

Supporting Information

Improvement of hole-transporting and electroluminescent properties of diketopyrrolopyrrole pigment by grafting with carbazole dendrons

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1. Synthesis and characterization

G1-hexyl bromide (2): 1,6-Dibromohexane (2.8 mL, 18.0 mmol) was added to a mixture of 3,6-di-*tert*-butyl-carbazole (**1**) (1.0 g, 3.6 mmol), KOH (0.81 g, 14.4 mmol), and *N,N*-dimethylformamide (DMF, 50 mL) at 0°C. The system was stirred at room temperature for 24 h and then diluted with water (100 mL). The solution was extracted with CH₂Cl₂ (3 x 50 mL), and the combined organic layers, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by column chromatography (CH₂Cl₂/hexane) to afford white solids (1.22 g, 77%); ¹H-NMR (600 MHz, CDCl₃): δ = 8.10 (s, 2H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.4 Hz, 2H), 4.25 (t, *J* = 7.2 Hz, 2H), 3.36 (t, *J* = 6.6 Hz, 2H), 1.81-1.90 (m, 4H), 1.44 (s, 18H), 1.41-1.39 (m, 4H); ¹³C-NMR (150 MHz, CDCl₃): δ = 141.5, 139.0, 123.3, 122.7, 116.3, 108.0, 43.0, 34.7, 33.7, 32.6, 32.4, 32.1, 29.0, 28.0, 26.5; *m/z* (MALDI-TOF): 441.3330 (C₂₆H₃₆BrN required *m/z* = 441.2031).

G2-hexyl bromide (4): 1,6-Dibromohexane (1.1 mL, 6.92 mmol) was added to a mixture of **3** (1.0 g, 1.40 mmol), KOH (0.31 g, 5.54 mmol), and *N,N*-dimethylformamide (DMF, 50 mL) at 0°C. The mixture was stirred at room temperature for 24 h and then quenched with water and CH₂Cl₂ (20 ml) was added. The organic phase was washed with water (50 mL × 2) and brine solution (50 ml), dried over anhydrous Na₂SO₄, and filtered. The solvent was removed to dryness, and the crude product was purified by column chromatography (SiO₂, CH₂Cl₂/hexane) to afford white solids (1.06 g, 86%); ¹H-NMR (600 MHz, CDCl₃): δ = 8.18 (s, 2H), 8.15 (s, 4H), 7.64 (m, 4H), 7.44 (m, 4H), 7.31 (m, 4H), 4.49 (t, *J* = 7.2 Hz, 2H), 3.43 (m, 2H), 2.09-1.91 (m, 4H), 1.46 (s, 36H), 1.44 (m, 4H); ¹³C-NMR (150 MHz, CDCl₃): δ = 142.5, 140.3, 139.9, 129.9, 125.7, 123.5, 123.4, 123.0, 119.5, 116.2, 109.9, 109.1, 43.5, 34.7, 33.7, 32.6, 31.9, 29.1, 28.0, 27.3, 26.6; *m/z* (MALDI-TOF): 883.6050 (C₅₈H₆₆BrN₃ required *m/z* = 883.4440).

2. Additional data

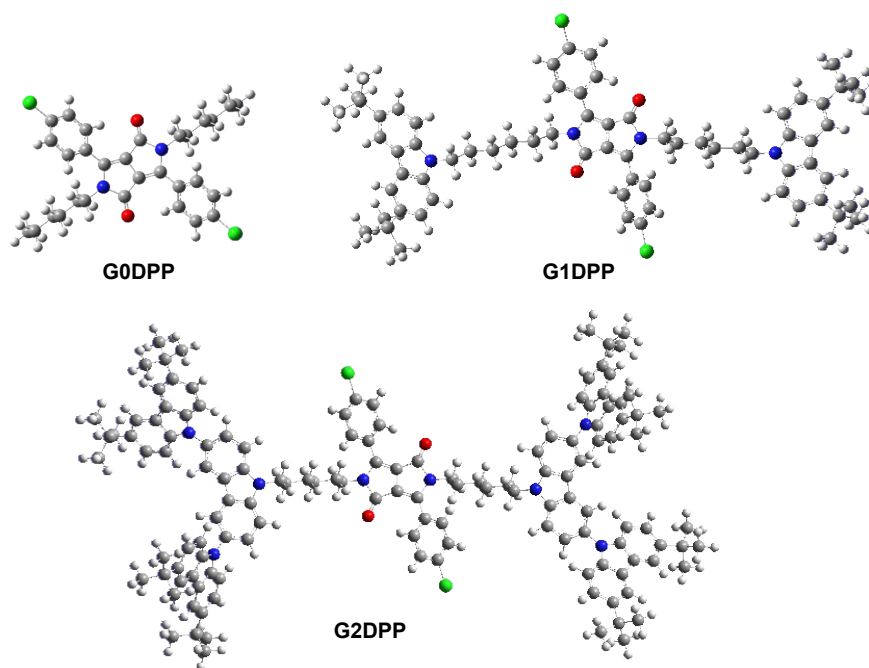


Fig. S1 Optimized geometry of DPP derivatives simulated with using B3LYP/6-31G(d) function.

