Supporting Information

Rationally Heteroarylated Pyridines as Hole Transport Materials for OLEDs

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General

All the synthesized molecules were characterised by NMR on a Jeol EXC NMR spectrometer. The optical properties such as UV-vis absorption and photoluminescence spectrum were recorded in Shimadzu UV-2450 and Carry Eclips Fluorescence Spectrometer, Agilent technologies, respectively. HRMS-ESI spectra of all the compounds were measured on Bruker Maxix Impact HD instrument and theoretical mass values were calculated from compass isotope pattern software. All the photophysical studies were performed in HPLC-grade solvents. The TGA and DSC analysis was investigated on NETZSCH STA448 F1 JUPITOR and (Perkin Elmer DSC 8000) instruments under a nitrogen and argon atmosphere, respectively, with a 10 °C/minute heating rate. Diffraction studies of **PrPzPy** were performed on an Agilent Technologies X-ray diffractometer (Rigaku corporations). The electrochemical properties of the molecules were measured by Cyclic Voltammetry on Metrohm Auto lab using three-electrode systems (Ag/AgCl, Pt-disc, and Pt-wire) in tetrabutylammonium hexafluorophosphate electrolyte, and DCM as solvent. For the photoluminescence study of the molecules, 1mg/ml stock solution was prepared in DCM solvent and experiments were done in 5 nm and 5nm slits for excitation and emission respectively. The excitation wavelength for **PrPzPy** and **MePzCzPy** was 330, and 338 nm, and photoluminescence and absorption studies were done using 10μM DCM. The compound **EtCz** was synthesized following a previous report.[1]

1. Experimantal Section:

Procedure for the synthesis of **MePz** [2]

NaH (1.5 eq.) and DMF (10 ml) were placed in a 100-ml two-neck round bottomed flask, then phenothiazine (1.0 eq.) was added to the RB. The mixture was stirred for 40 minutes at room temperature, then iodomethane (1.1 eq.) was added dropwise. The mixture was stirred for 6h at room temperature. The crude product was poured into the ice-water and extracted with DCM. The organic layer was evaporated on rota-evaporator and the crude product was purified by column chromatography with 3% ethyl acetate-hexane as the eluent; White solid; Yield: 80%; ^{1}H NMR (500 MHz, $CDCl_3$): 7.24-7.13 (m, 4H), 6.92 (t, J = 7.55 Hz, 2H), 6.81 (d, J = 8.25 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 145.78, 127.39, 127.11, 123.33, 122.41,114.03, 35.26.

Procedure for the synthesis of **PrPz** [2]

NaH (1.5 eq.) and DMF (10 ml) were placed in a 100-ml two-necked round bottomed flask, then phenothiazine (1.0 eq.) was added to the RB. The mixture was stirred for 40 minutes at room temperature, then iodopropane (1.1 eq.) was added dropwise. The mixture was stirred for 6h at room temperature. The crude product was poured into the ice-water and extracted with DCM. The organic layer was evaporated on rota-evaporator and the crude product was purified by column chromatography with 2% ethyl acetate-hexane as the eluent; Oily compound was obtained which become yellow solid after some time; Yield: 75%; ^{1}H NMR (500 MHz, $CDCl_3$): 7.35-7.30 (m, 4H), 7.08 (t, J = 7.55 Hz, 2H), 7.00 (d, J = 7.55 Hz, 2H), 3.92 (t, J = 6.15 Hz, 2H), 1.99-1.95 (m, 2H), 1.16 (t, J =7.55 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 144.98, 127.09, 126.92, 124.60, 122.04, 115.19, 48.71, 19.82, 11.10.

Synthetic Procedure for **MePzCHO** [3]

A mixture of 10-methyl-10*H*-phenothiazine (1 eq.), $POCl_3$ (1.5 eq.), and DMF (2 eq.) in RB was stirred at room temperature for 1h. After that, the reaction mixture was refluxed at 95 °C for 12h. Then the reaction mixture was quenched with aq. solution of $NaHCO_3$ and extracted with DCM. The organic solvent was evaporated using rota-evaporator and the crude solid was purified by column chromatography with 8% ethyl acetate-hexane as the eluent; Yellow solid; Yield: 50%; ^{1}H NMR (500 MHz, $CDCl_3$): 9.73 (s, 1H), 7.58-7.55 (m, 1H), 7.50-7.50 (m, 1H), 7.15-7.12 (m, 1H), 7.07-7.05 (m, 1H), 6.95-6.94 (m, 1H), 6.78-6.74 (m, 2H), 3.33 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 189.92, 150.75, 143.76, 130.83, 130.33, 127.60, 127.56, 127.02, 123.58, 123.41, 122.16, 114.61, 113.50, 35.58.

Synthetic Procedure for **PrPzCHO** [3]

A mixture of 10-propyl-10*H*-phenothiazine (1 eq.), $POCl_3$ (1.5 eq.), and DMF (2 eq.) in RB was stirred at room temperature for 1h. After that, the reaction mixture was refluxed at 95 °C for 12h. Then the reaction mixture was quenched with aq. solution of $NaHCO_3$ and extracted with DCM. The organic solvent was evaporated using rota-evaporator and the crude solid was purified by column chromatography with 6% ethyl acetate-hexane as the eluent; Oily compound was obtained; Yield: 55%; ^{1}H NMR (500 MHz, $CDCl_3$): 9.74 (s, 1H), 7.59-7.57 (m, 1H), 7.52-7.52 (m, 1H), 7.15-7.11 (m, 1H), 7.07-7.05 (m, 1H), 6.94-6.91 (m, 1H), 6.84-6.82 (m, 2H), 3.80 (t, J = 7.55 Hz, 2H), 1.82-1.77 (m, 2H), 0.99 (t, J = 7.55 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 189.86, 150.50, 143.14, 130.77, 129.97, 128.07, 127.41, 127.34, 124.71, 123.49, 123.39, 115.83, 114.62, 49.47, 19.82, 11.06.

Synthetic Procedure for **EtCzAc** [4]

To a solution of 9-ethyl-9*H*-carbazole (1eq.) in 20 ml dichloromethane was added $AlCl_3$ (3.5 eq.) and acetyl chloride (2 eq.). The reaction mixture was stirred at room temperature for 6 hours, and then poured into 20 ml diluted HCl ice water. The organic phase was collected, dried over anhydrous Na_2SO_4, and concentrated in vacuum. The crude product was purified by

column chromatography (10% ethyl acetate/ hexane) to afford desired product as a white solid. Yield: 70%. ^{1}H NMR (500 MHz, DMSO-d_6): 8.86 (s, 1H), 8.30 (d, J= 8.25 Hz, 1H), 8.07 (d, J = 8.95 Hz, 1H), 7.65 (t, J= 7.55 Hz, 1H), 4.45 (q, J = 7.60 Hz, 2H), 2.67 (s, 3H), 1.30 (t, J = 6.85 Hz, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 196.97, 142.17, 140.27, 128.37, 126.45, 126.02, 122.55, 122.04, 121.89, 120.80, 119.76, 109.66, 108.82, 37.22, 26.68, 13.69.

Synthetic Procedure for **PrPzPy)** [4]

A mixture of 4-methoxyacetophenone (3 eq.), 10-propyl-10*H*-phenothiazine-3-carbaldehyde (1 eq.), ammonium acetate (8 eq.) and AcOH (20 ml) in 100 ml RB was refluxed at 130 °C for 12h. Then the reaction mixture was quenched with water and extracted with DCM. The organic solvent was evaporated using rota-evaporator and the crude solid was purified by column chromatography with 8% ethyl acetate-hexane as the eluent; Yellow solid; Yield: 48%; ^{1}H NMR (500 MHz, DMSO-d_6): 8.28 (d, J = 8.95 Hz, 4H), 7.99 (s, 2H), 7.83-7.82 (m, 2H), 7.20-7.16 (m, 2H), 7.10-7.08 (m, 5H), 7.06-7.03 (m, 1H), 7.01-6.96 (m, 1H), 3.87 (t, J = 6.85 Hz, 2H), 3.83 (s, 6H), 1.76-1.69 (m, 2H), 0.95 (t, J = 6.90 Hz, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 160.12, 155.89, 147.82, 145.42, 144.16, 131.76, 131.43, 128.13, 127.56, 127.04, 126.37, 125.50, 124.19, 123.06, 122.58, 115.82, 115.79, 114.00, 113.88, 55.13, 55.11, 48.22, 19.43, 10.86; HRMS (ESI): Calculated for $C_{34}H_{30}N_2O_2S$ $[M+H]^+$: 531.2101, found: 531.2101, Melting Point: 141°C.

Synthetic Procedure for **MePzCzPy** [5]

A mixture of 1-(9-ethyl-9*H*-carbazol-3-yl)ethan-1-one (3 eq.), 10-methyl-10*H*-phenothiazine-3-carbaldehyde (1 eq.), ammonium acetate (8 eq.) and AcOH (20 ml) in 100 ml RB was refluxed at 130 °C for 12h. Then the reaction mixture was quenched with water and extracted with DCM. The organic solvent was evaporated using rota-evaporator and the crude solid was purified by column chromatography with 6% ethyl acetate-hexane as the eluent; Yellow color

solid; Yield 35%; ^{1}H NMR (500 MHz, $CDCl_3$): 8.95 (s, 2H), 8.42 (d, *J* = 8.20 Hz, 2H), 8.27 (d, *J* = 7.55 Hz, 2H), 7.89 (s, 2H), 7.64 (d, *J* = 6.15 Hz, 2H), 7.53-7.42 (m, 6H), 7.30-7.19 (m, 4H), 6.98-6.91 (m, 2H), 6.85 (d, *J* = 8.25 Hz, 1H), 4.41 (q, *J* = 6.90 Hz, 4H), 3.41 (s, 3H), 1.47 (t, *J* = 6.9 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): 158.29, 148.53, 146.37, 145.31, 140.60, 140.43, 133.59, 130.97, 127.61, 127.24, 126.35, 125.74, 125.57, 125.31, 124.10, 123.37, 123.29, 122.80, 122.76, 120.75, 119.35, 119.03, 115.17, 114.36, 114.23, 108.60, 108.51, 37.68, 35.43, 13.85; HRMS (ESI): Calculated for $C_{46}H_{36}N_4S$ $[M+H]^+$: 677.2730, found: 677.2730, Melting Point: 210 °C.

