**	**-1.4221**	**-3.0451**
C	**9.48754**	**-0.647**	**-2.2349**
C	**10.5589**	**2.08003**	**0.38072**
C	**11.1677**	**2.98704**	**1.2459**
C	**10.7637**	**3.07466**	**2.57953**
C	**9.74833**	**2.23681**	**3.04518**
C	**9.14578**	**1.31451**	**2.19184**
C	**-10.737**	**2.95245**	**-0.1962**
N	**-11.817**	**2.63495**	**0.11139**
C	**-9.1972**	**4.66768**	**-0.9572**
N	**-9.0008**	**5.77052**	**-1.2814**
C	**-6.2409**	**-3.9649**	**-1.2007**
N	**-6.5666**	**-5.0815**	**-1.2456**
C	**-5.8247**	**-1.9818**	**-2.4931**
N	**-5.8089**	**-1.535**	**-3.5674**
H	**-2.9442**	**-2.1489**	**-0.6833**
H	**-5.0222**	**2.17604**	**-1.1984**
H	**-6.8456**	**3.75907**	**-1.2831**
H	**-9.5752**	**0.71404**	**0.15318**
H	**-7.7516**	**-0.8781**	**0.24939**
H	**-5.5217**	**-4.6283**	**1.04215**
H	**-5.3727**	**-4.8442**	**3.63471**
H	**-5.2804**	**-0.4709**	**2.36836**
H	**0.12515**	**2.3457**	**0.35647**
H	**2.56383**	**1.60686**	**0.24236**
H	**2.96286**	**-1.356**	**-0.4668**
H	**5.13123**	**-2.1959**	**-0.6397**
H	**7.57077**	**-1.9588**	**-0.5608**

H	7.12053	2.213	0.40112
H	4.69683	1.97714	0.33317
H	11.1248	-1.0295	0.72361
H	12.6072	-2.3829	-0.7274
H	12.0899	-2.6451	-3.1471
H	10.0835	-1.5237	-4.1013
H	8.6199	-0.1479	-2.6536
H	10.8658	2.01993	-0.6581
H	11.9534	3.63617	0.87079
H	11.2361	3.78657	3.24909
H	9.43222	2.28853	4.08293
H	8.36889	0.65241	2.55962

2h			
Symbol	X	Y	Z
C	-2.722	-1.1632	-0.3383
C	-3.7277	-0.1995	-0.1955
S	-3.0096	1.40519	0.12025
C	-1.4022	0.75137	0.03121
C	-1.4352	-0.6278	-0.2224
C	-5.1377	-0.4638	-0.1939
C	-5.4867	-1.9135	0.05682
C	-5.4584	-2.3834	1.425
C	-6.1874	0.44949	-0.3737
C	-5.7973	-2.6809	-1.0484
C	-5.9973	1.79365	-0.8633
C	-7.0297	2.67184	-0.9851
C	-8.3738	2.30779	-0.622
C	-8.5844	0.95566	-0.1778
C	-7.5511	0.07648	-0.0751
C	-9.4292	3.2223	-0.7151
C	-0.1067	1.28968	0.14372
C	0.88012	0.32599	-0.0227
S	0.18393	-1.2795	-0.324
C	2.29496	0.55993	0.03259
C	3.26974	-0.3669	-0.1565
C	4.70481	-0.159	-0.1145
C	5.56529	-1.2506	-0.3529
C	6.94482	-1.1187	-0.3278
C	7.5383	0.13174	-0.0671
C	6.68854	1.23422	0.17116
C	5.31296	1.08775	0.15041
N	8.93585	0.28167	-0.0477

