Electronic Supplementary Material (ESI) for RSC Advances.

Effects of Cyano Groups on the Properties of Thiazole-based β-Ketoiminate Boron Complexes: Aggregation-Induced Emission and Mechanofluorochromism

Lin Zhou,[a] Defang Xu,[b] Huaizhi Gao,[a] Aixia Han[a] Yan Yang,[a] Chao Zhang,[a] Xingliang Liu,[a]* and Feng Zhao[c]*

[a]Chemical Engineering College, Qinghai University, Xining 810016, China

[b]Key Lab of Comprehensive and Highly Efficient Utilization of Salt Lake Resources, Qinghai Institute of Salt Lakes, Chinese Academy of Sciences, Xining 810008, China

[c]Henan Province Key Laboratory of New Optoelectronic Functional Materials, College of Chemistry and Chemical Engineering, Anyang Normal University, Anyang, Henan 455000, China

*To whom correspondence should be addressed. E-mail: liuxingliangqhu@163.com, zhaofeng@aynu.edu.cn

Table S1. Photophysical data of **BF_2-TT-CN**, **BPh_2-TT-CN**, **BF_2-TT** and **BPh_2-TT** in different solvents.

	solvent	λ_{abs} (nm)	ε^{max}(M^{-1} cm^{-1})	λ_{em} (nm)	$\Delta\nu_{st}$(cm^{-1})	Φ_f
BF_2-TT-CN	cyclohexane	293, 456	60900	506	2167	0.380
	toluene	293, 457	58600	543	3466	0.289
	THF	292, 451	56000	596	5394	0.026
	DCM	293, 457	57900	603	5298	0.039
	DMF	290, 452	51800	612	5784	0.005
	Acetonitrile	289, 447	55900	618	6190	0.004
BPh_2-TT-CN	cyclohexane	288, 451	55200	498	2093	0.392
	toluene	292, 458	52400	524	2750	0.365
	THF	288, 451	50900	564	4442	0.142
	DCM	291, 454	51300	571	4513	0.169
	DMF	449	47400	600	5605	0.005
	Acetonitrile	445	50300	606	5970	0.008
BF_2-TT	cyclohexane	431	57100	474	2105	0.553
	toluene	436	51800	496	2774	0.458
	THF	434	52100	526	4030	0.420
	DCM	448	53600	545	3973	0.354
	DMF	445	50900	568	4866	0.048
	Acetonitrile	448	54200	575	4930	0.036
BPh_2-TT	cyclohexane	442	45500	489	2175	0.389
	toluene	446	51700	497	2301	0.334
	THF	444	50800	506	2760	0.475
	DCM	446	52200	520	3191	0.451
	DMF	444	48800	528	3583	0.354
	Acetonitrile	440	52800	530	3859	0.378

a. $\Delta\nu_{st} = \nu_{abs}-\nu_{em}$. b. The fluorescence quantum yield (Φ_f) was measured using fluorescein (Φ=0.79 in 0.1 M sodium hydroxide water solution) as standard.

Table S2. Dihedral angles between boron chelate ring A and phenyl ring B.

BF_2-TT-CN	**BPh_2-TT-CN**	**BF_2-TT**	**BPh_2-TT**
22.5°	22.4°	9.3°	2.3°

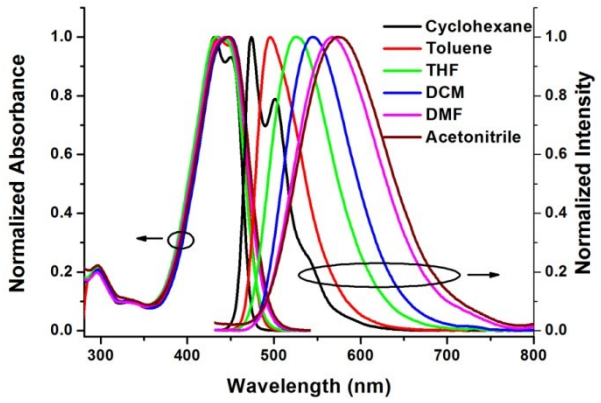

Fig. S1 Normalized UV-vis absorption spectra (left) and normalized PL spectra (right, excited at 410 nm) of **BF_2-TT** in different solvents (1.0×10^{-5} mol L^{-1}).

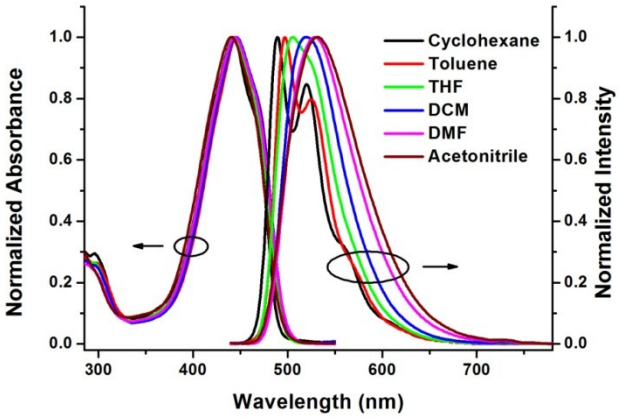

Fig. S2 Normalized UV-vis absorption spectra (left) and normalized PL spectra (right, excited at 420 nm) of **BPh_2-TT** in different solvents (1.0×10^{-5} mol L^{-1}).