1.1 Hole-only device fabrication for **PrPzPy** compound.

The hole-only device (HOD) with **PrPzPy** was fabricated to evaluate the change in current density with the enhancement in operating voltage. The developed device contained two electrodes i.e. (i) anode, which contained an indium tin oxide (ITO) glass of ~125 nm thickness, and (ii) cathode, which contained aluminum (Al) of ~100 nm thickness, respectively. The hole was injected by a hole injection layer i.e. poly(3,4-ethylenedioxythiophene): polystyrene sulphonate (PEDOT:PSS) with a thickness of ~40 nm. The charge carrier hole was then transported by a hole transport layer (HTL) comprised of **PrPzPy** that had a thickness of ~10 nm. Similarly, the electron was injected by the electron injection layer (EIL) i.e. lithium fluoride (LiF) which had a thickness of ~1 nm. Initially, the ITO-coated glass substrate was properly washed in acetone at 45°C for 30 minutes, followed by washing in 2-propanol at 60 °C for 60 mins (both under an ultrasonic bath), and then it was carefully treated in an ozone atmosphere under ultraviolet light for 15 minutes. After that, the substrate was shifted into a nitrogen-filled glove box for spin-coating the HIL and HTL. The HIL was spin-coated at 4,000 rpm for 20 seconds. The **PrPzPy** was dissolved in toluene and then spin-coated onto the specimen at 2,500 rpm for 20 seconds to coat the HTL. After coating the HTL, the specimen was shifted into a high-vacuum chamber with a base pressure of $\sim 1 \times 10^{-7}$ torr for sequential

deposition of EIL and cathode via thermal evaporation. The current density of the developed device was measured with a Keithley 2400 electrometer.

2. TD spectrum

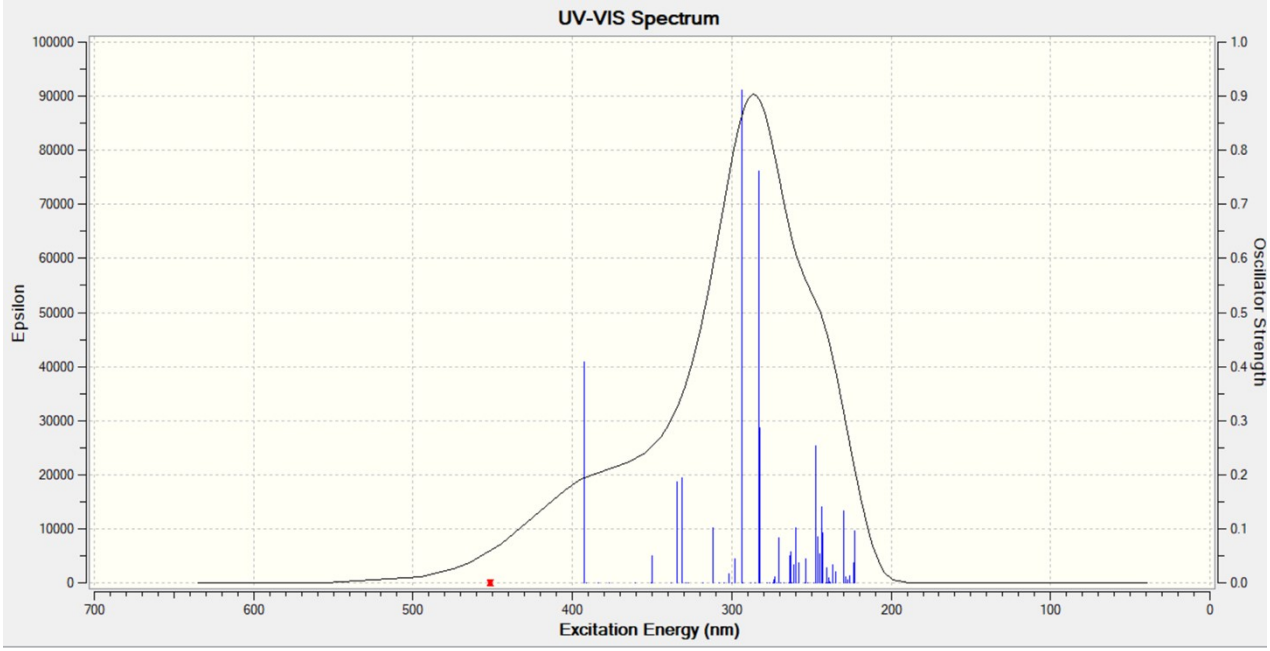


Fig. S1. TD Spectrum of **PrPzPy**

Table **S1**. TD-DFT analysis of **PrPzPy (**transition, oscillator strength, and energy) with B3LYP functional. MO number 140 corresponds to HOMO and 141 corresponds to LUMO. Transitions with oscillator strengths and coefficients greater than 0.10 are tabulated.

S.No.	Transition Energy/Wavelength	Nature of transitions MOs involved	 Coefficients	oscillator strength (f)
1.	3.1564 eV 92.81 nm	140 ->141	0.68011	f=0.4080
2.	3.7056 eV 334.59 nm	139 ->141	0.47978	f=0.1865
3.	3.7433 eV 331.22 nm	139 ->141 140 ->142 140 ->143	0.43778 0.26124 0.45651	f=0.1947
4.	4.2262eV 293.37 nm	137 ->141 139 ->142	0.24986 0.51084	f=0.9104
5	4.3766 eV 283.29 nm	137 ->141 138 ->142	0.16940 0.66081	f=0.7622
6	4.3931eV 282.23 nm	137 ->141 138 ->141	0.52141 0.15468	f=0.2861
7.	5.0070 eV 247.62 nm	137 ->143 138 ->143	0.38740 0.36615	f=0.2531

8.	5.0096 eV 247.50 nm	137 ->143 0.26203 138 ->143 0.14315 139 ->144 0.22506 139 ->145 0.55289	f=0.1124
9.	5.0892 eV 243.62 nm	134 ->141 0.38023 135 ->141 0.26471 137 ->144 0.10913 138 ->146 0.16874	f=0.1410
10.	5.3913 eV 229.97 nm	139 ->148 0.63261	f=0.1332

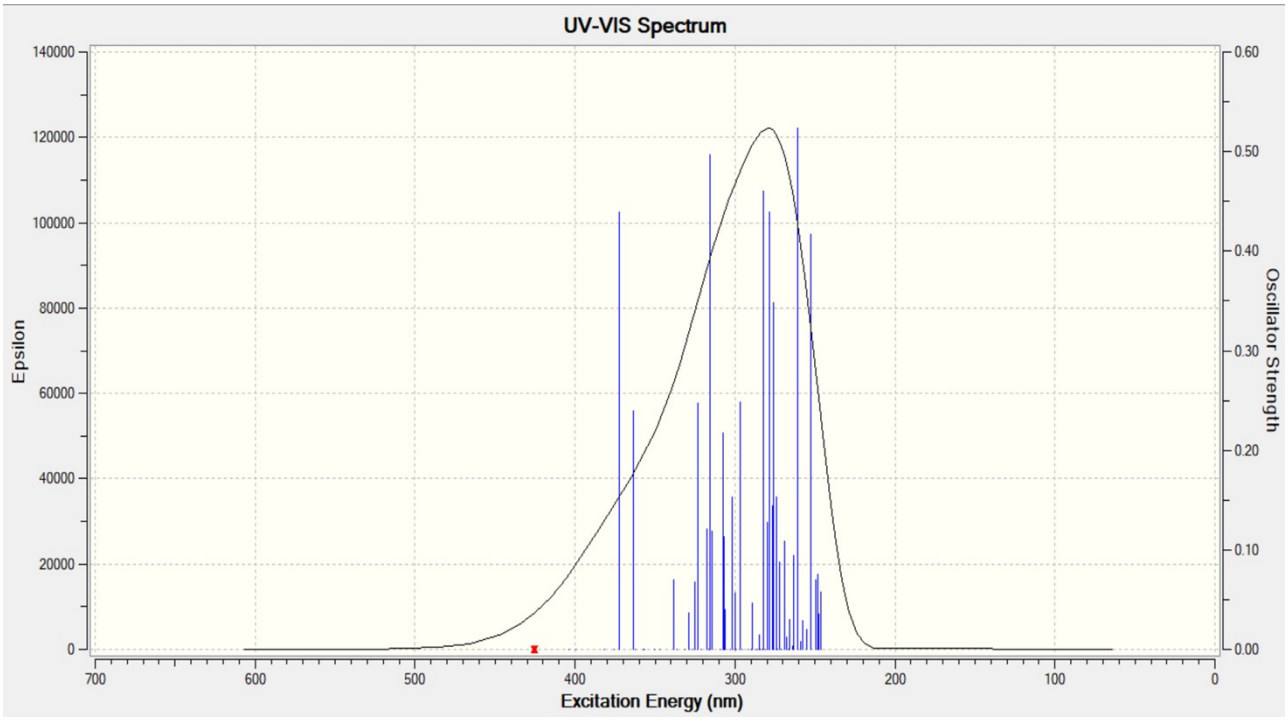


Fig. S2. TD Spectrum of **MePzCzPy** with B3LYP functional

Table S2. TD-DFT analysis of **MePzCzPy (**transition, oscillator strength, and energy) with B3LYP functional. MO number 178 corresponds to HOMO and 179 corresponds to LUMO. Transitions with oscillator strengths and coefficients greater than 0.10 are tabulated.

S.No.	Transition Energy/Wavelength	Nature of transitions MOs involved Coefficients	oscillator strength (f)
1.	3.3276 eV 372.59 nm	178 -> 179 0.67474	f=0.4396
2.	3.4132eV 363.25 nm	177 -> 179 0.68860	f=0.2394
3.	3.8364 eV 323.18 nm	175 -> 179 0.23000 177 -> 181 0.17683 177 -> 182 0.43000	f=0.2477
4.	3.9283 eV 315.62 nm	176 -> 182 0.18560 177 -> 180 0.45804 177 -> 182 0.13002	f=0.4964
5.	4.0314 eV 307.55 nm	175 -> 179 0.46428 176 -> 180 0.16659 178 -> 182 0.22428	f=0.2178

6.	4.0372 eV 307.10 nm	175 -> 179 0.42819 178 -> 181 0.30193	f=0.1129
7.	4.1060 eV 301.96 nm	174 -> 179 0.57495	f=0.1531
8.	4.1749 eV 296.97 nm	174 -> 179 0.26022 175 -> 180 0.11879 176 -> 182 0.55336 177 -> 181 0.23847	f=0.2483
9.	4.3962 eV 282.02 nm	173 -> 179 0.24924 178 -> 185 0.26249	f=0.4607

10.	4.4336 eV 279.65 nm	172 -> 179 0.10702 173 -> 179 0.31961 174 -> 181 0.20361 175 -> 181 0.13778 175 -> 182 0.13002 176 -> 182 0.10137 178 -> 185 0.27320	f=0.1272
11.	4.4496 eV 278.64 nm	173 -> 179 0.22185 174 -> 180 0.37536 177 -> 184 0.10956 178 -> 185 0.17465	f=0.4396
12.	4.4834 eV 276.54 nm	176 -> 181 0.11732 177 -> 184 0.45436	f=0.1442
13.	4.4962 eV 275.75 nm	174 -> 182 0.16989 175 -> 180 0.31371 175 -> 181 0.38228 176 -> 184 0.12476 177 -> 184 0.13734 177 -> 187 0.11795	f=0.3483

14.	4.5267 eV 273.89 nm	169 -> 179 0.44056	f=0.1534
15.	4.7507 eV 260.98 nm	176 -> 184 0.61399	f=0.5237
16.	4.9084 eV 252.60 nm	176 -> 184 0.21681 176 -> 185 0.61972	f=0.4175

Table S3: Charge transfer distances and magnitude of charge transfer for each molecule.