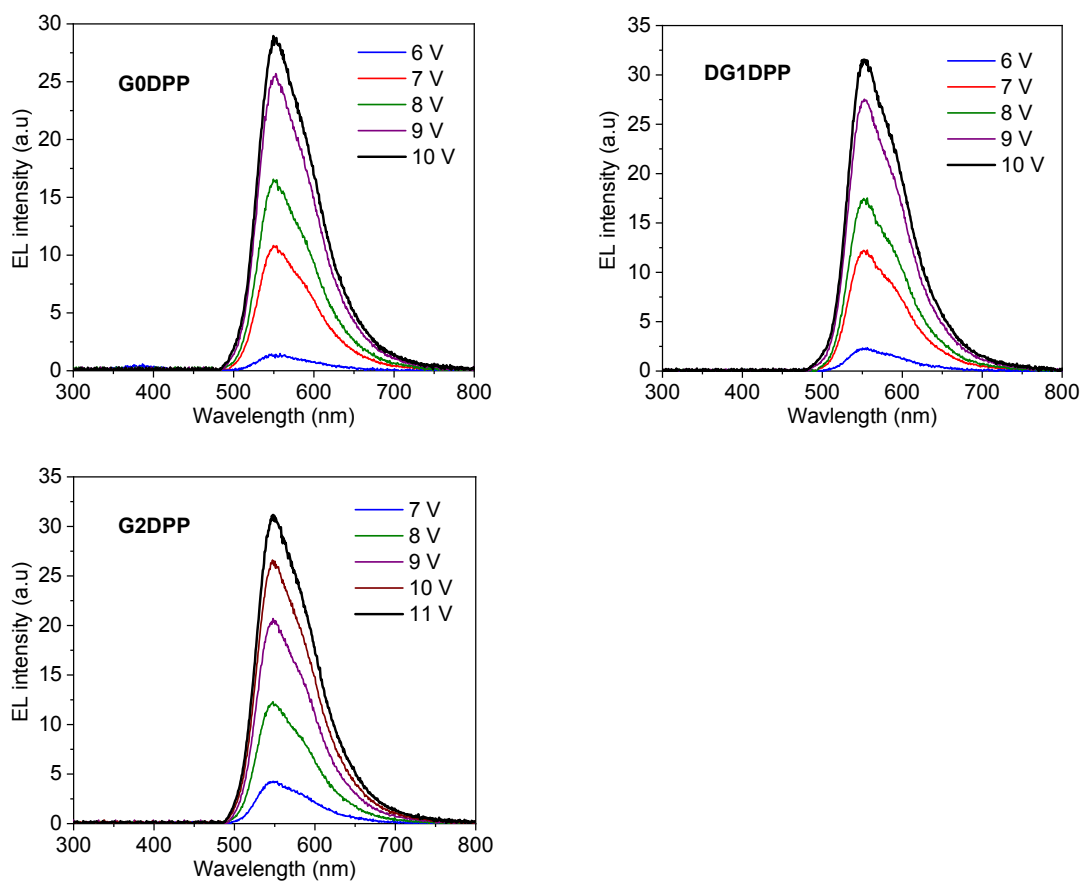
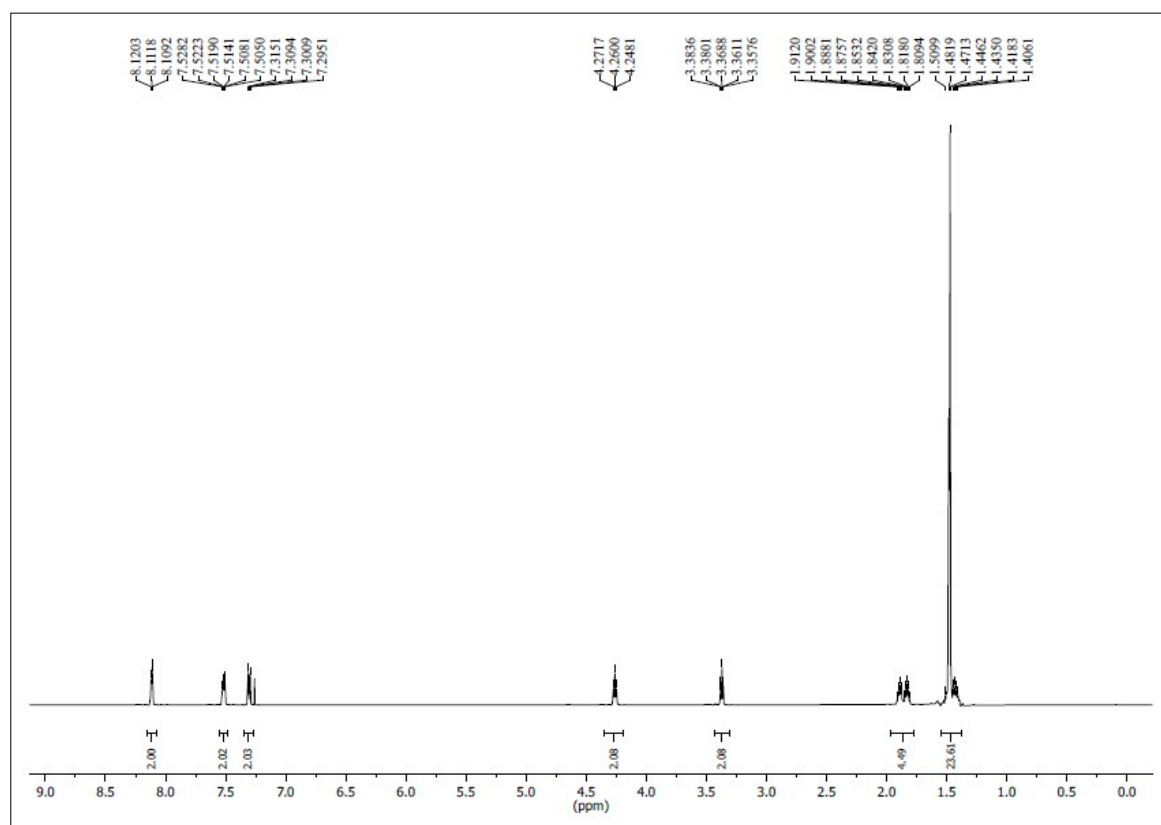
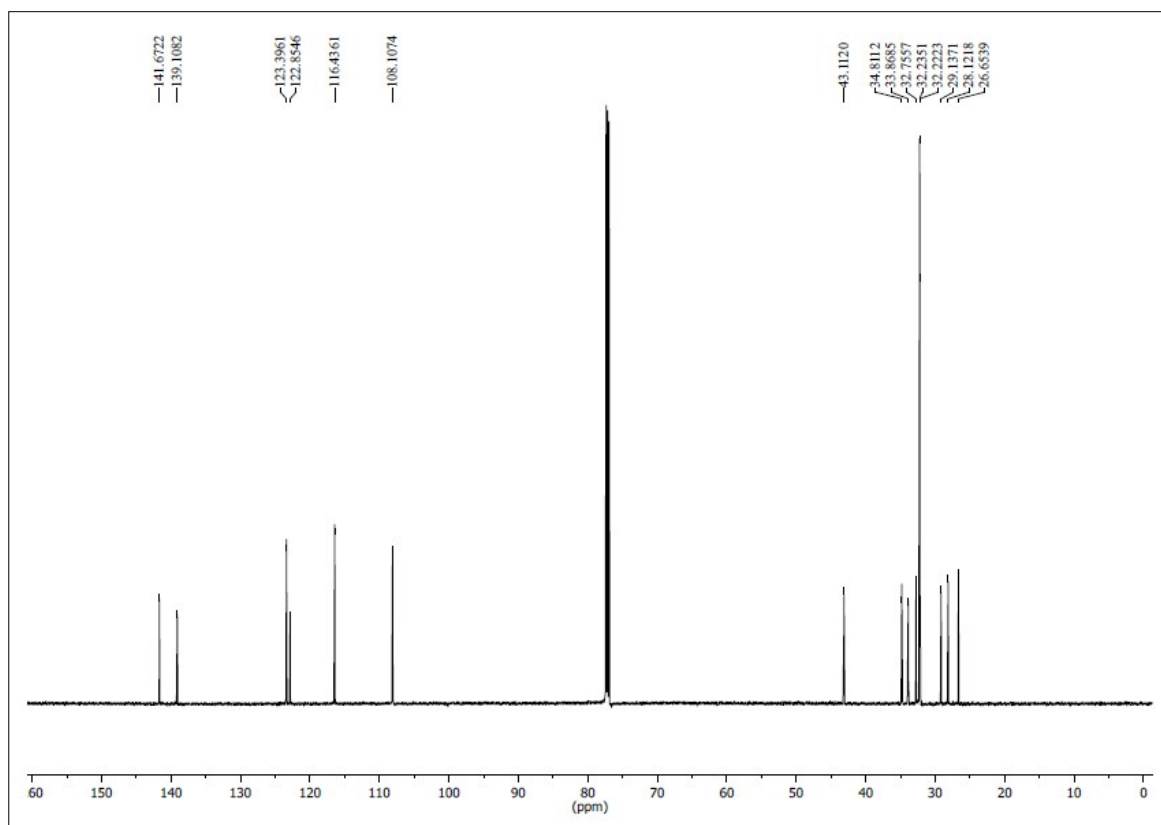


Fig. S2 Electroluminescence (EL) spectra at various applied voltages of the fabricated OLEDs.