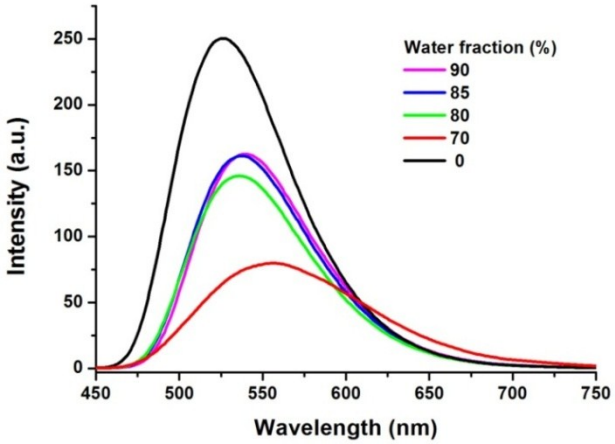

Fig. S3 PL spectra of **BF_2-TT** (λ_{ex} = 420 nm) in water–THF mixtures with different water fractions ($0 < f_w < 90\%$).

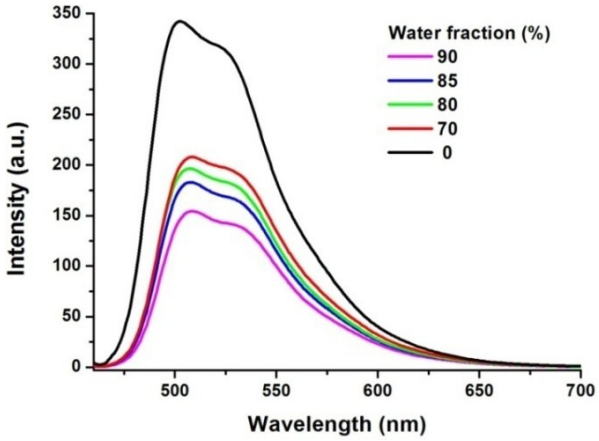

Fig. S4 PL spectra of **BPh_2-TT** (λ_{ex} = 400 nm) in water–THF mixtures with different water fractions (0 <f_w< 90%).

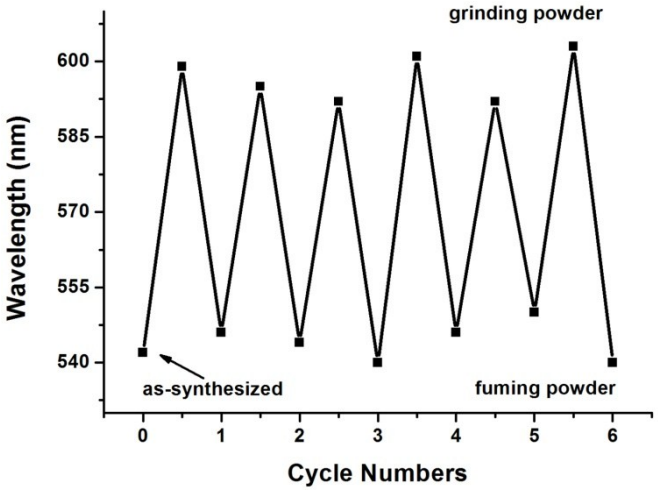

Fig. S5 Maximum fluorescent emission of **BF_2-TT-CN** upon repeating treated by grinding and fuming with CH_2Cl_2.

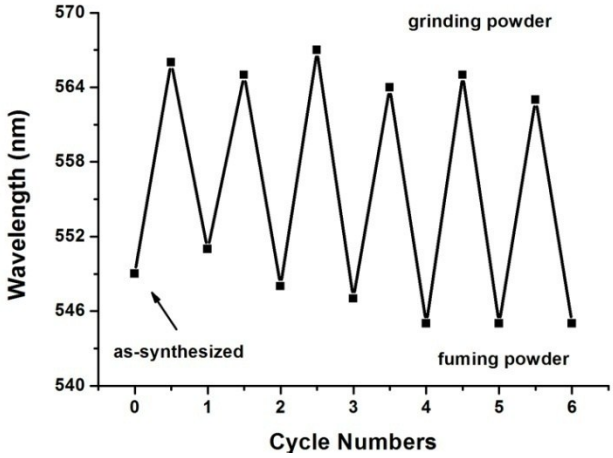

Fig. S6 Maximum fluorescent emission of **BPh_2-TT-CN** upon repeating treated by grinding and fuming with CH_2Cl_2.