Molecule	Method	S_1		S_2		T_1		T_2	
		D_{CT} (Å)	Q_{CT}	D_{CT} (Å)	Q_{CT}	D_{CT} (Å)	Q_{CT}	D_{CT} (Å)	Q_{CT}
PrPzPy	B3LYP	4.13	0.79	5.15	0.96	3.25	0.65	1.14	0.37
MePzCzPy		4.57	0.83	3.67	0.76	3.45	0.61	2.71	0.58
PrPzPy	wB97X-D	1.16	0.66	2.35	0.62	1.13	0.51	0.71	0.36
MePzCzPy		1.59	0.66	1.18	0.52	0.21	0.33	1.00	0.41

Table S4: A comparison of HOMO and LUMO energies (in eV), $\lambda_{max}\,(in\ nm)$ of the UV spectrum (for transition to S_1 state) for B3LYP and wB97X-D results against experimental values

Molecule	HOMO			LUMO			λ_{max}(nm)		
	B3LYP	wB97X-D	Exp.	B3LYP	wB97X-D	Exp.	B3LYP	wB97X-D	Exp.
PrPzPy	-5.28	-7.17	-5.10	-1.60	0.22	-2.14	392.81	317.76	330
MePzCzPy	-5.43	-7.33	-5.10	-1.58	0.21	-2.04	372.59	297.97	338