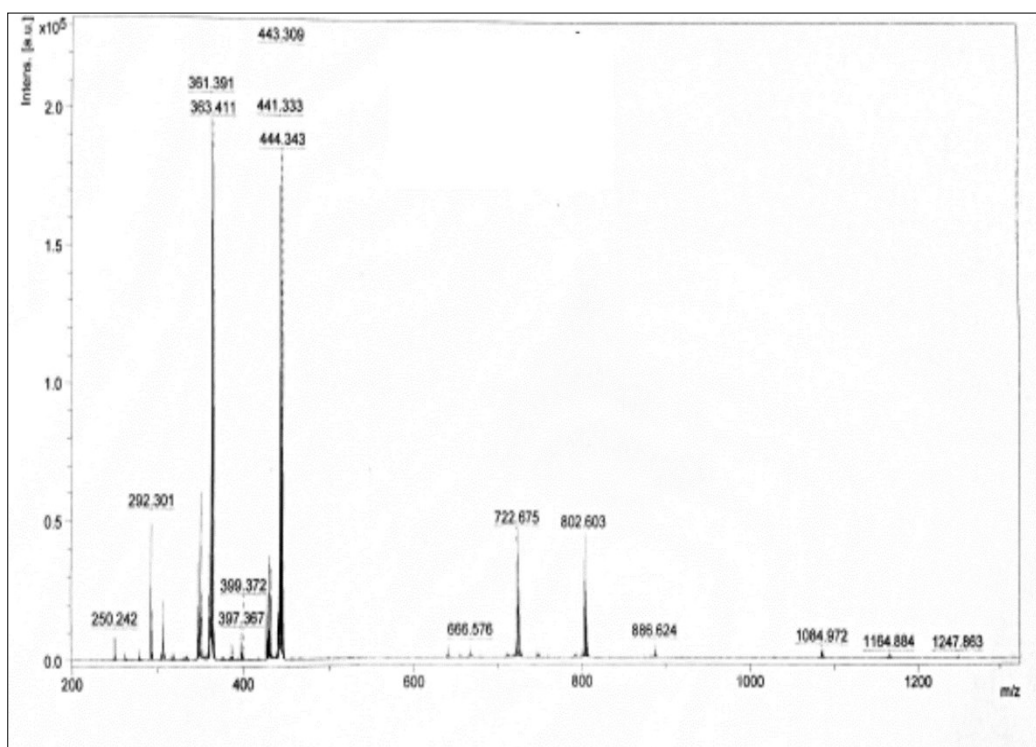
Fig. S3 Copies of ^1H NMR, ^{13}C NMR and HRMS mass spectra of **Compound 2**



^1H -NMR (600 MHz, CDCl_3)

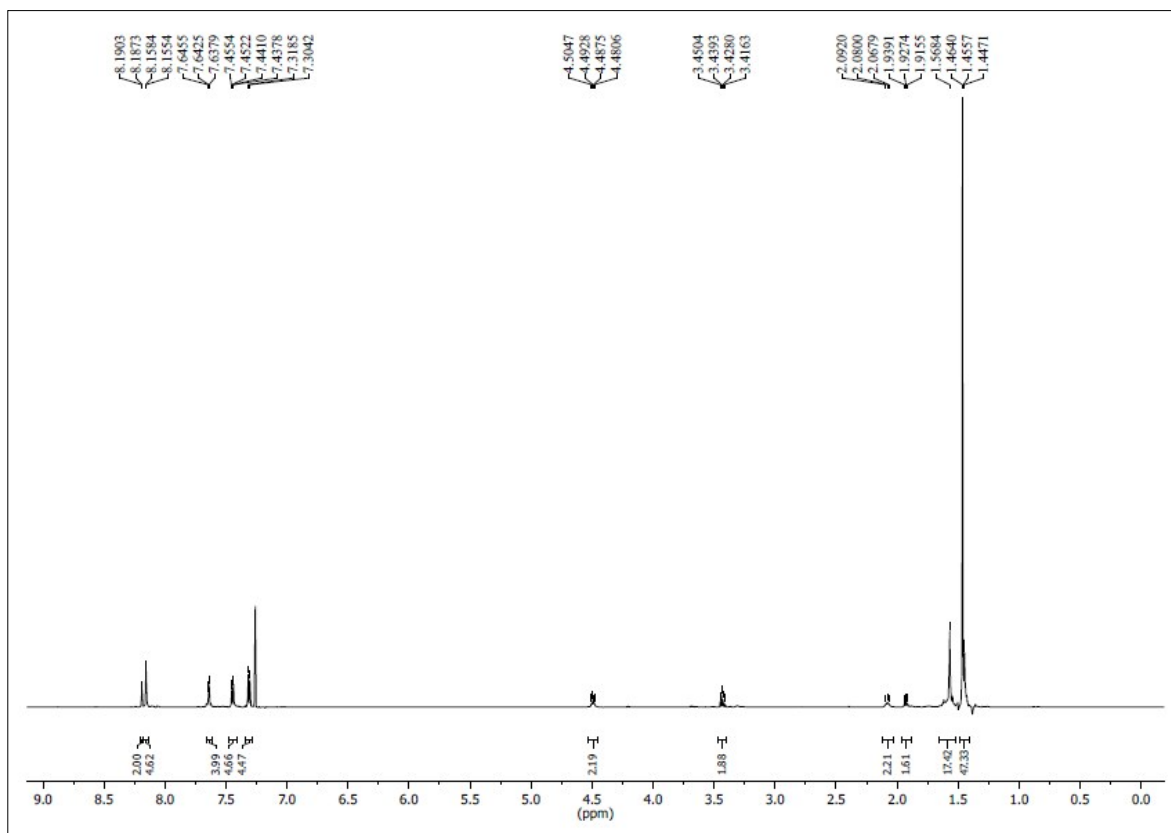


^{13}C -NMR (150 MHz, CDCl_3)