C	**9.55352**	**1.2485**	**0.80095**
C	**9.76677**	**-0.5298**	**-0.8779**
C	**10.9083**	**-1.1454**	**-0.3444**
C	**11.7309**	**-1.9198**	**-1.1602**
C	**11.4206**	**-2.1033**	**-2.5091**
C	**10.2813**	**-1.4951**	**-3.0402**
C	**9.46209**	**-0.7051**	**-2.2361**
C	**10.5583**	**2.08768**	**0.29788**
C	**11.1753**	**3.01827**	**1.13174**
C	**10.7906**	**3.13596**	**2.46879**
C	**9.78663**	**2.30468**	**2.9695**
C	**9.17616**	**1.35922**	**2.14767**
C	**-5.5865**	**-3.662**	**1.95888**
C	**-5.5211**	**-3.6905**	**3.36977**
C	**-5.3477**	**-2.4427**	**3.92008**
S	**-5.2549**	**-1.2105**	**2.7259**
C	**-10.762**	**2.85827**	**-0.3709**
N	**-11.846**	**2.54188**	**-0.0805**
C	**-9.2173**	**4.56089**	**-1.1509**
N	**-9.023**	**5.65398**	**-1.5077**
C	**-6.1647**	**-4.0615**	**-0.9952**
N	**-6.4599**	**-5.1876**	**-0.9695**
C	**-5.7517**	**-2.1295**	**-2.3703**
N	**-5.7144**	**-1.7261**	**-3.4614**
H	**-2.9375**	**-2.2048**	**-0.5369**
H	**-5.0171**	**2.10118**	**-1.204**
H	**-6.8503**	**3.66365**	**-1.3864**
H	**-9.5901**	**0.64342**	**0.08282**
H	**-7.7575**	**-0.9278**	**0.27673**
H	**0.12366**	**2.33057**	**0.33507**
H	**2.5646**	**1.59245**	**0.24287**
H	**2.96581**	**-1.3913**	**-0.3708**
H	**5.134**	**-2.2288**	**-0.5497**
H	**7.57365**	**-1.9837**	**-0.5038**
H	**7.12255**	**2.20872**	**0.36314**
H	**4.69884**	**1.96496**	**0.32864**
H	**11.1445**	**-1.0112**	**0.70595**
H	**12.612**	**-2.3912**	**-0.735**
H	**12.0605**	**-2.7121**	**-3.1401**
H	**10.0348**	**-1.6225**	**-4.0901**
H	**8.58584**	**-0.2201**	**-2.6534**
H	**10.8501**	**2.00395**	**-0.7437**
H	**11.9519**	**3.66198**	**0.72938**
H	**11.2692**	**3.86601**	**3.11402**

H	**9.48566**	**2.37995**	**4.01032**
H	**8.40794**	**0.70257**	**2.54247**
H	**-5.7166**	**-4.5501**	**1.35691**
H	**-5.5989**	**-4.5978**	**3.95651**
H	**-5.2712**	**-2.1835**	**4.96736**

2i			
Symbol	**X**	**Y**	**Z**
C	**-5.4878**	**0.71214**	**-0.0236**
C	**-5.7002**	**-0.6626**	**-0.1219**
S	**-4.1484**	**-1.4873**	**-0.1599**
C	**-3.2609**	**0.02033**	**-0.0344**
C	**-4.1397**	**1.11577**	**0.01989**
C	**-1.8252**	**-0.0422**	**0.00319**
C	**-1.043**	**-1.1765**	**0.18603**
C	**0.34065**	**-0.9407**	**0.1349**
C	**0.67442**	**0.38751**	**-0.0888**
S	**-0.7784**	**1.35731**	**-0.2389**
C	**1.97805**	**0.98415**	**-0.1898**
C	**-6.9277**	**-1.4037**	**-0.1436**
C	**-6.8547**	**-2.8151**	**0.37869**
C	**-6.7503**	**-2.9898**	**1.82559**
C	**-8.1575**	**-0.8994**	**-0.5908**
C	**-6.8855**	**-3.8315**	**-0.5491**
C	**-8.2692**	**0.29643**	**-1.391**
C	**-9.4757**	**0.80541**	**-1.7615**
C	**-10.709**	**0.17868**	**-1.3635**
C	**-10.607**	**-1.0472**	**-0.6161**
C	**-9.3977**	**-1.5639**	**-0.2663**
C	**-11.951**	**0.72492**	**-1.7092**
C	**-6.3361**	**-4.1691**	**2.54933**
C	**-6.3588**	**-3.9959**	**3.89857**
S	**-6.891**	**-2.4001**	**4.33998**
C	**-7.0707**	**-1.9563**	**2.69314**
C	**-3.6994**	**2.55799**	**0.15015**
C	**-4.8243**	**3.57695**	**0.37927**
C	**-4.2966**	**5.00878**	**0.53341**
C	**-5.407**	**6.04528**	**0.74241**
C	**-4.8844**	**7.47862**	**0.89929**
C	**-5.9999**	**8.50812**	**1.10184**
S	**3.43264**	**0.00075**	**-0.058**
C	**4.47531**	**1.39785**	**-0.2795**
C	**3.70735**	**2.53964**	**-0.4438**