3. **Cyclic Voltammetry**

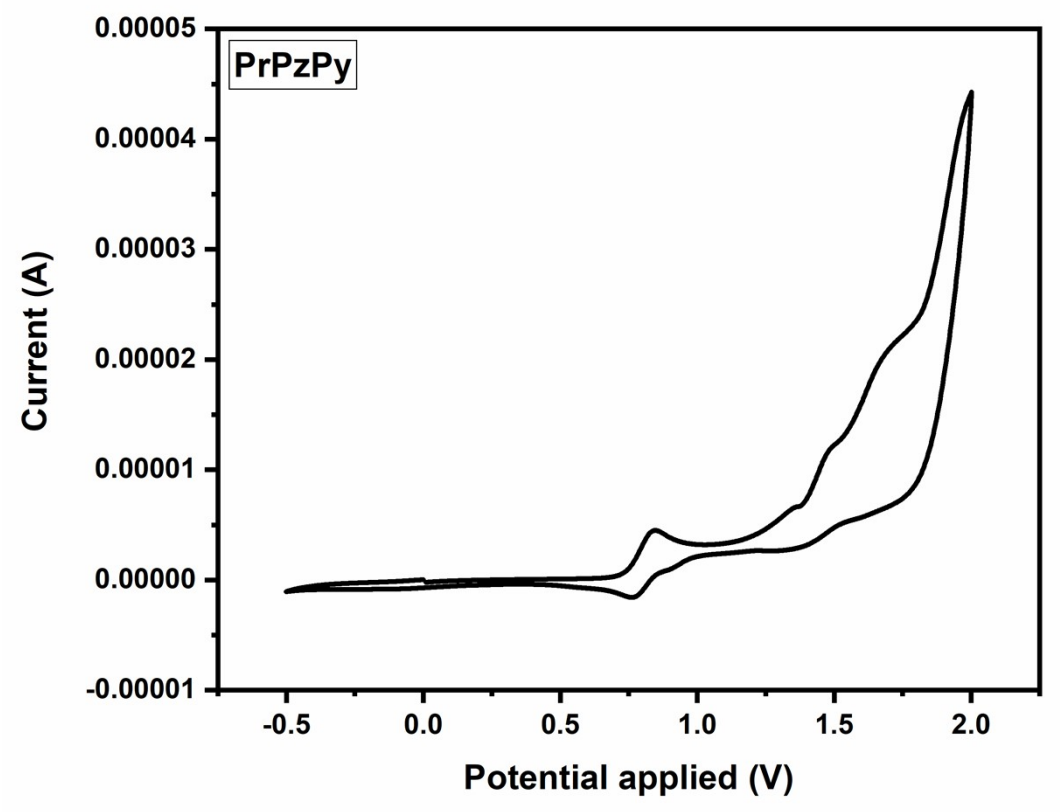


Fig. S3. Cyclic Voltagrmmograms of **PrPzPy**

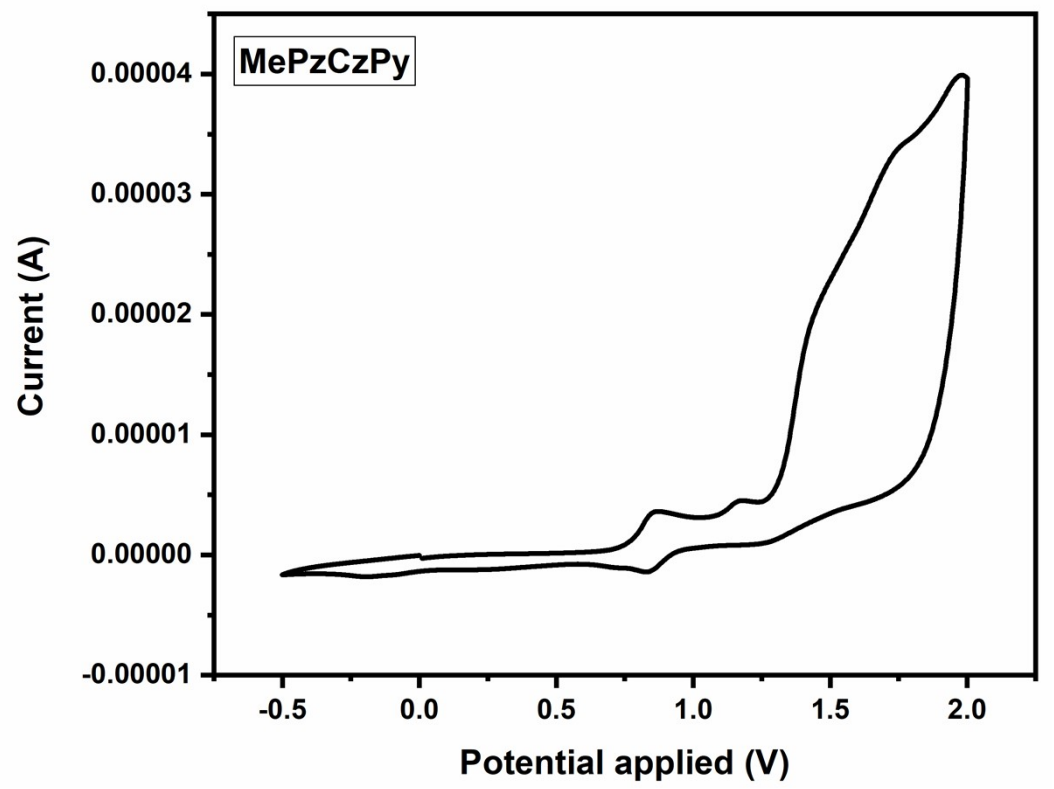


Fig. S4. Cyclic Voltagrmmograms of **MePzCzPy**

4. TGA analysis

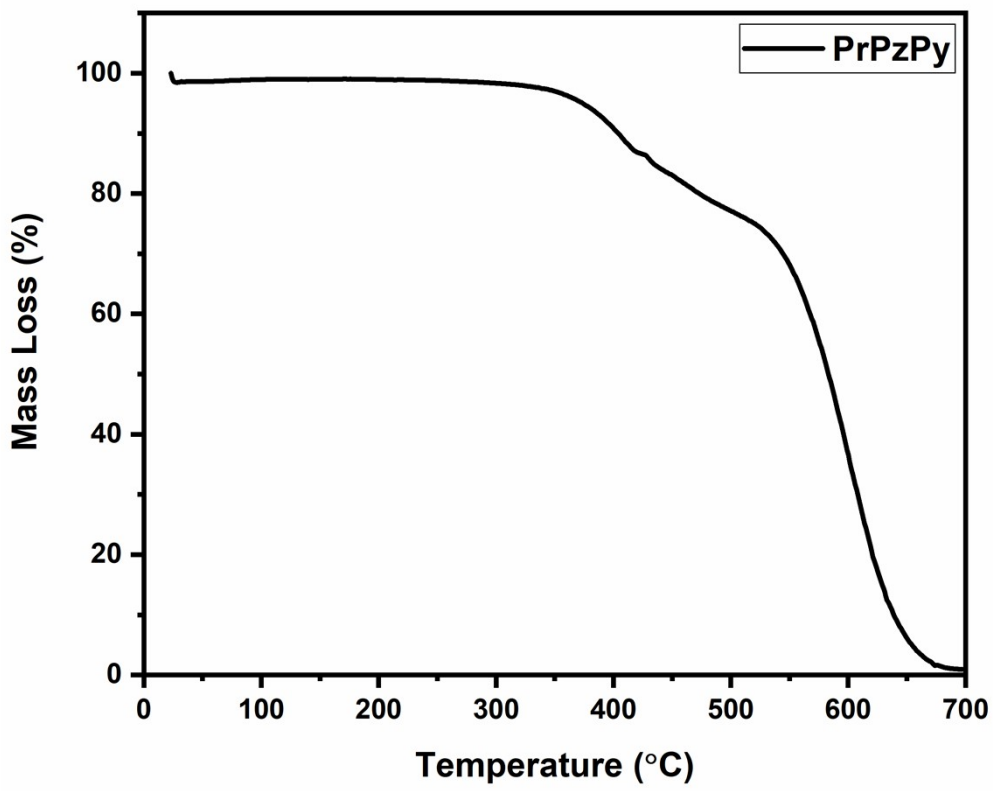


Fig. S5. TGA graph of **PrPzPy**

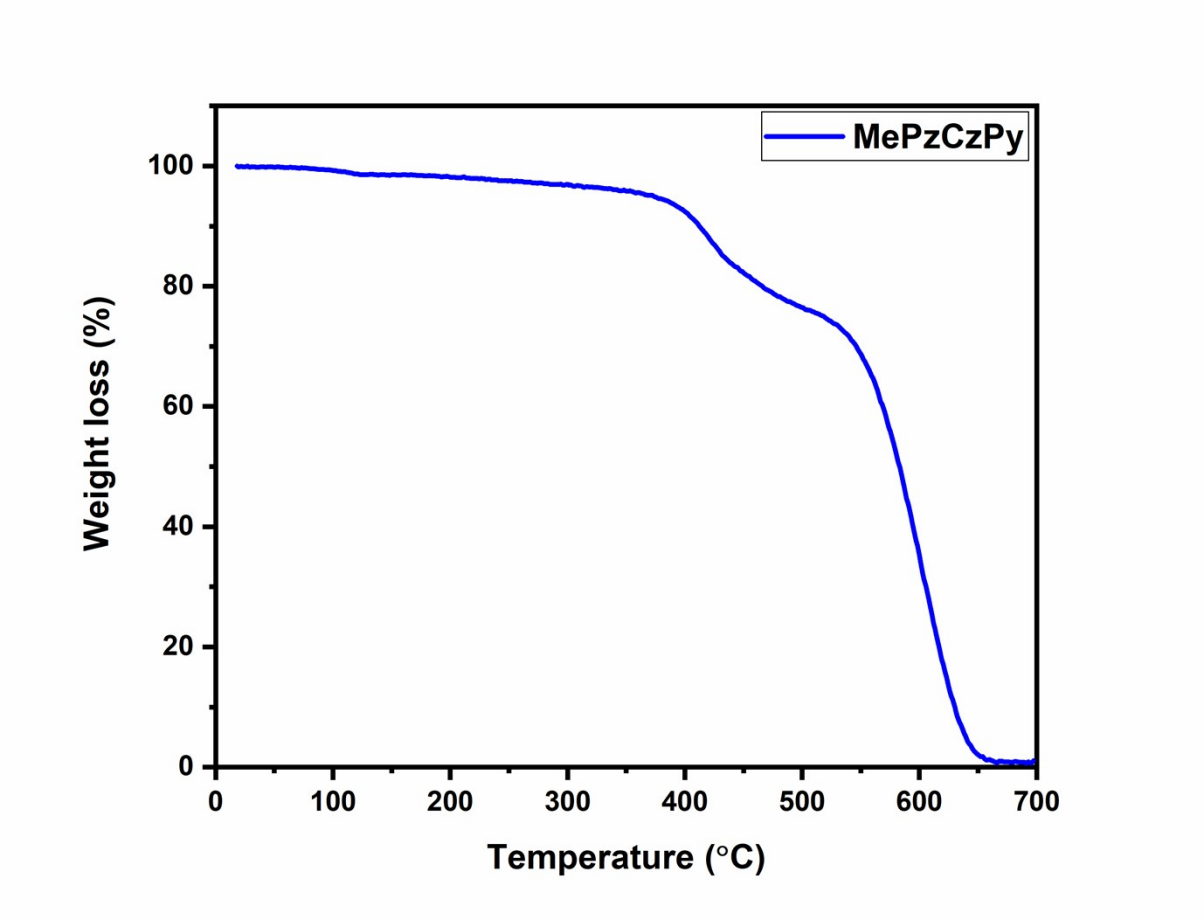


Fig. S6. TGA graph of **MePzCzPy**

5. DSC analysis

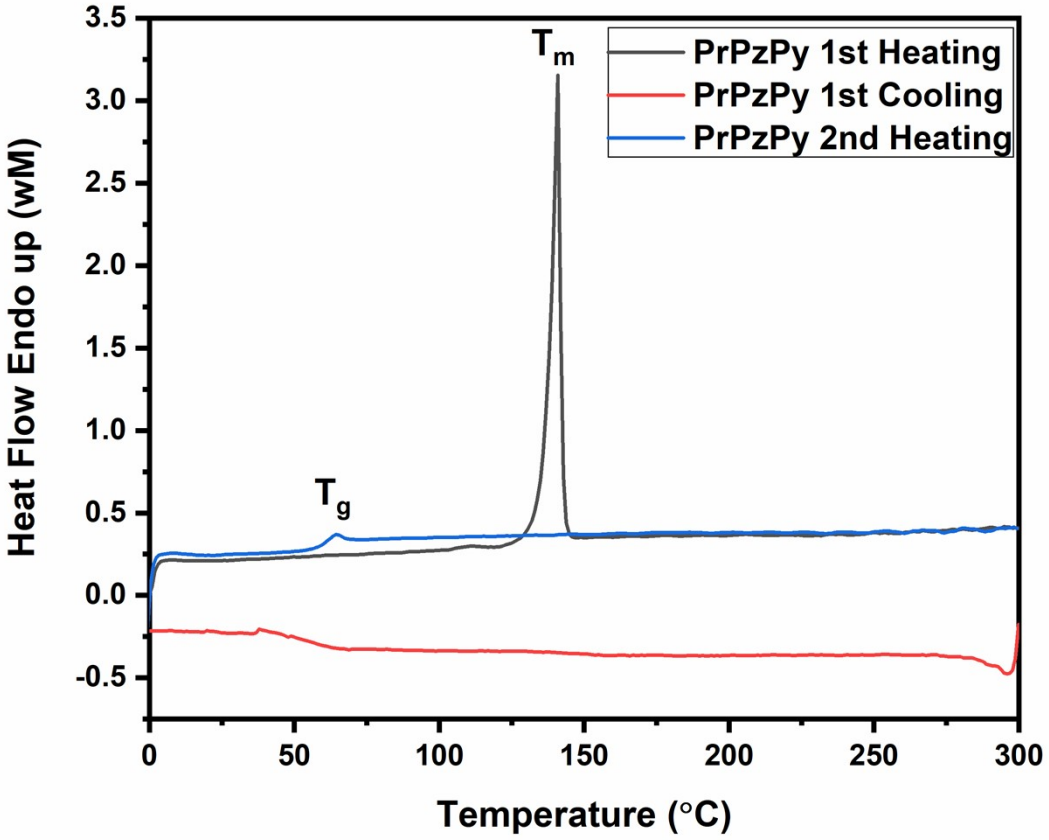


Fig. S7. DSC graph of **PrPzPy**

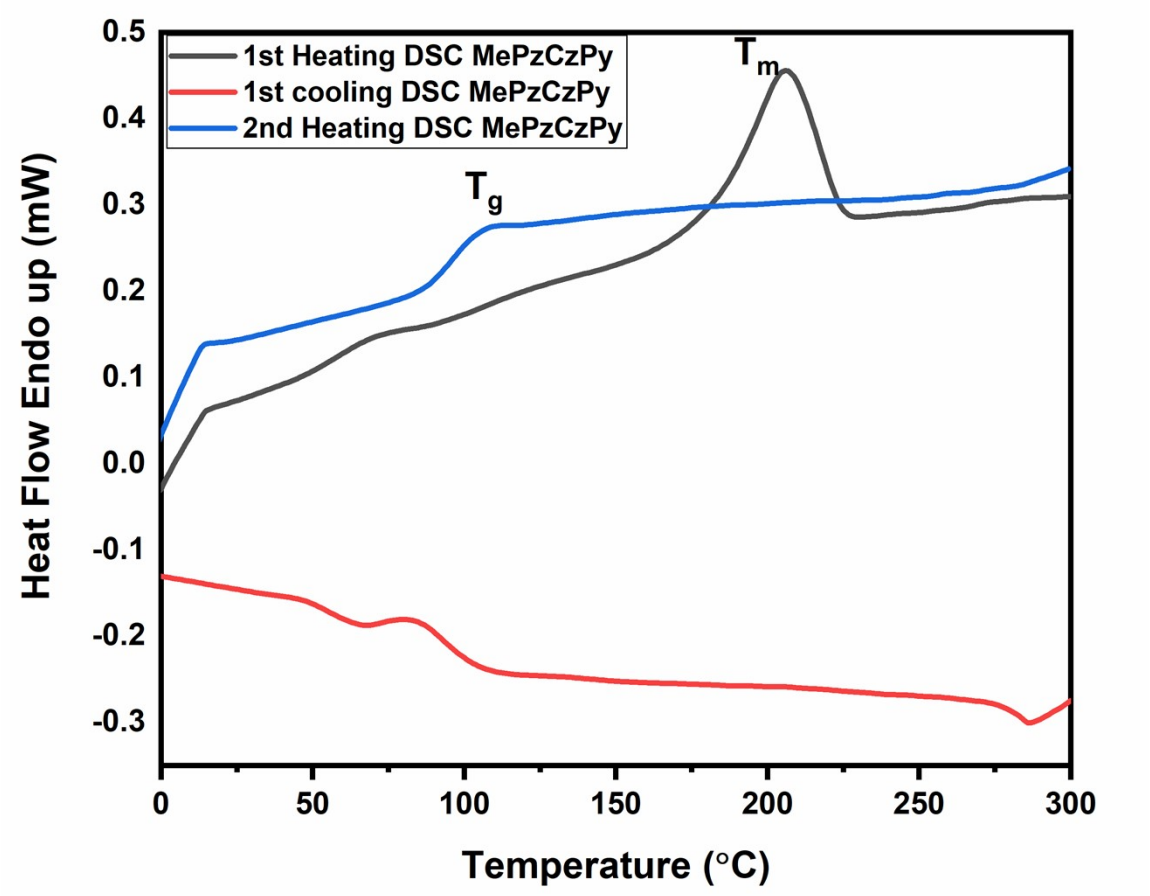


Fig. S8. DSC graph of **MePzCzPy**

6. X-ray analysis

Single-crystal X-ray diffraction data of **PrPzPy** was gathered on an Agilent Supernova X-ray diffractometer equipped with a CCD detector at room temperature (150 or 296 K) using the source graphite-monochromatic Cu Kα radiation (λ = 1.54184Å). For single crystal analysis, the same methods and software were used as mentioned in the previous report.[6-10] Crystallographic data have been illustrated in Table S5. CCDC 2192347 contains the supplementary crystallographic data for this paper. These data can be acquired free of cost from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Table **S5 Crystal data and structure refinement for** PrPzPy (CCDC No. 2192347)

Identification code	**PrPzPy**
Empirical formula	$C_{34}H_{30}N_2O_2S$
Formula weight	530.66
Temperature/K	296(2)
Crystal system	Monoclinic
Space group	$P2_1/c$
a/Å	15.6071(7)
b/Å	10.1092(4)
c/Å	19.5816(8)
α/°	90.00
β/°	110.641(5)
γ/°	90.00
Volume/Å^3	2891.2(2)
Z	4
ρ_{calc}g/cm^3	1.219
μ/mm^{-1}	1.245
F(000)	1120
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.04 to 133.74

Index ranges	$-18 \leq h \leq 18$ $-12 \leq k \leq 5$ $-23 \leq l \leq 17$
Reflections collected	9730
Independent reflections	5084
Data/restraints/parameters	5084/6/356
Goodness-of-fit on F^2	1.022
Final R indexes [I>=2σ (I)]	$R_1 = 0.0507$, $wR_2 = 0.1370$
Final R indexes [all data]	$R_1 = 0.0643$, $wR_2 = 0.1530$
CCDC No	2192347