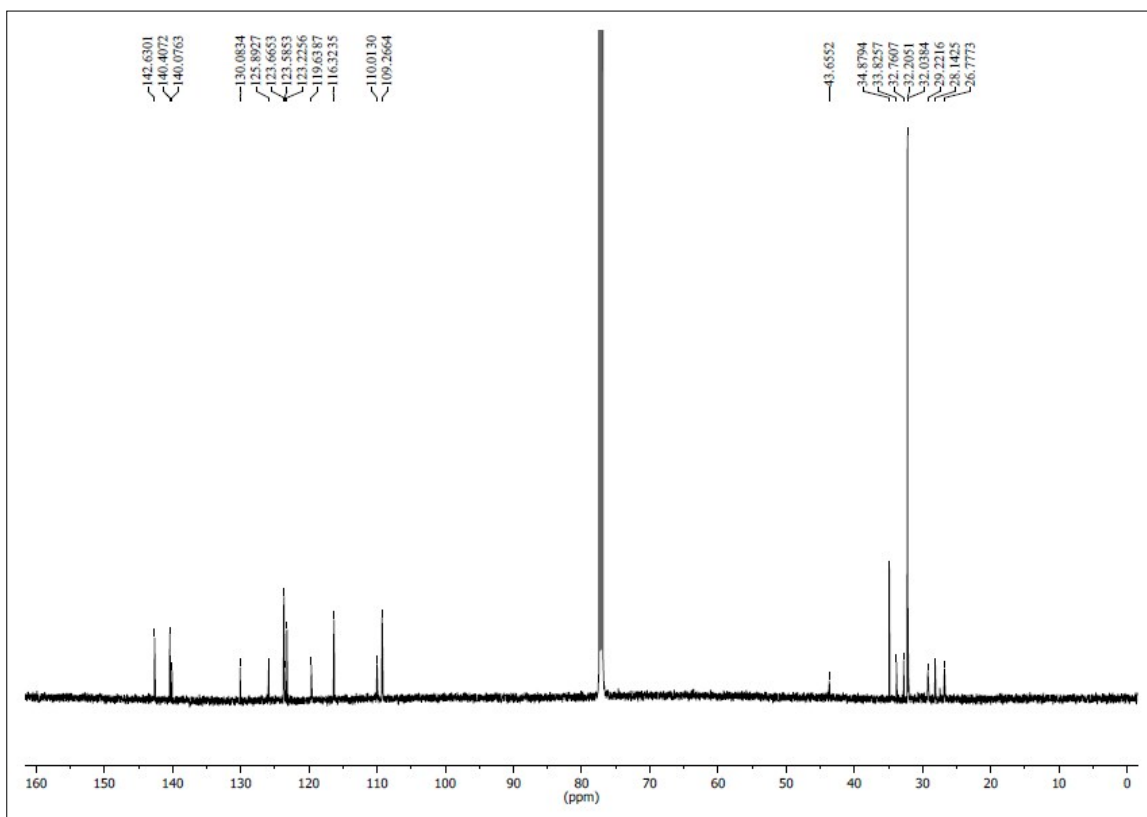


HRMS

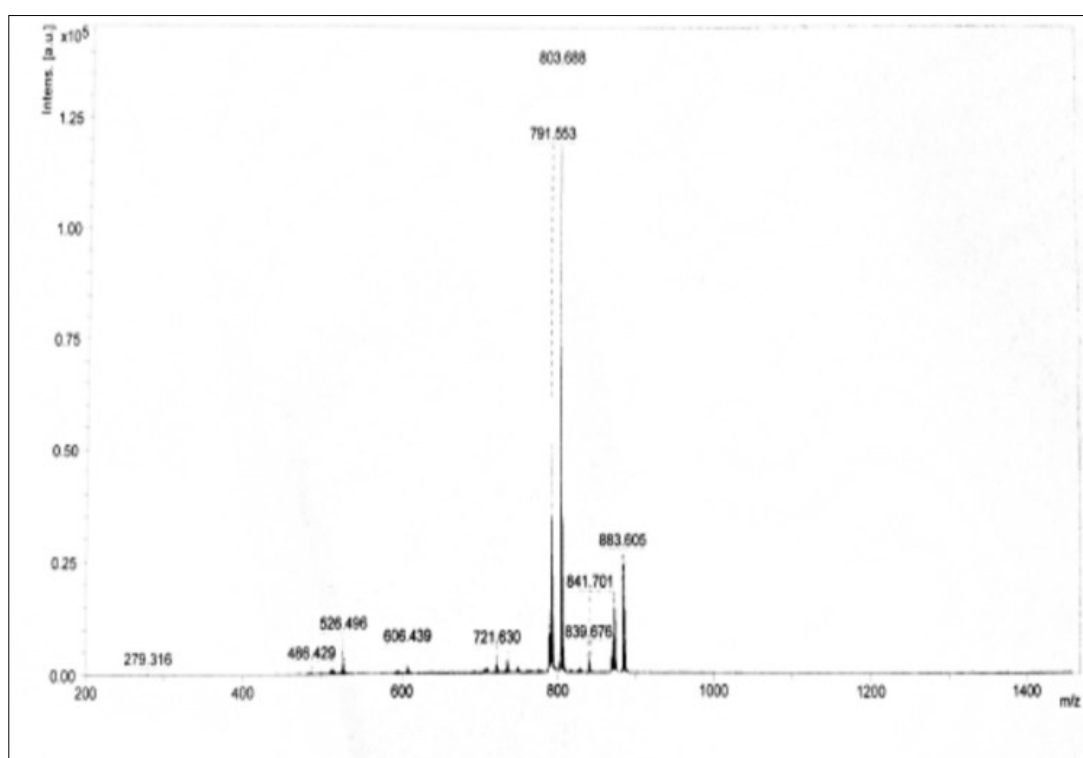
Fig. S4 Copies of ¹H NMR, ¹³C NMR and HRMS mass spectra of **Compound 4**



¹H-NMR (600 MHz, CDCl₃)

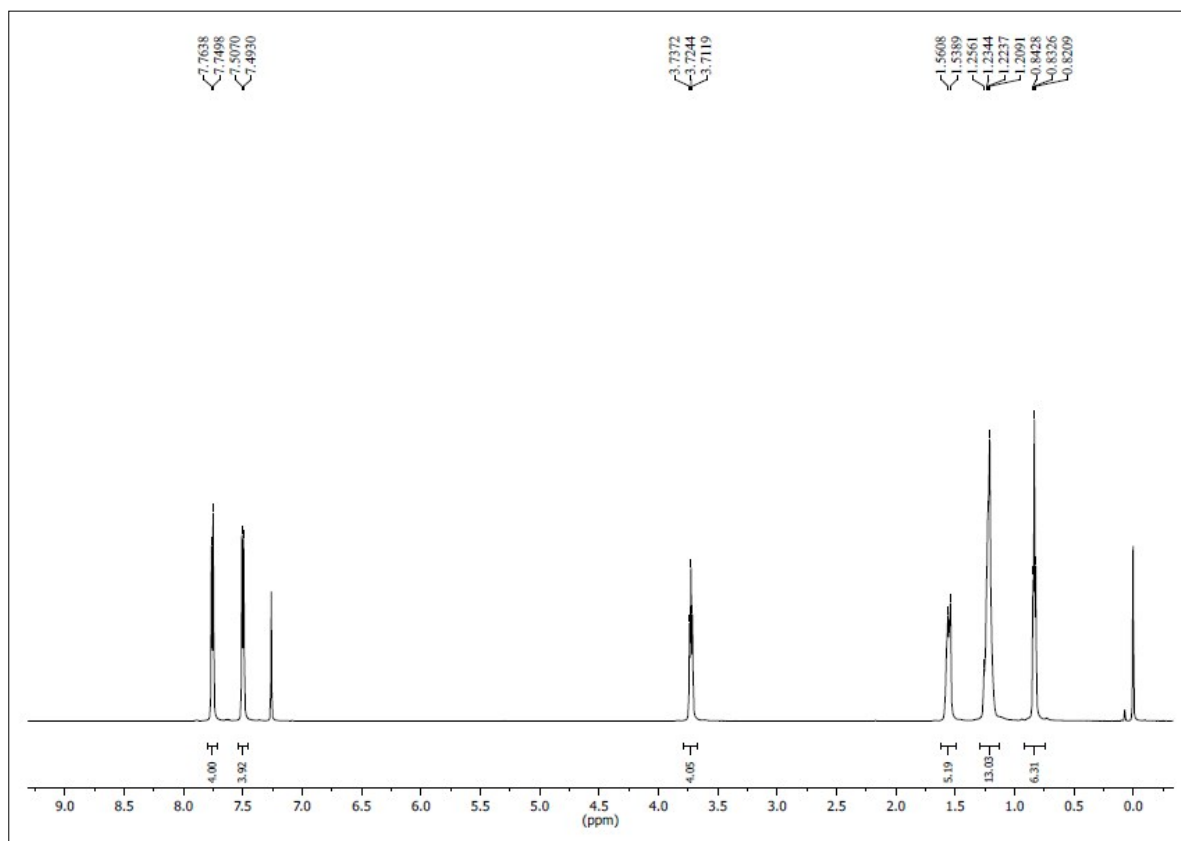


^{13}C -NMR (150 MHz, CDCl_3)