C	**2.31696**	**2.3106**	**-0.394**
C	**5.91237**	**1.32408**	**-0.2856**
C	**6.66207**	**0.20687**	**-0.1199**
C	**8.11293**	**0.10404**	**-0.1309**
C	**8.71368**	**-1.1512**	**0.09128**
C	**10.0911**	**-1.317**	**0.09649**
C	**10.942**	**-0.2218**	**-0.1369**
C	**10.3552**	**1.03967**	**-0.3668**
C	**8.97889**	**1.1949**	**-0.3585**
N	**12.3439**	**-0.3804**	**-0.1487**
C	**13.1932**	**0.65561**	**0.33677**
C	**12.9293**	**-1.5797**	**-0.6498**
C	**13.973**	**-2.2039**	**0.04986**
C	**14.5549**	**-3.367**	**-0.4508**
C	**14.0971**	**-3.933**	**-1.6421**
C	**13.0538**	**-3.3169**	**-2.3362**
C	**12.4778**	**-2.1439**	**-1.8529**
C	**14.343**	**1.02137**	**-0.3796**
C	**15.1817**	**2.02296**	**0.10506**
C	**14.8811**	**2.68509**	**1.29694**
C	**13.7338**	**2.32725**	**2.00781**
C	**12.8985**	**1.3145**	**1.5405**
C	**-13.171**	**0.09373**	**-1.3375**
N	**-14.16**	**-0.436**	**-1.0188**
C	**-12.048**	**1.94307**	**-2.4392**
N	**-12.105**	**2.94476**	**-3.0338**
C	**-6.8641**	**-5.2279**	**-0.2305**
N	**-6.8484**	**-6.3704**	**-0.0089**
C	**-6.9384**	**-3.5563**	**-1.9566**
N	**-6.969**	**-3.3802**	**-3.1064**
H	**-6.3089**	**1.40779**	**0.08124**
H	**-1.4693**	**-2.157**	**0.36515**
H	**1.08345**	**-1.7186**	**0.26724**
H	**-7.3642**	**0.76302**	**-1.7595**
H	**-9.5217**	**1.68478**	**-2.3953**
H	**-11.52**	**-1.5567**	**-0.3253**
H	**-9.3671**	**-2.4802**	**0.3129**
H	**-6.0235**	**-5.0937**	**2.08657**
H	**-6.0904**	**-4.7087**	**4.66531**
H	**-7.4136**	**-0.9663**	**2.43158**
H	**-2.9749**	**2.63817**	**0.97134**
H	**-3.1487**	**2.84698**	**-0.7562**
H	**-5.5305**	**3.54444**	**-0.4608**
H	**-5.3943**	**3.30217**	**1.2768**

H	-3.5964	5.04847	1.3796
H	-3.7117	5.27755	-0.3575
H	-6.1054	6.00585	-0.1055
H	-5.995	5.77511	1.63118
H	-4.1891	7.5189	1.74877
H	-4.2947	7.74686	0.01221
H	-5.5956	9.51958	1.2098
H	-6.6915	8.51541	0.25199
H	-6.5856	8.28644	2.00113
H	4.15174	3.51671	-0.5965
H	1.57772	3.09619	-0.5049
H	6.40008	2.28403	-0.4421
H	6.14261	-0.7376	0.04166
H	8.07913	-2.0137	0.27875
H	10.5179	-2.296	0.28332
H	10.9925	1.89512	-0.5611
H	8.56975	2.18151	-0.5527
H	14.3224	-1.7719	0.9817
H	15.3621	-3.839	0.10176
H	14.5486	-4.8427	-2.0256
H	12.6943	-3.7419	-3.2689
H	11.6778	-1.659	-2.4023
H	14.573	0.51678	-1.312
H	16.0682	2.29494	-0.4605
H	15.5336	3.46923	1.66812
H	13.493	2.82755	2.94133
H	12.0167	1.02749	2.10364

2j			
Symbol	X	Y	Z
C	-2.7938	-1.4312	-0.6355
C	-3.5757	-0.7901	0.32685
S	-2.5472	0.23466	1.33153
C	-1.1077	-0.217	0.44373
C	-1.4305	-1.1165	-0.5702
C	0.17733	0.31447	0.7889
C	0.4894	1.32604	1.68419
C	1.86724	1.59452	1.77822
C	2.65763	0.79755	0.96029
S	1.64818	-0.3173	0.05278
C	4.08951	0.84408	0.84988
C	4.86218	0.04685	0.0687