7. ^{1}H and ^{13}C NMR spectra

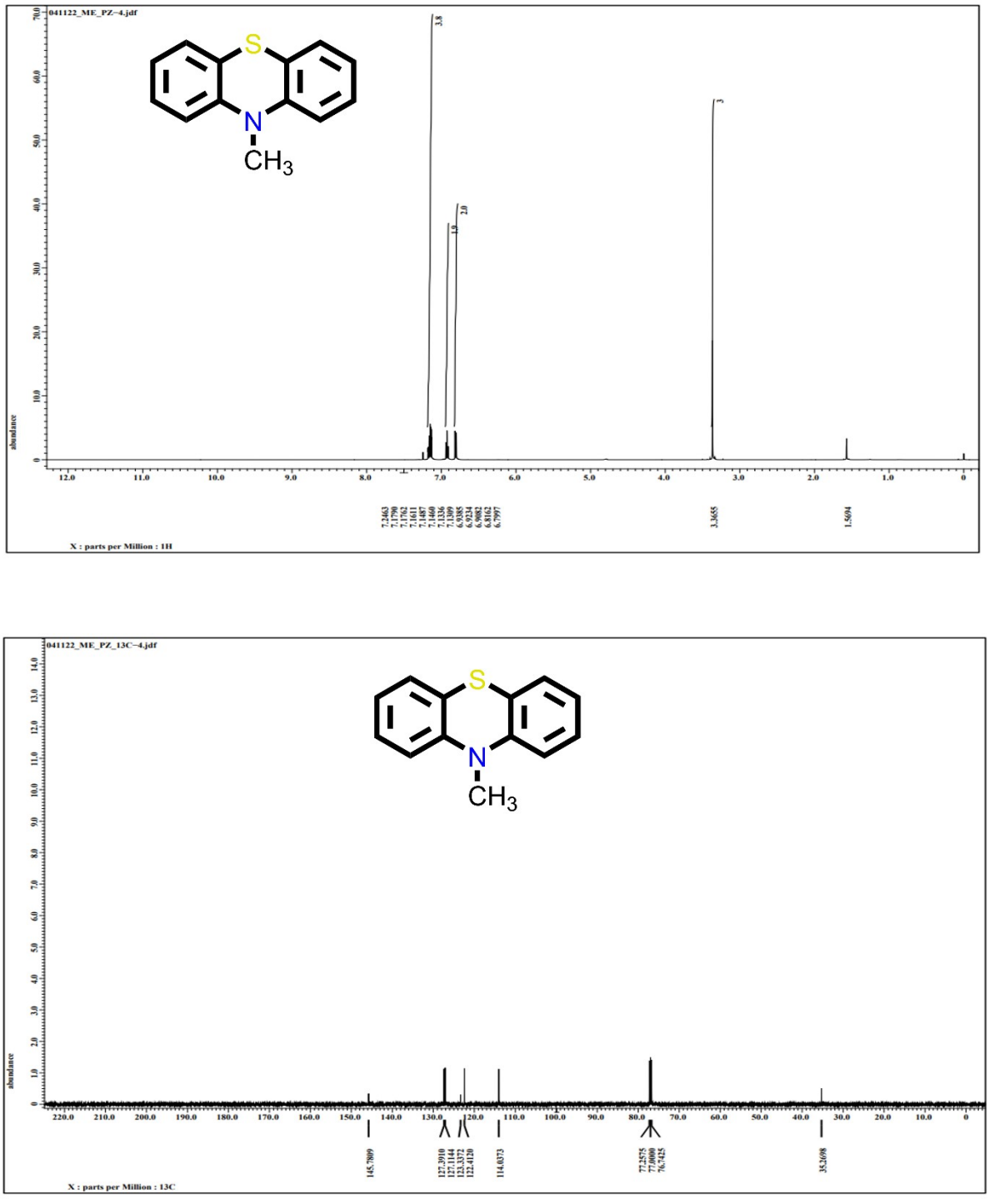
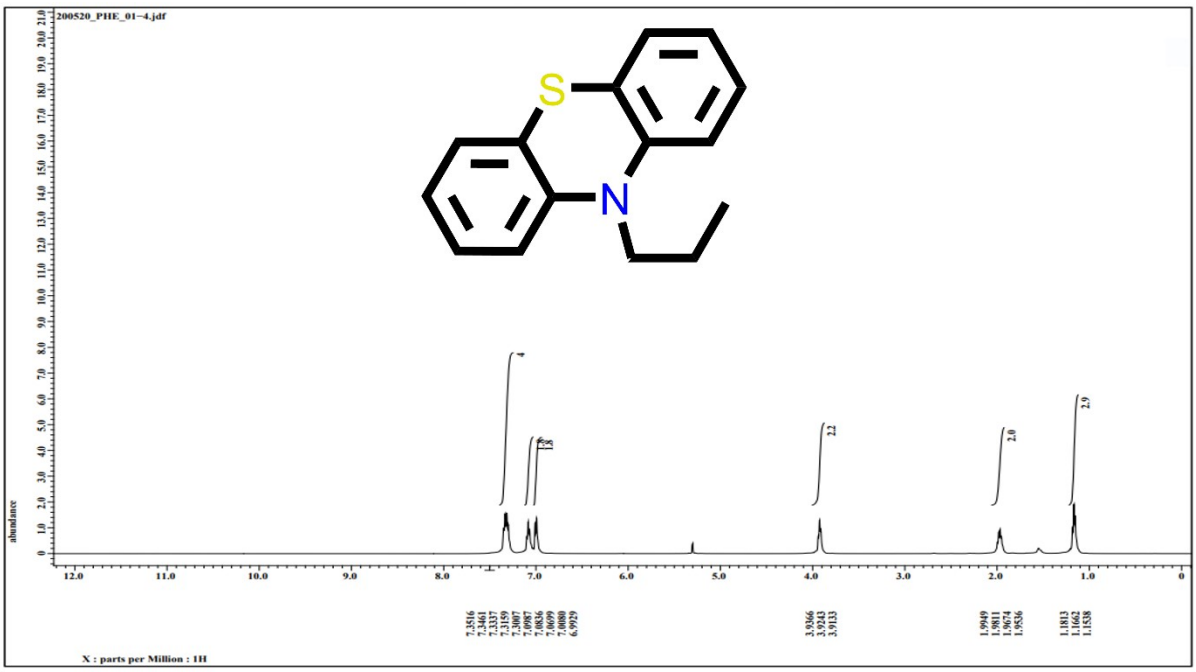