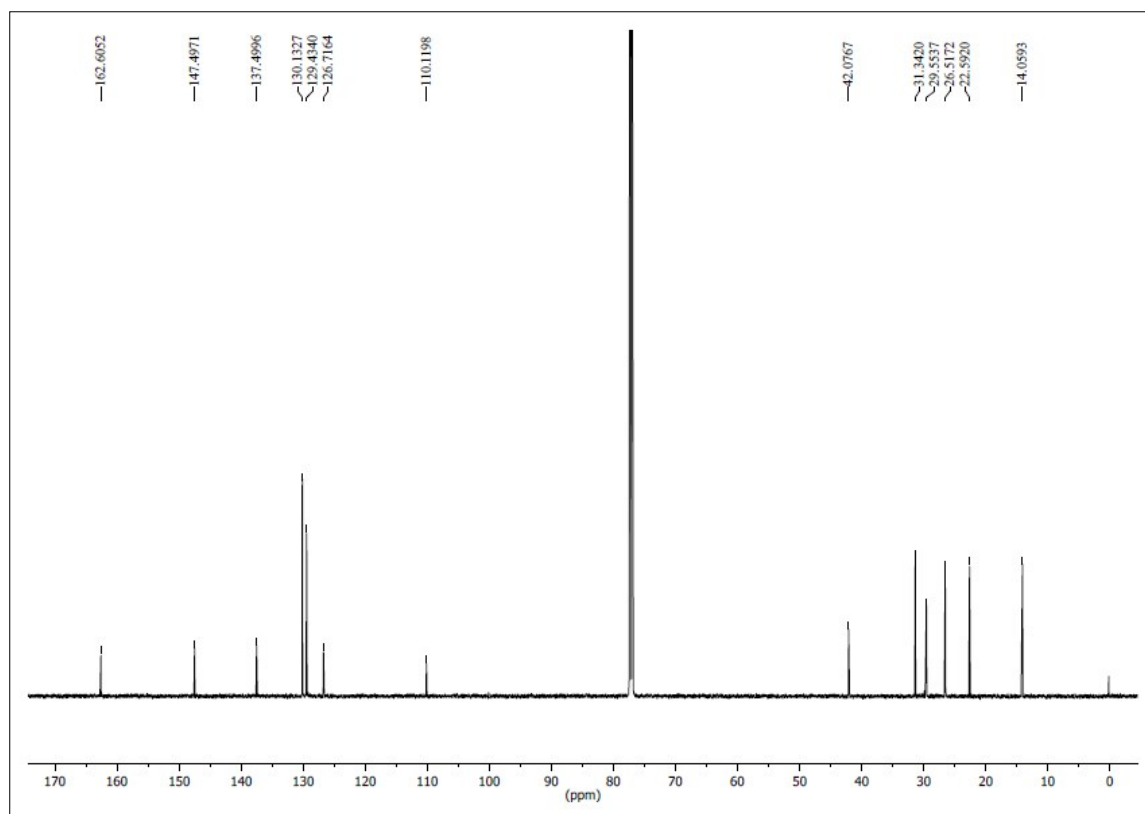


HRMS

Fig. S5 Copies of ^1H NMR, ^{13}C NMR, FTIR and HRMS mass spectra of **G0DPP**



^1H -NMR (600 MHz, CDCl_3)



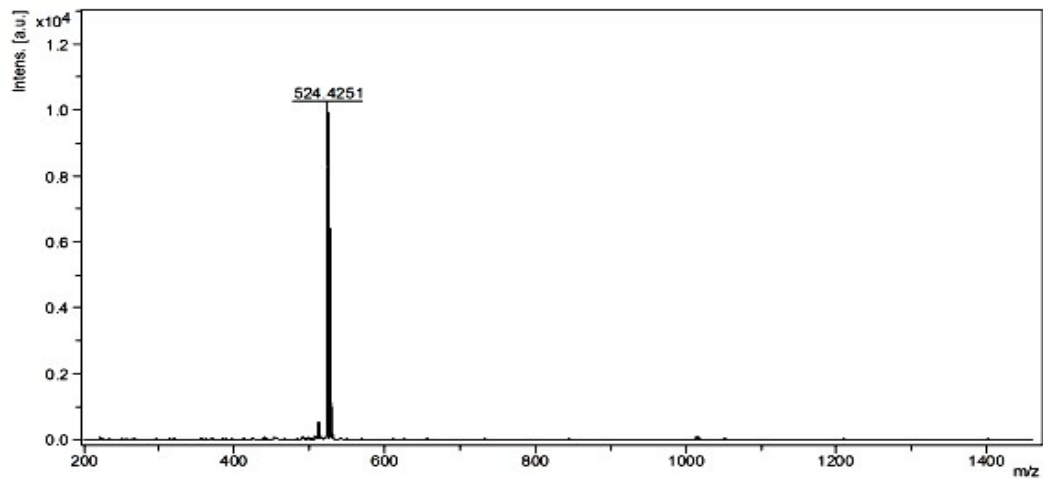
^{13}C -NMR (150 MHz, CDCl_3)