C	**6.30669**	**0.0693**	**-0.0647**
C	**6.94474**	**-0.8999**	**-0.8647**
C	**8.32002**	**-0.9432**	**-1.0198**
C	**9.16389**	**-0.0026**	**-0.3819**
C	**8.52242**	**0.9877**	**0.40567**
C	**7.14584**	**1.01334**	**0.5593**
N	**10.5515**	**-0.066**	**-0.5185**
C	**11.3674**	**0.89516**	**0.232**
C	**11.1279**	**-0.5596**	**-1.7827**
C	**12.8195**	**0.47177**	**0.47969**
C	**13.5618**	**1.49731**	**1.34825**
C	**15.019**	**1.10984**	**1.61509**
C	**11.902**	**-1.8885**	**-1.7047**
C	**11.0804**	**-3.1174**	**-1.2995**
C	**11.9357**	**-4.3828**	**-1.1802**
C	**-4.9936**	**-0.8455**	**0.54329**
C	**-5.6246**	**0.38253**	**1.13056**
C	**-5.7929**	**-1.9499**	**0.20707**
C	**-7.2265**	**-1.8278**	**0.08326**
C	**-8.0066**	**-2.8631**	**-0.3317**
C	**-7.4412**	**-4.1513**	**-0.6351**
C	**-6.023**	**-4.3042**	**-0.4411**
C	**-5.2439**	**-3.2594**	**-0.0491**
C	**-8.2371**	**-5.2148**	**-1.0775**
C	**-5.628**	**1.60969**	**0.31414**
C	**-6.1644**	**0.2949**	**2.39299**
C	**-5.5158**	**2.89637**	**0.86879**
C	**-5.5362**	**4.02763**	**0.05775**
C	**-5.6755**	**3.92558**	**-1.3323**
C	**-5.7733**	**2.63747**	**-1.8853**
C	**-5.7381**	**1.50325**	**-1.0881**
C	**-5.7236**	**5.12996**	**-2.2534**
C	**-5.5311**	**6.50566**	**-1.6078**
C	**-5.5927**	**7.64981**	**-2.6276**
C	**-5.4048**	**9.03047**	**-1.9927**
C	**-7.6741**	**-6.485**	**-1.3873**
N	**-7.192**	**-7.5165**	**-1.6397**
C	**-9.6429**	**-5.0719**	**-1.2485**
N	**-10.792**	**-4.9334**	**-1.3879**
C	**-6.8953**	**1.35069**	**3.03219**
N	**-7.5054**	**2.17122**	**3.58805**
C	**-6.0422**	**-0.8935**	**3.18908**
N	**-5.9528**	**-1.8273**	**3.8775**
H	**-3.2218**	**-2.0634**	**-1.4031**

H	**-0.6934**	**-1.5044**	**-1.2636**
H	**-0.265**	**1.86258**	**2.24904**
H	**2.29091**	**2.35398**	**2.42545**
H	**4.55576**	**1.60016**	**1.47797**
H	**4.36371**	**-0.7133**	**-0.5331**
H	**6.33936**	**-1.6514**	**-1.3657**
H	**8.74681**	**-1.7356**	**-1.6195**
H	**9.0987**	**1.7695**	**0.88204**
H	**6.71458**	**1.80529**	**1.16441**
H	**11.3604**	**1.88294**	**-0.2634**
H	**10.9031**	**1.02886**	**1.2117**
H	**10.3248**	**-0.6458**	**-2.5199**
H	**11.8025**	**0.21638**	**-2.1698**
H	**12.8302**	**-0.5068**	**0.97532**
H	**13.3604**	**0.35519**	**-0.4666**
H	**13.528**	**2.48016**	**0.85919**
H	**13.0336**	**1.61463**	**2.30397**
H	**15.5214**	**1.8577**	**2.23641**
H	**15.0847**	**0.14745**	**2.13457**
H	**15.584**	**1.02053**	**0.68053**
H	**12.3462**	**-2.06**	**-2.6956**
H	**12.7428**	**-1.7811**	**-1.0117**
H	**10.5797**	**-2.9197**	**-0.3441**
H	**10.2862**	**-3.29**	**-2.0385**
H	**11.3296**	**-5.2479**	**-0.8936**
H	**12.4287**	**-4.6217**	**-2.1294**
H	**12.7191**	**-4.2606**	**-0.4237**
H	**-7.6914**	**-0.8687**	**0.28257**
H	**-9.0763**	**-2.7241**	**-0.4472**
H	**-5.5824**	**-5.2851**	**-0.5853**
H	**-4.191**	**-3.4283**	**0.14003**
H	**-5.3853**	**3.02066**	**1.9369**
H	**-5.4365**	**5.00107**	**0.52447**
H	**-5.8768**	**2.52691**	**-2.9617**
H	**-5.8172**	**0.52332**	**-1.5469**
H	**-4.9667**	**4.99186**	**-3.0383**
H	**-6.6882**	**5.11497**	**-2.781**
H	**-6.301**	**6.66721**	**-0.8415**
H	**-4.5646**	**6.53878**	**-1.0868**
H	**-4.8243**	**7.49176**	**-3.3965**
H	**-6.5574**	**7.6156**	**-3.1515**
H	**-5.4533**	**9.82424**	**-2.7446**
H	**-6.1805**	**9.23244**	**-1.2457**
H	**-4.4341**	**9.10752**	**-1.4902**