Fig. S9. ^{1}H and ^{13}C NMR spectrum of **MePz**



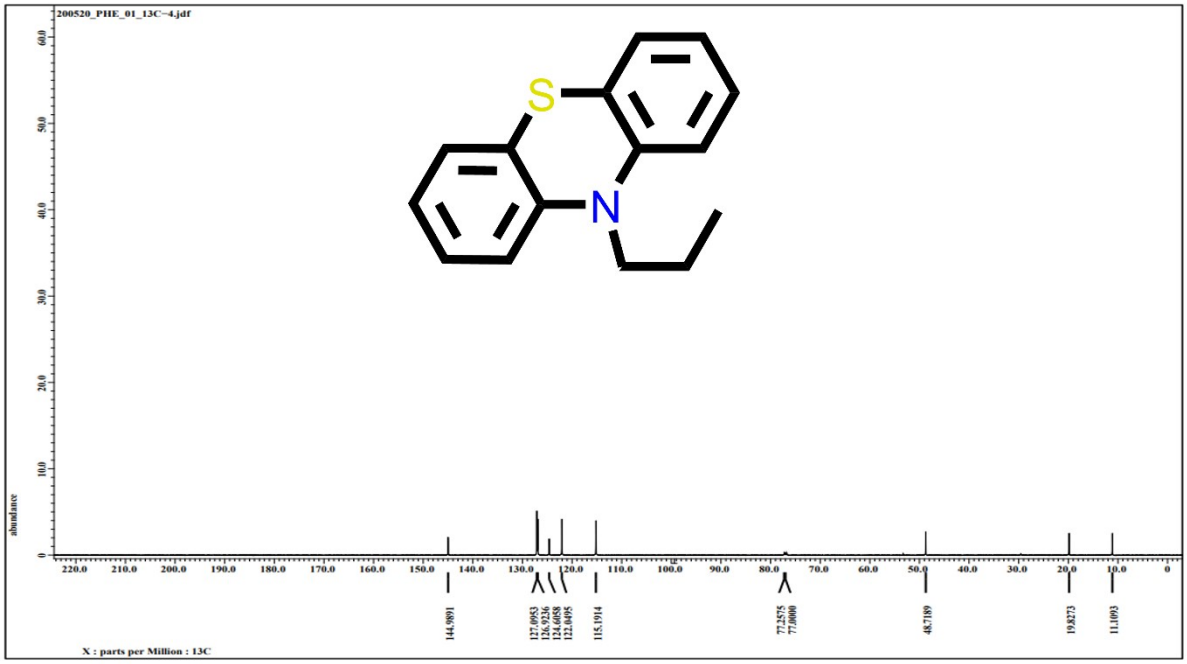


Fig. S10. ^{1}H and ^{13}C NMR spectrum of **PrPz**

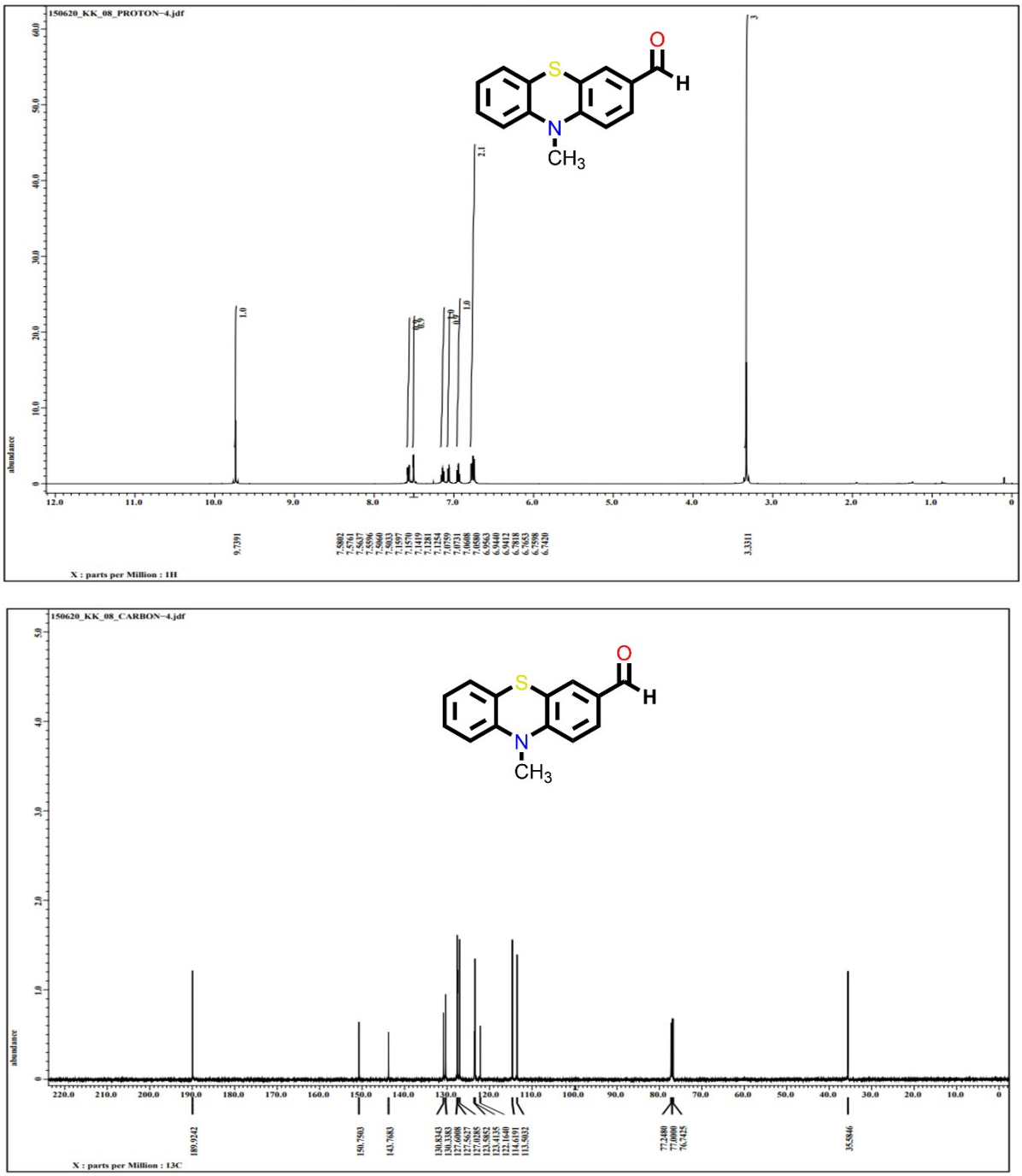


Fig. S11. ^{1}H and ^{13}C NMR spectrum of **MePzCHO**

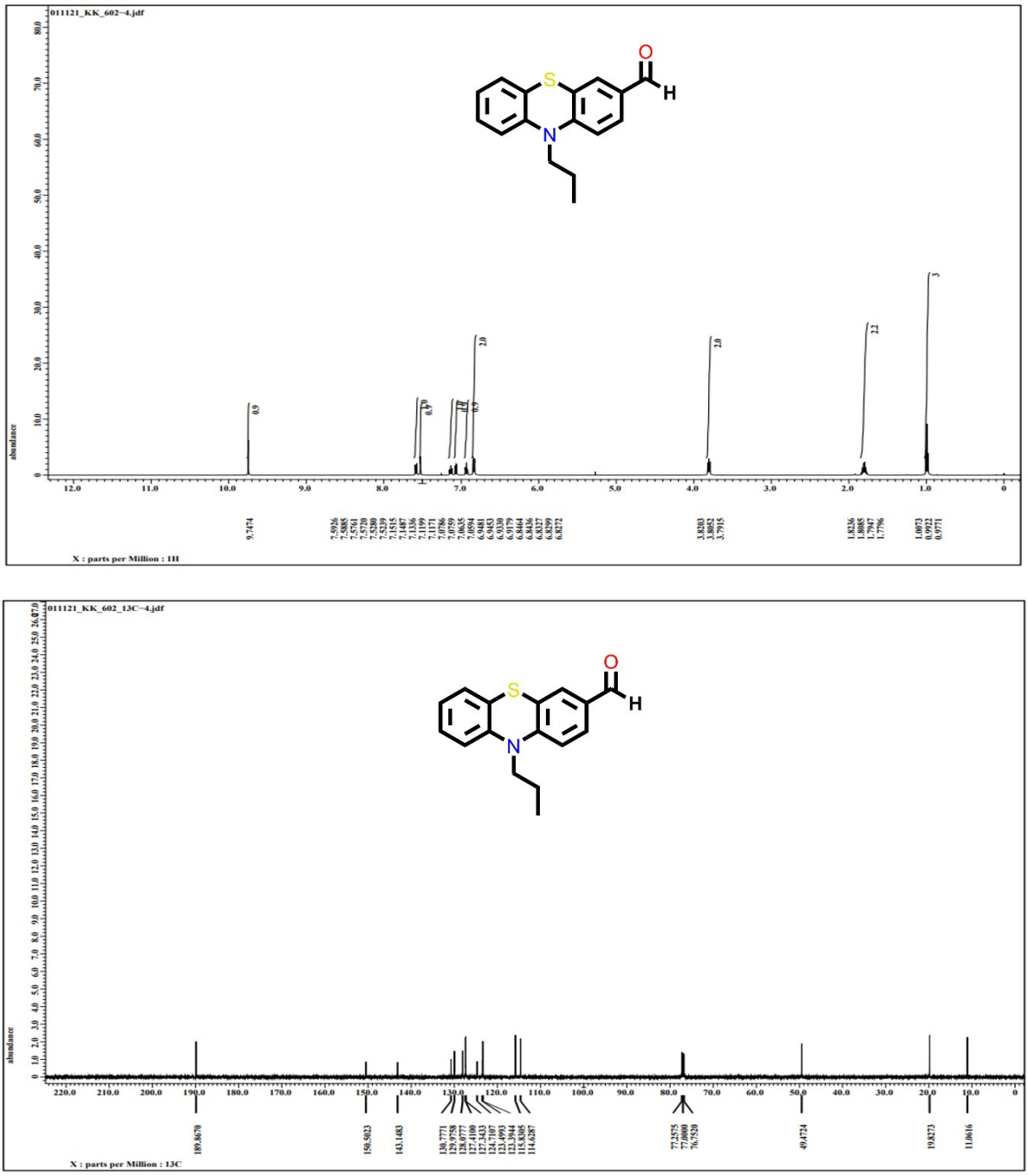


Fig. S12. ^{1}H and ^{13}C NMR spectrum of **PrPzCHO**

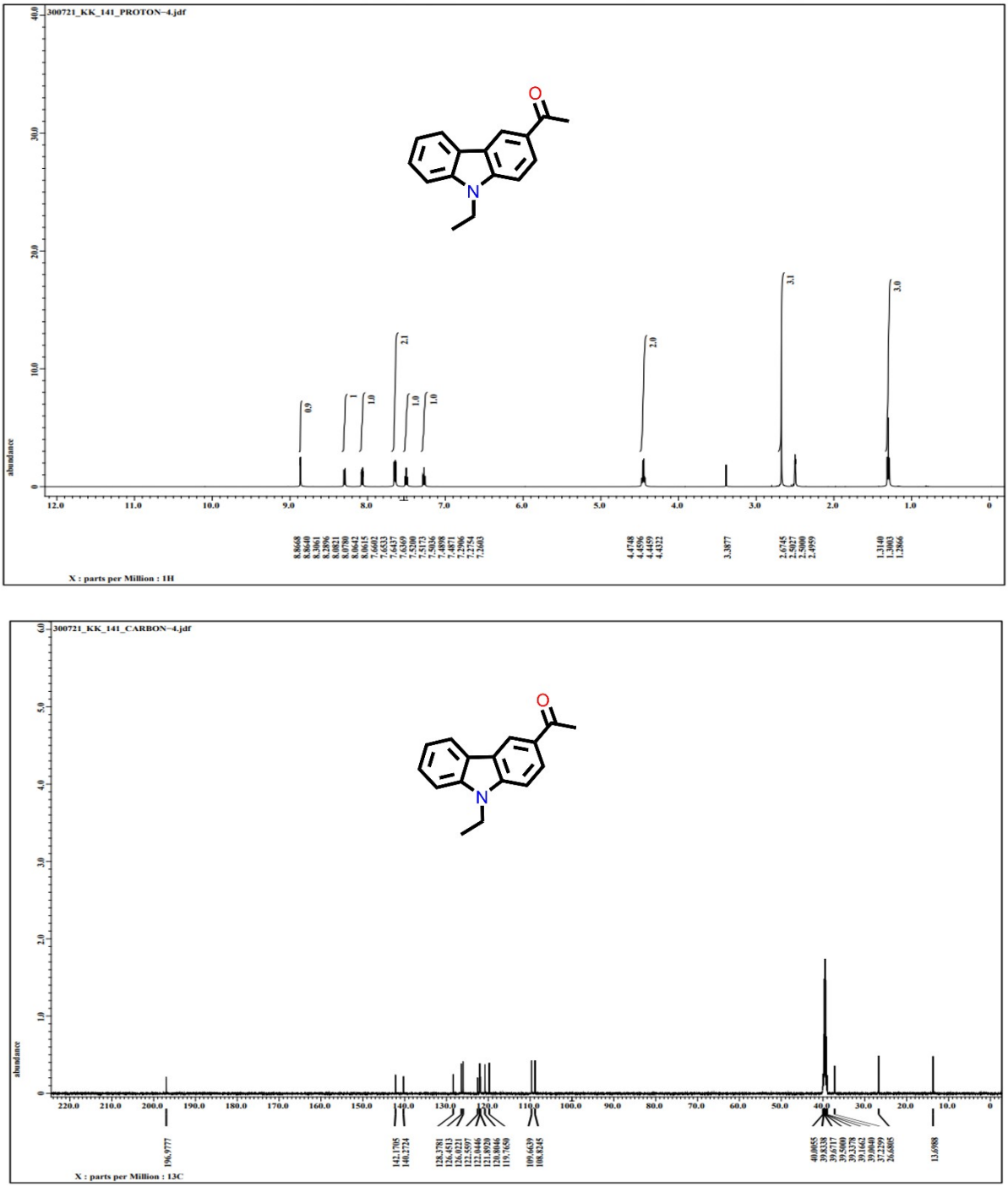


Fig. S13. ^{1}H and ^{13}C NMR spectrum of **EtCzAc**

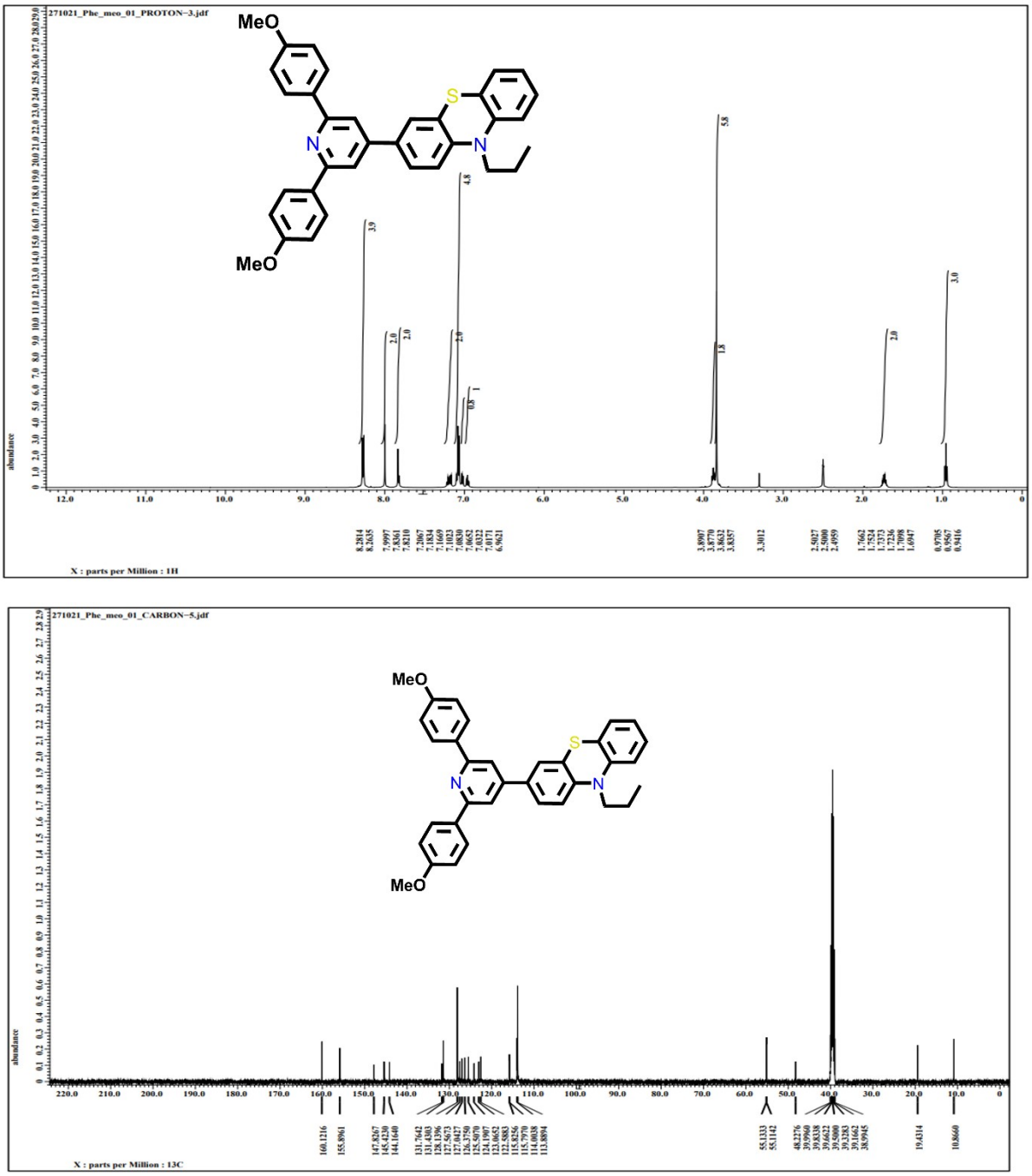


Fig. S14. ^{1}H and ^{13}C NMR spectrum of **PrPzPy**

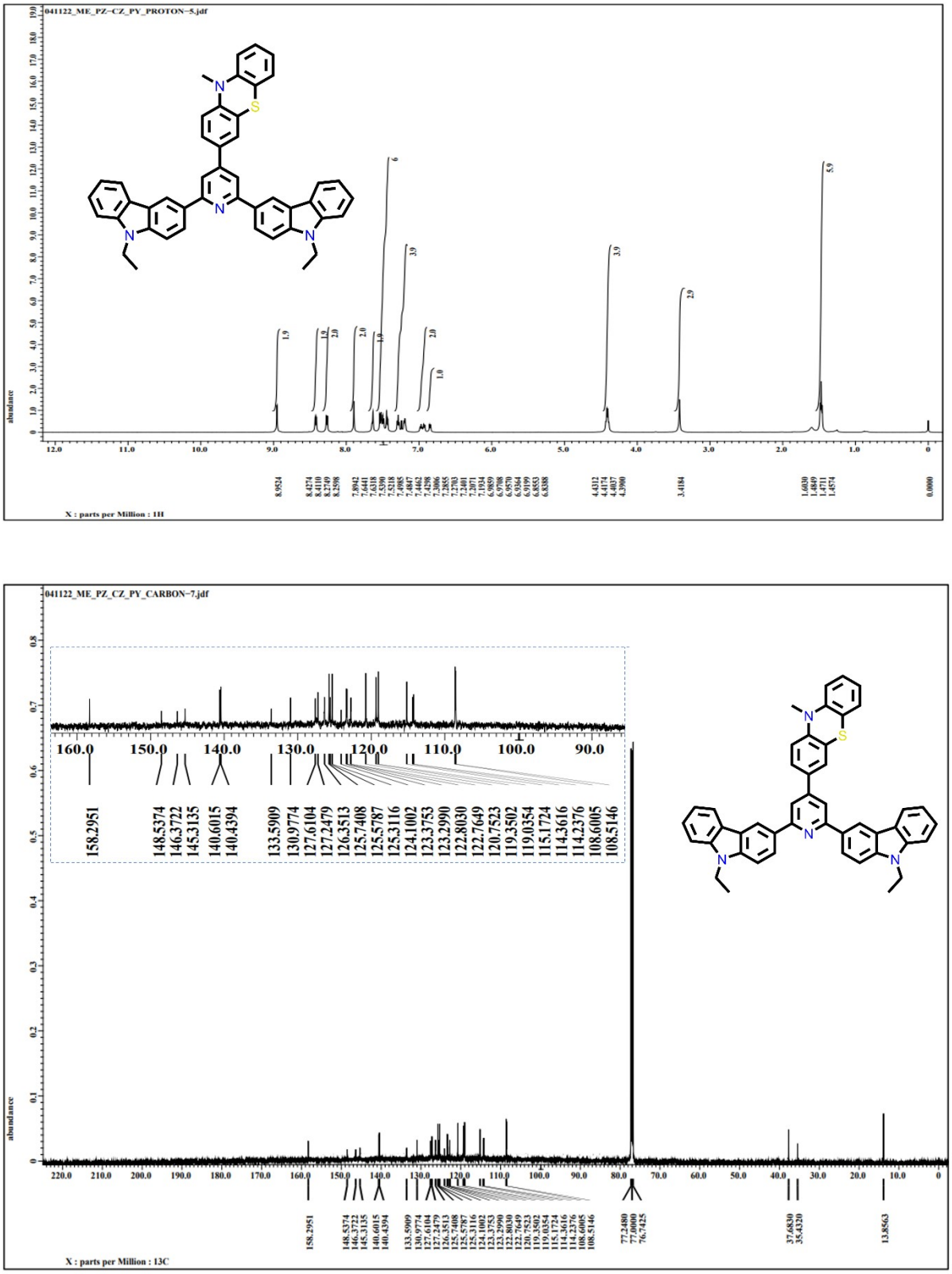


Fig. S15. ^{1}H and ^{13}C NMR spectrum of **MePzCzPy**

8. HRMS spectrum

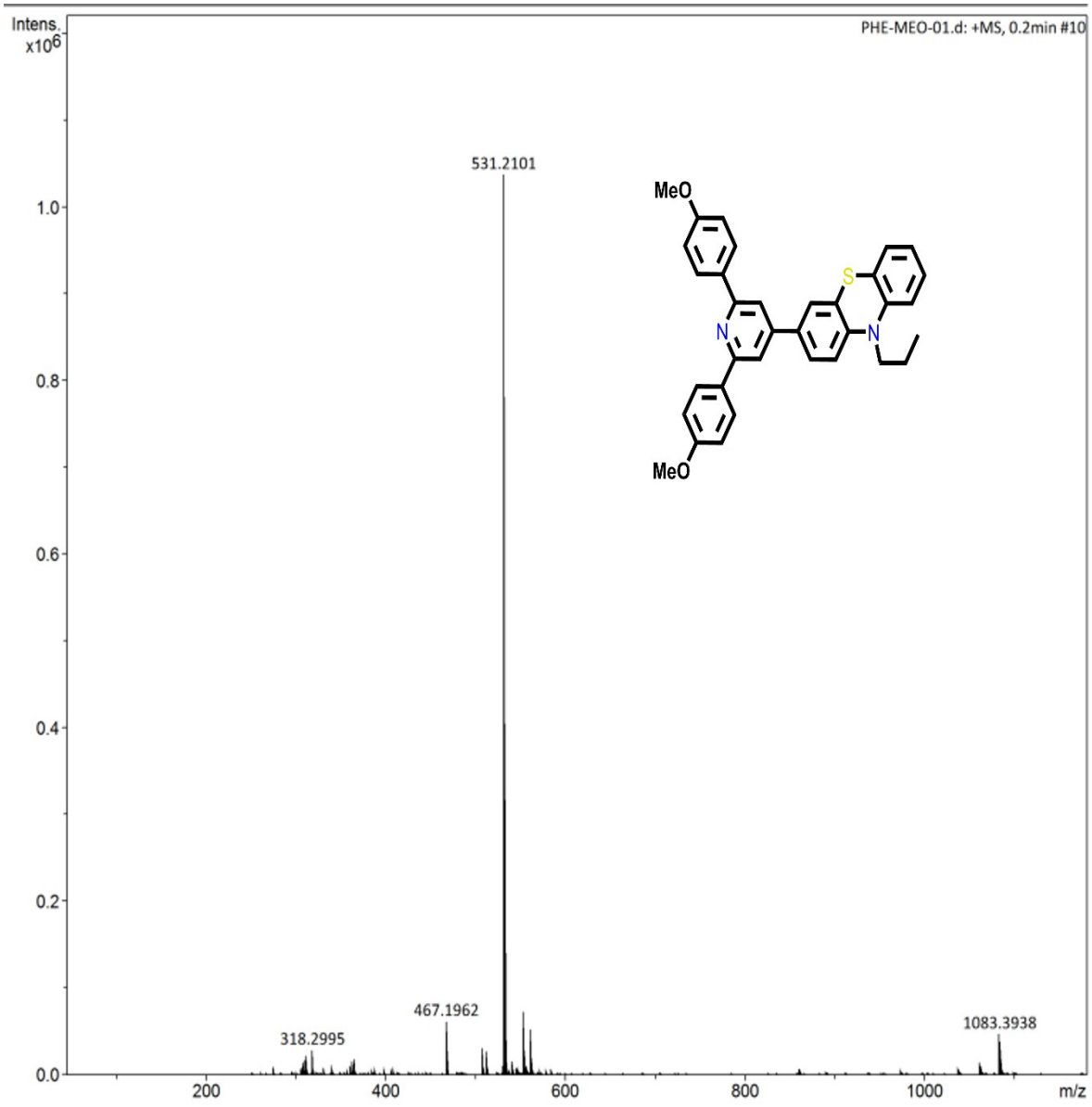


Fig. S16. HRMS spectrum of **PrPzPy**

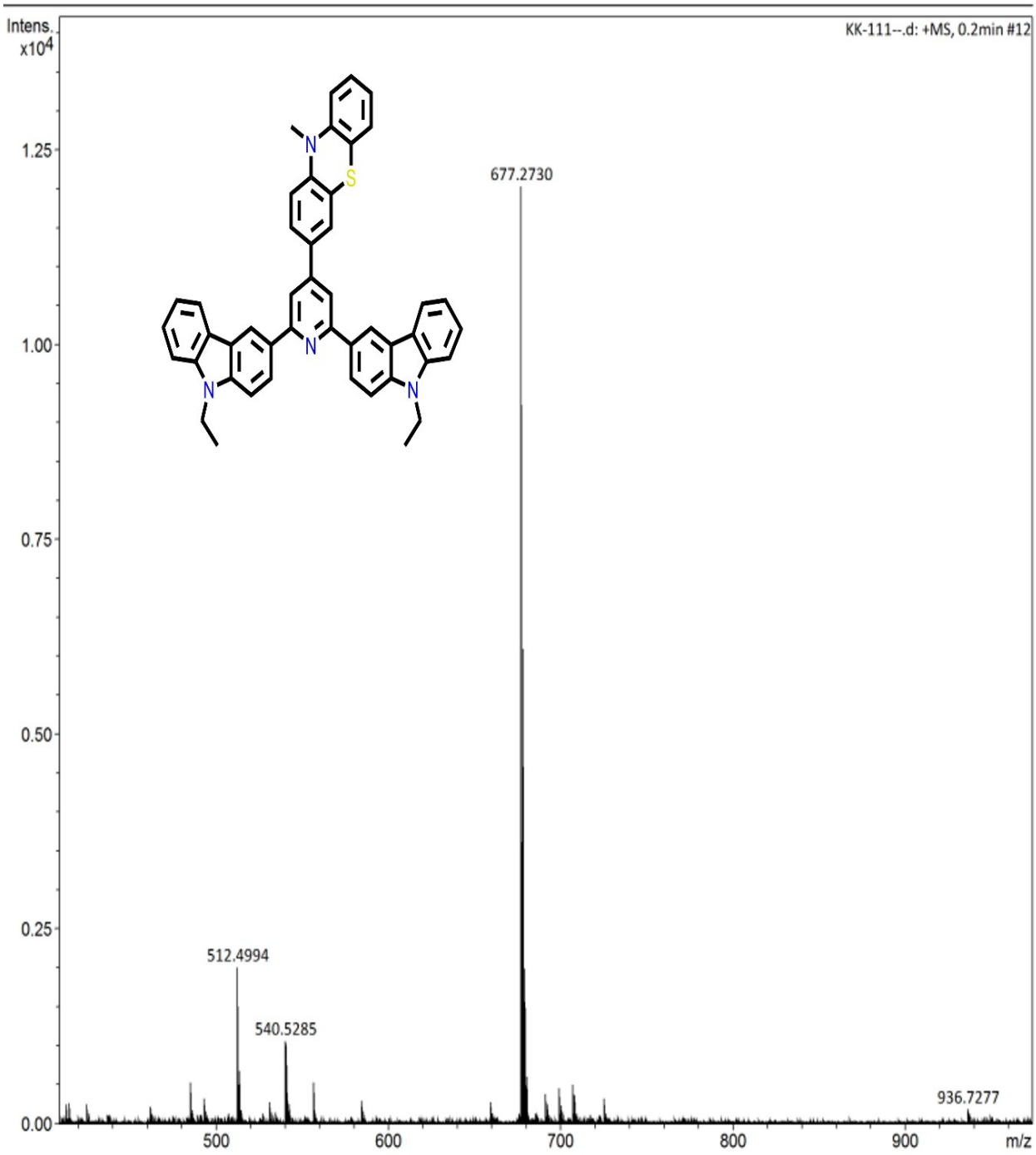


Fig. S17. HRMS spectrum **MePzCzPy**

9. Coordinates of the optimized structures:

1.1 Coordinates of the optimized structure of **PrPzPy** with B3LYP functional.

Atomic No.	X-coordinate	Y-coordinates	Z-coordinates
6	7.621008647	-1.688739081	2.241225075
6	8.097876672	-0.596083002	1.526995018
6	7.296480592	0.039294050	0.580424949
6	5.998910513	-0.417257983	0.294429926
6	5.547570475	-1.550559069	0.999782980
6	6.335614514	-2.155155115	1.975818056
7	5.184548447	0.220707067	-0.670302148
6	3.779391342	0.182932066	-0.592291140
6	3.105065287	-0.889032013	0.027923906
16	4.011070354	-2.329766128	0.549212947
6	2.976257285	1.195556146	-1.144574183
6	1.589160179	1.153667142	-1.062259175
6	0.926711127	0.111772064	-0.406234127
6	1.720626186	-0.905262017	0.141923914
6	5.812811522	1.169315141	-1.603702218
6	5.998735514	2.616273248	-1.109457182
6	6.679008584	3.479635312	-2.175966264
6	-0.550765987	0.076511064	-0.296418119
6	-1.294390041	1.252082156	-0.150899108
6	-2.687483149	1.184076154	-0.030942099
7	-3.345663201	0.015243063	-0.084959103
6	-2.652977151	-1.124389024	-0.240516115

6	-1.256096045	-1.130915028	-0.332836122
6	-3.441145213	-2.383650120	-0.289399118
6	-3.514217209	2.406314247	0.147428915
6	-4.719041313	-2.438667123	0.278204925
6	-5.480929385	-3.604062209	0.259812924
6	-4.970642335	-4.756438301	-0.347434123
6	-3.696779238	-4.716212299	-0.930709167
6	-2.948680176	-3.550812208	-0.899140166
6	-2.994951170	3.584236334	0.695052959
6	-3.779802227	4.724456421	0.861053968
6	-5.122244330	4.704255423	0.471352940
6	-5.659517393	3.529927334	-0.075794102
6	-4.869169316	2.404434250	-0.228611114
8	-5.624152371	-5.946959383	-0.426513129
6	-6.929801505	-6.048794412	0.142304914