MALDI-TOF-MS Report

Frontier Research Center, Vidyasirimedhi Institute of Science and Technology

Comment 1 Ms 524.1897

Comment 2

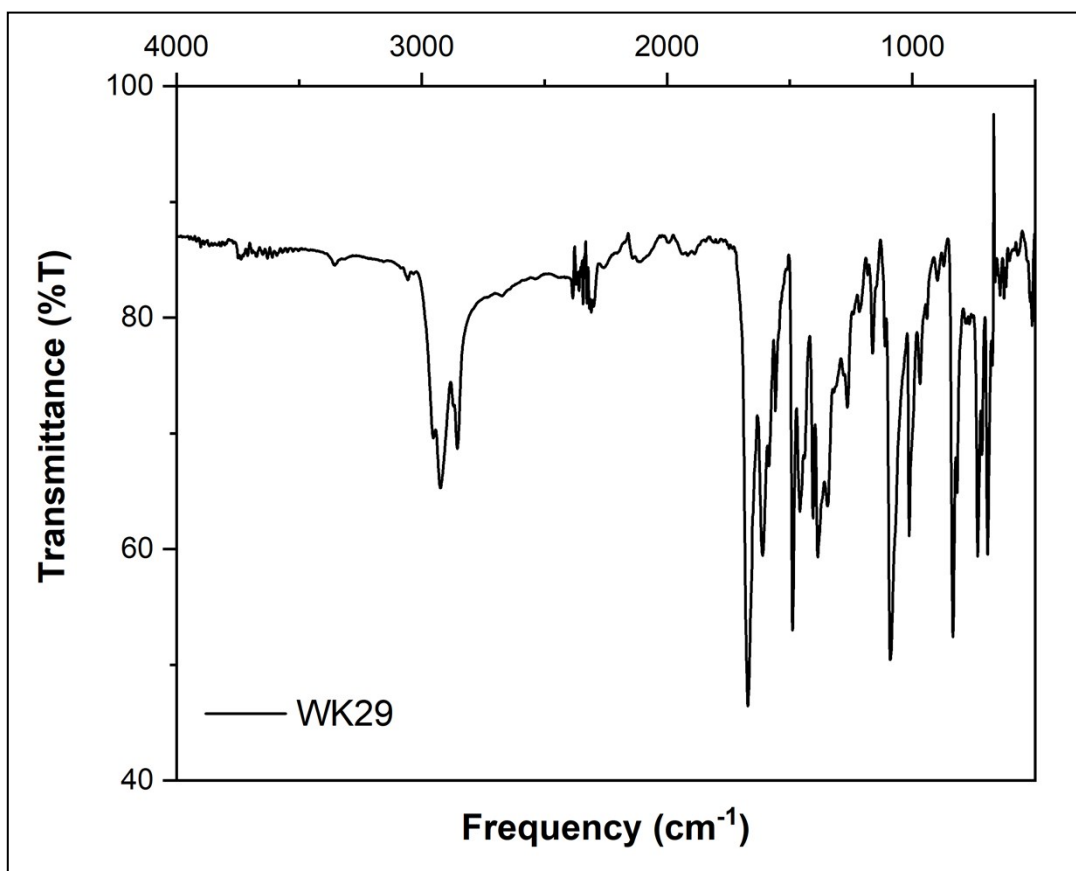


m/z	S/N	Quality Fac.	Res.	Intens.	Area
524.4251	753		5876	8196	855

Bruker Autoflex Speed

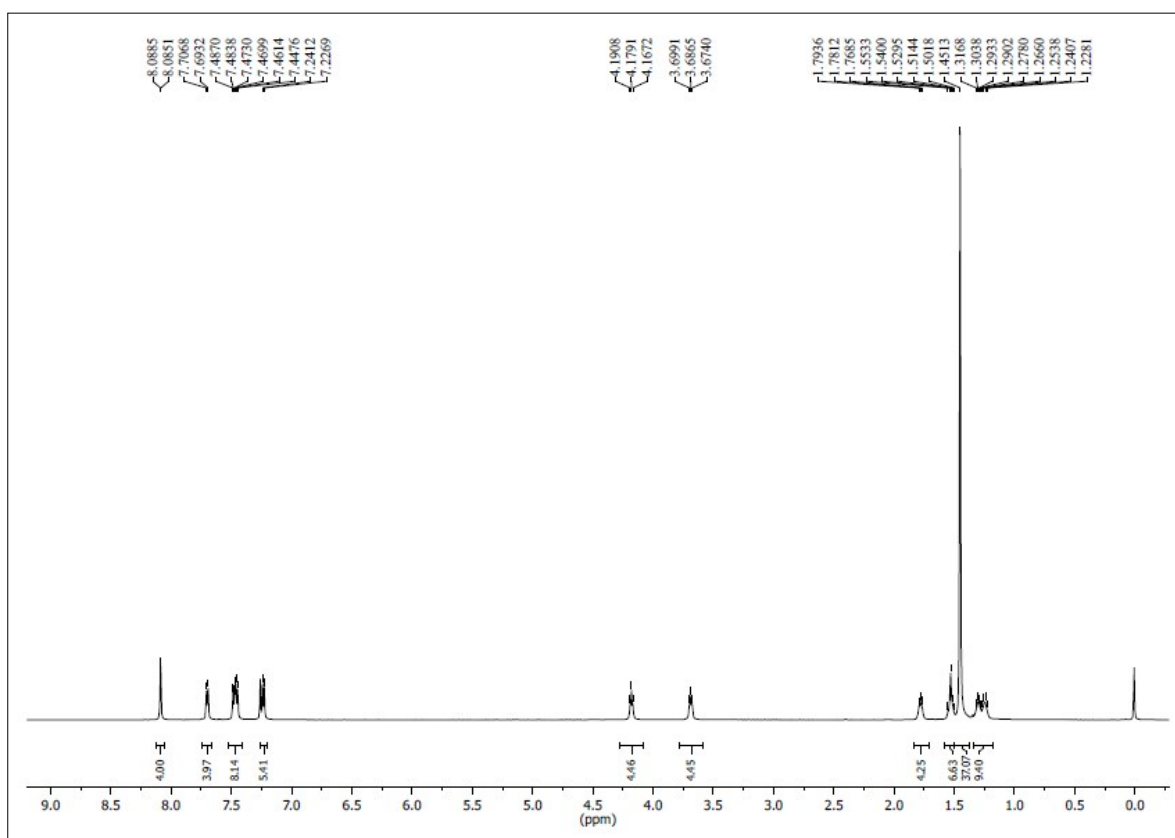
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HRMS

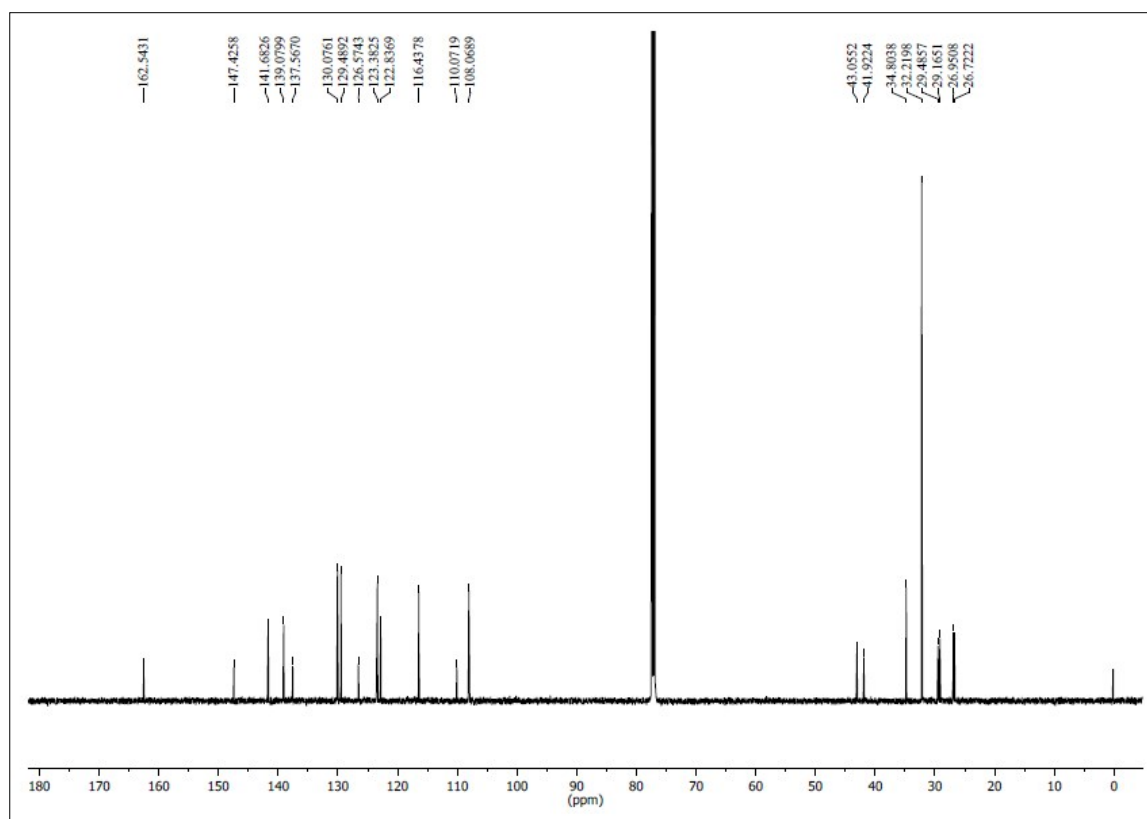


FT-IR

Fig. S6 Copies of ^1H NMR, ^{13}C NMR, FTIR and HRMS mass spectra of **G1DPP**



^1H -NMR (600 MHz, CDCl_3)



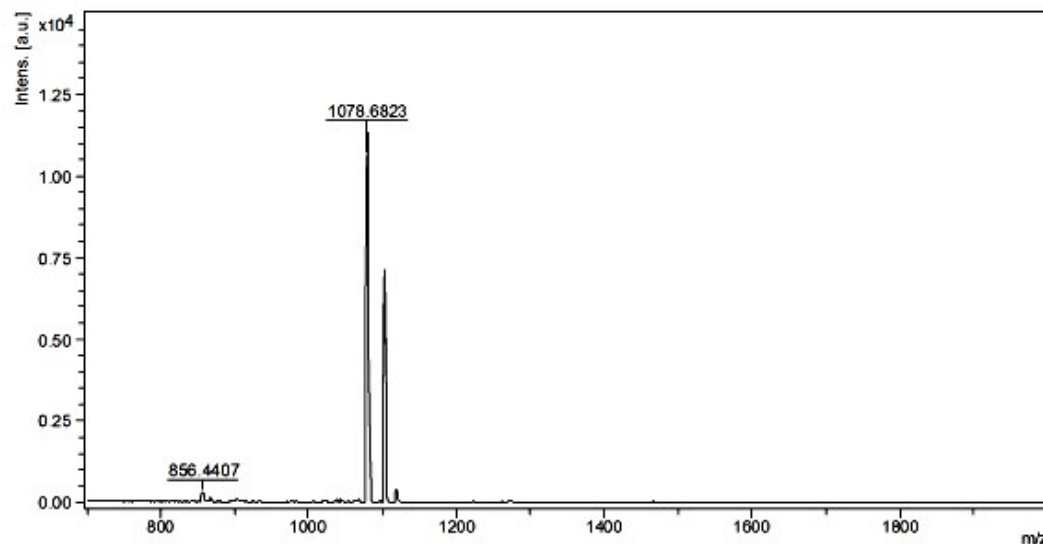
^{13}C -NMR (150 MHz, CDCl_3)