8	-5.978699382	5.755212484	0.583531949
6	-5.491718356	6.977240605	1.138386990
1	8.234139655	-2.176228122	2.989283131
1	9.096502723	-0.216067972	1.708594034
1	7.699022656	0.896572117	0.063037909
1	5.943713516	-3.013268180	2.509947097
1	3.427249320	2.031498208	-1.656841224
1	1.020564136	1.947894204	-1.530905215
1	1.256219147	-1.731816078	0.666509953
1	6.782552591	0.750805105	-1.882547238

1	5.213118452	1.168680138	-2.516927289
1	5.032139441	3.050844284	-0.843973163
1	6.591043556	2.627689247	-0.191452111
1	6.087738524	3.513920314	-3.096153334
1	6.807080591	4.506002389	-1.824566234
1	7.668841667	3.088964281	-2.431308284
1	-0.791519003	2.208997228	-0.121360106
1	-0.722908003	-2.065453099	-0.440761130
1	-5.116933338	-1.548328053	0.747621961
1	-6.459698429	-3.603074208	0.719937958
1	-3.317892207	-5.610213366	-1.411431205
1	-1.977437101	-3.548376209	-1.379162204
1	-1.964668091	3.622219338	1.028344983
1	-3.338834195	5.609187503	1.299376002
1	-6.700879427	3.527552338	-0.375622125
1	-5.290750347	1.500817180	-0.649263146
1	-7.628037550	-5.356538335	-0.338000122
1	-7.252316517	-7.071919464	-0.040002099
1	-6.909682504	-5.860747361	1.220121999
1	-4.678071294	7.391675610	0.535248944
1	-6.335786443	7.663858669	1.127226991
1	-5.150281331	6.837733607	2.168664068

1.2 Coordinates of the optimized structure of **MePzCzPy** with B3LYP functional.

Atomic No.	**X-coordinate**	**Y-coordinates**	**Z-coordinates**
6	10.064860205	0.898319847	0.281374249

6	10.285734872	-0.309343753	0.935408493
6	9.336768826	-1.329397085	0.881483231
6	8.158024228	-1.173137092	0.139234912
6	7.949410121	0.050551773	-0.523158389
6	8.882737445	1.079450440	-0.435384333
7	7.193767023	-2.202755773	0.042278249
6	5.826359148	-1.869858747	0.076729240
6	5.362621862	-0.715012683	-0.581923478
16	6.510689843	0.235651099	-1.563458855
6	4.881103412	-2.659211568	0.746995542
6	3.531252907	-2.323858854	0.736857729
6	3.071154413	-1.168780502	0.094541164
6	4.020290516	-0.361678518	-0.550680192
6	1.634695024	-0.800688073	0.099999479
6	0.636392026	-1.776958263	0.025639693
6	-0.710727200	-1.394451813	0.017325354
7	-1.079050636	-0.106881555	0.113019159
6	-0.137278204	0.846109208	0.201935109
6	1.227967856	0.534676681	0.180276004
6	-0.615653389	2.250885417	0.302472940
6	-1.804833087	-2.397433478	-0.077782656
6	-1.885927151	2.586272465	-0.178400580
6	-2.336180397	3.902280243	-0.097189473
6	-1.509047162	4.899223060	0.485634168
6	-0.241087852	4.579437475	0.978562459

6	0.185642258	3.261837450	0.879186893