MALDI-TOF-MS Report

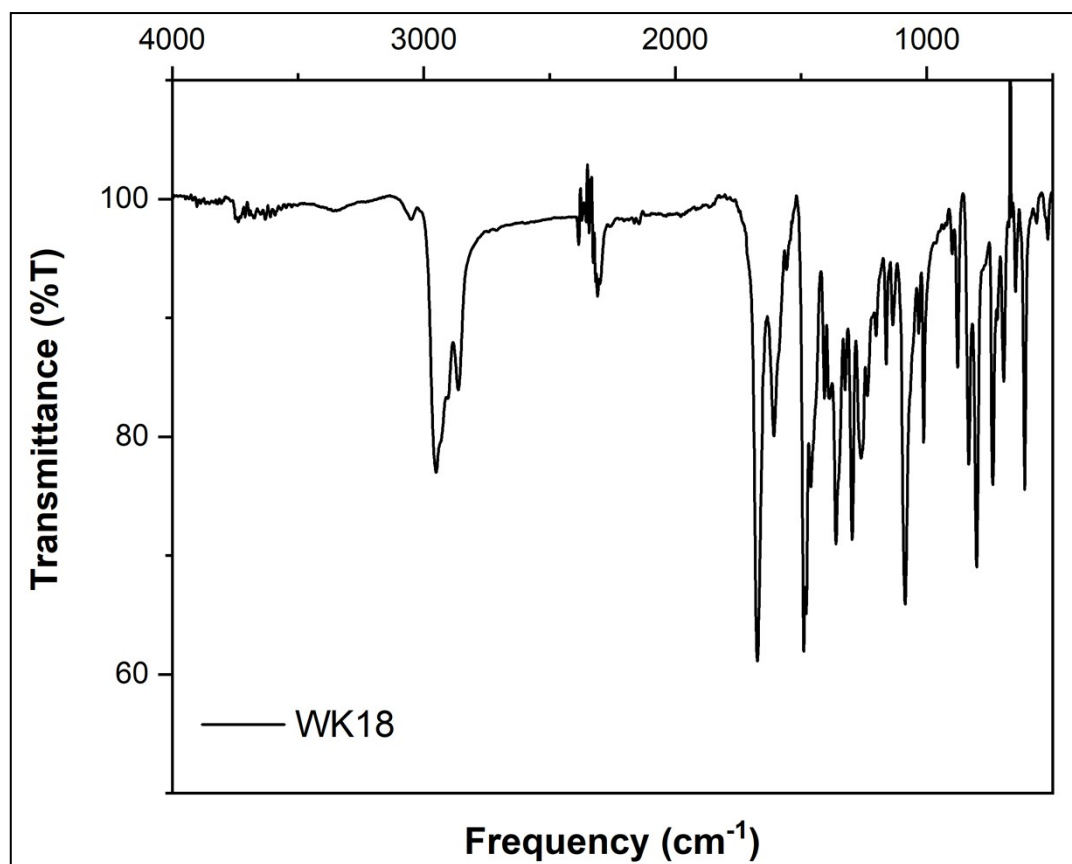
Frontier Research Center, Vidyasirimedhi Institute of Science and Technology