6	-1.596472900	-3.656861858	-0.683559028
6	-2.604789975	-4.606128250	-0.785313357
6	-3.860254097	-4.290595631	-0.258662804
6	-4.099126655	-3.029324312	0.349360490
6	-3.071568034	-2.091958826	0.431431669
6	7.586514334	-3.553608952	0.431613397
6	-3.558548711	4.566765749	-0.498275830
6	-3.412289781	5.932145331	-0.137119882
7	-2.173047555	6.114553787	0.466636104
7	-5.018862421	-5.048176089	-0.213884895
6	-6.015635636	-4.296296590	0.398235024
6	-5.483556803	-3.034262943	0.773100555
6	-4.738495874	4.136155547	-1.112134290
6	-5.747799451	5.060087027	-1.360286177
6	-5.587213524	6.408082586	-1.000813717
6	-4.423291753	6.863477551	-0.388645311
6	-7.347295896	-4.630413374	0.658935283
6	-8.138447898	-3.686061742	1.306303599
6	-7.625269953	-2.435269175	1.685986053
6	-6.300584885	-2.104048758	1.422326155
6	-5.186155379	-6.380575635	-0.784170959
6	-5.621570039	-6.365073705	-2.251826755
6	-1.633838635	7.387080076	0.933767859
6	-0.868352195	8.157735298	-0.145153472

1	10.796873739	1.695400656	0.329346611
1	11.194155940	-0.463035458	1.506245068
1	9.519110235	-2.248003391	1.422176843
1	8.688593267	2.016291348	-0.944849741
1	5.196195734	-3.538905704	1.291266371
1	2.835005531	-2.956099558	1.274698705
1	3.704293909	0.532265776	-1.075299309
1	0.906430509	-2.822427327	-0.033731583
1	1.967276178	1.322007368	0.233376402
1	-2.502878623	1.811609895	-0.615449783
1	0.398262807	5.326129852	1.433072015
1	1.158417899	3.008654982	1.282521664
1	-0.629905212	-3.889338891	-1.113643985
1	-2.414123073	-5.553796986	-1.273623718
1	-3.234507424	-1.124102189	0.888195749
1	7.604107520	-3.706579950	1.518263615
1	6.890803999	-4.266247725	-0.009970697
1	8.579396007	-3.761403919	0.034358553
1	-4.864454019	3.096018113	-1.391864009
1	-6.667185759	4.740149786	-1.836688806
1	-6.385477722	7.112552074	-1.205896132
1	-4.313358174	7.907639515	-0.122512736
1	-7.760667096	-5.588542870	0.368397733
1	-9.174858104	-3.923111612	1.518999012
1	-8.270161650	-1.723178148	2.187597395

1	-5.906700213	-1.137136523	1.715502152
1	-4.239328436	-6.912966631	-0.670812582
1	-5.916779294	-6.915129537	-0.173721472
1	-6.579473731	-5.853871549	-2.370738926
1	-4.882244053	-5.856595912	-2.874689888
1	-5.732008008	-7.388719573	-2.618915536
1	-2.466500439	7.983234708	1.312876446
1	-0.986785852	7.181375333	1.789057874
1	-1.513887594	8.386241601	-0.996112728
1	-0.494719101	9.100059852	0.263806336
1	-0.015023966	7.580263904	-0.507651940

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