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Comment 2

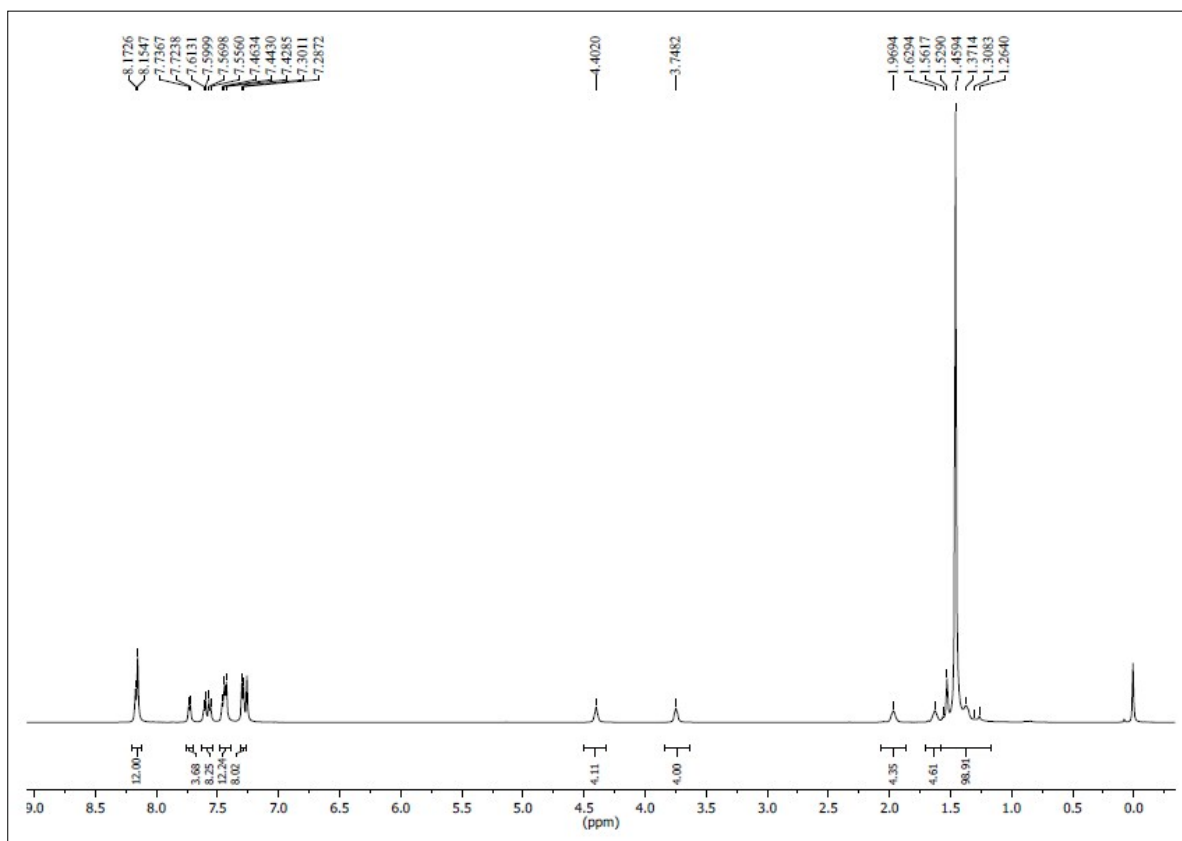


HRMS

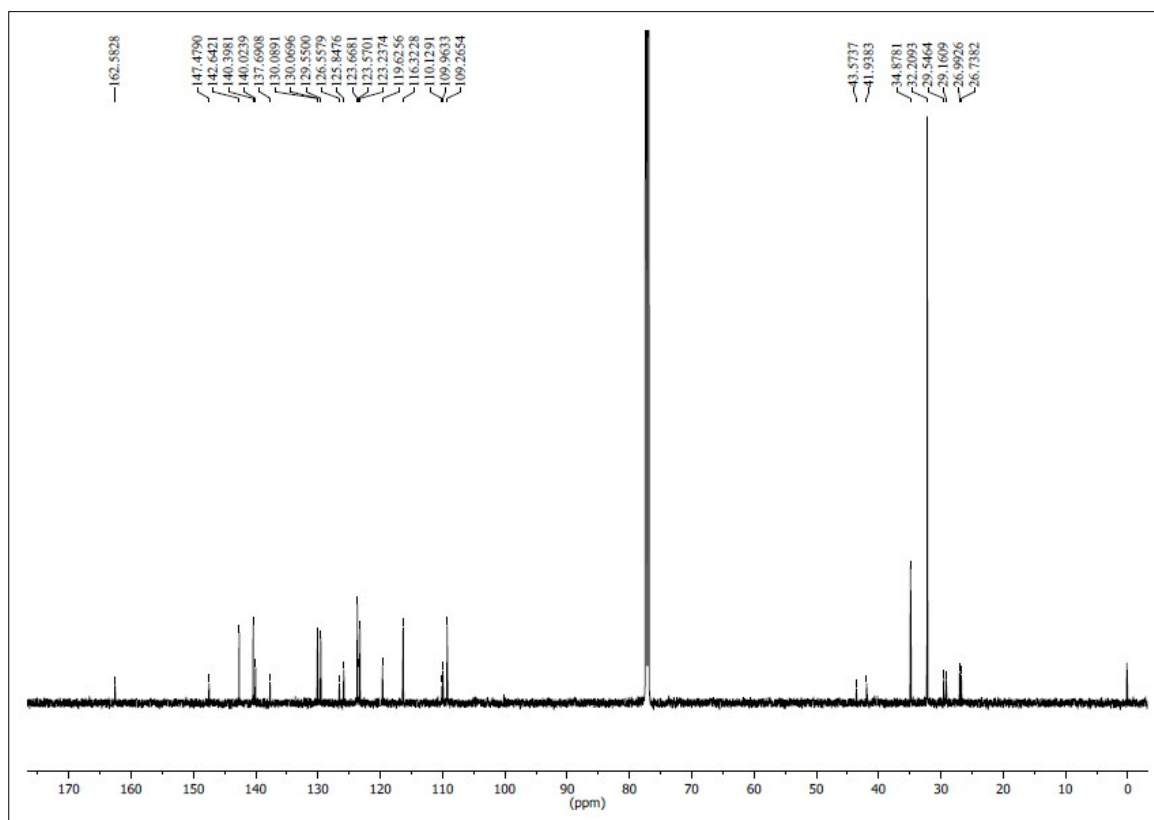


FT-IR

Fig. S7 Copies of ^1H NMR, ^{13}C NMR, FTIR and HRMS mass spectra of **G2DPP**



^1H -NMR (600 MHz, CDCl_3)

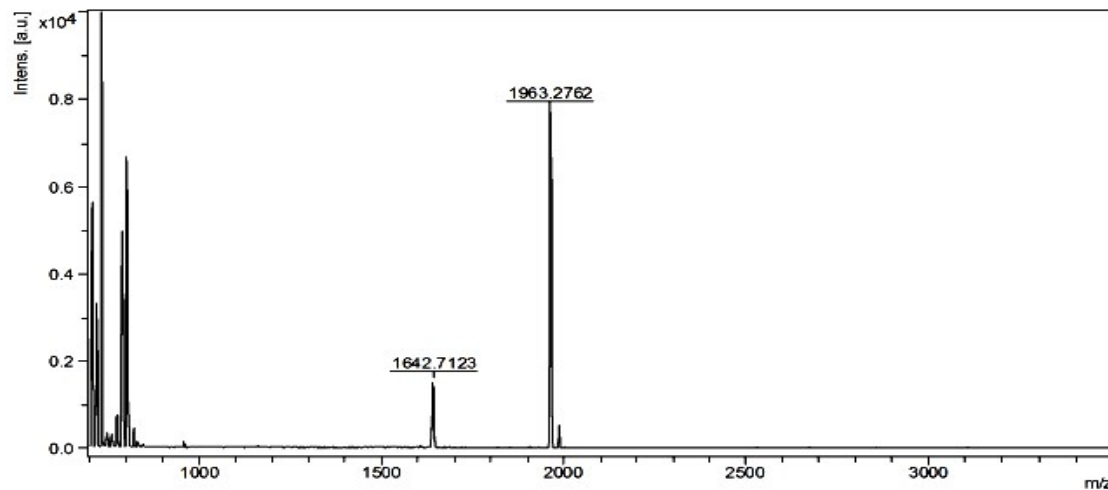


^{13}C -NMR (150 MHz, CDCl_3)

MALDI-TOF-MS Report

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Comment 1 Ms 1963.0476
Comment 2

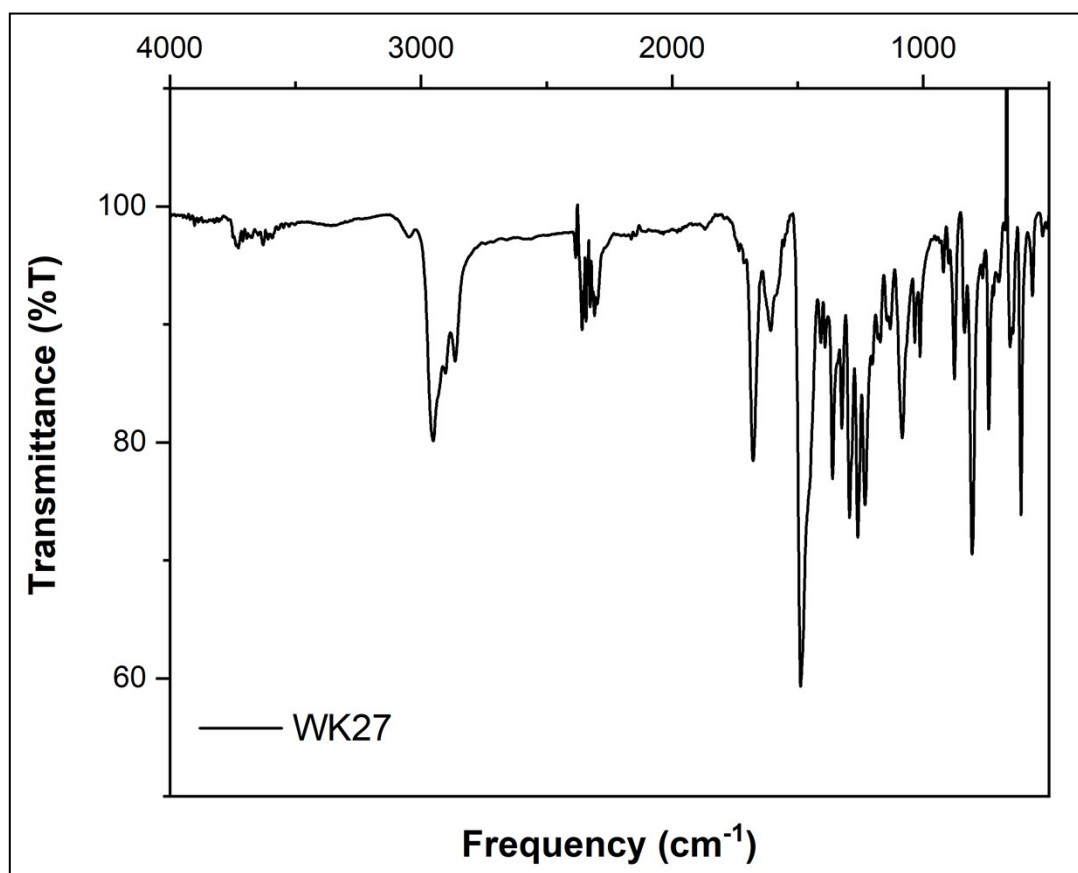


m/z	S/N	Quality Fac.	Res.	Intens.	Area
1642.7123	123		2285	1531	1333
1963.2762	296		17950	2744	333

Bruker Autoflex Speed

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HRMS



FT-IR