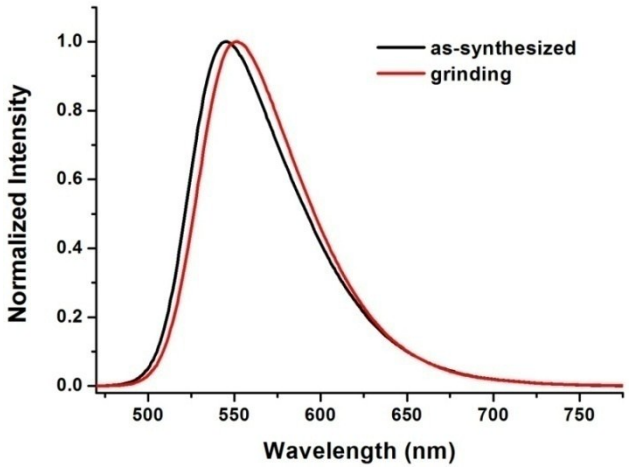

Fig. S7 Normalized fluorescent spectra of **BF_2-TT** in different solid-states: as-synthesized and grinding, λ_{ex} = 450 nm.

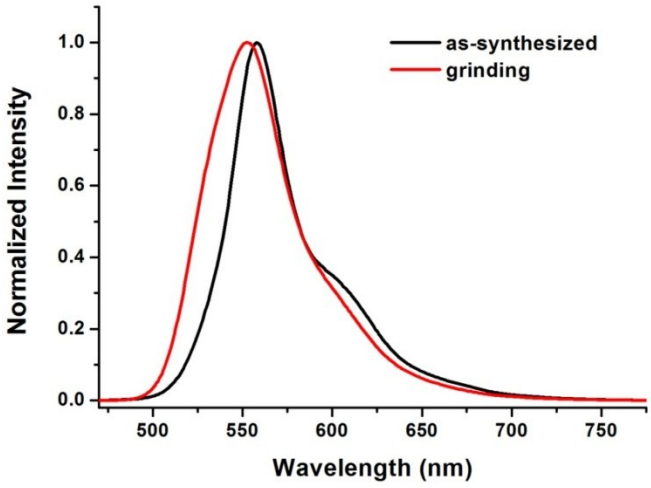

Fig. S8 Normalized fluorescent spectra of **BPh_2-TT** in different solid-states: as-synthesized and grinding, λ_{ex} = 460 nm.

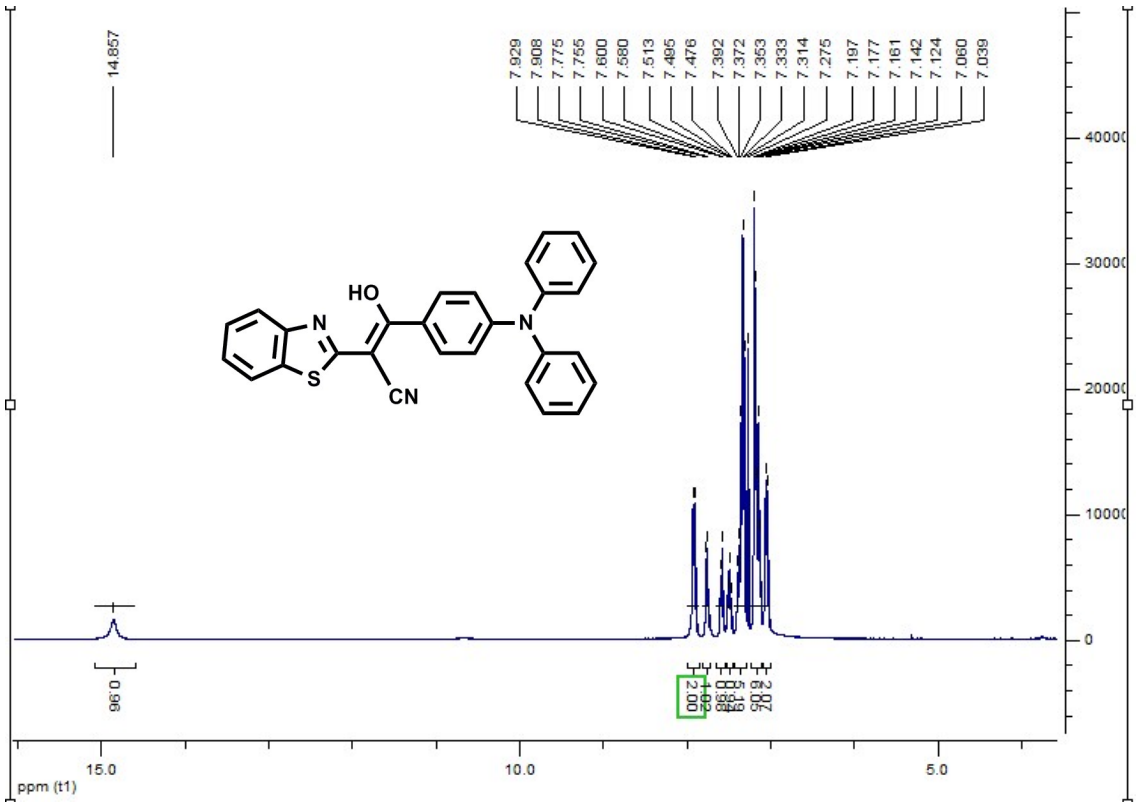

Fig. S9 ^{1}H NMR (400 MHz) spectrum of compound **3**.

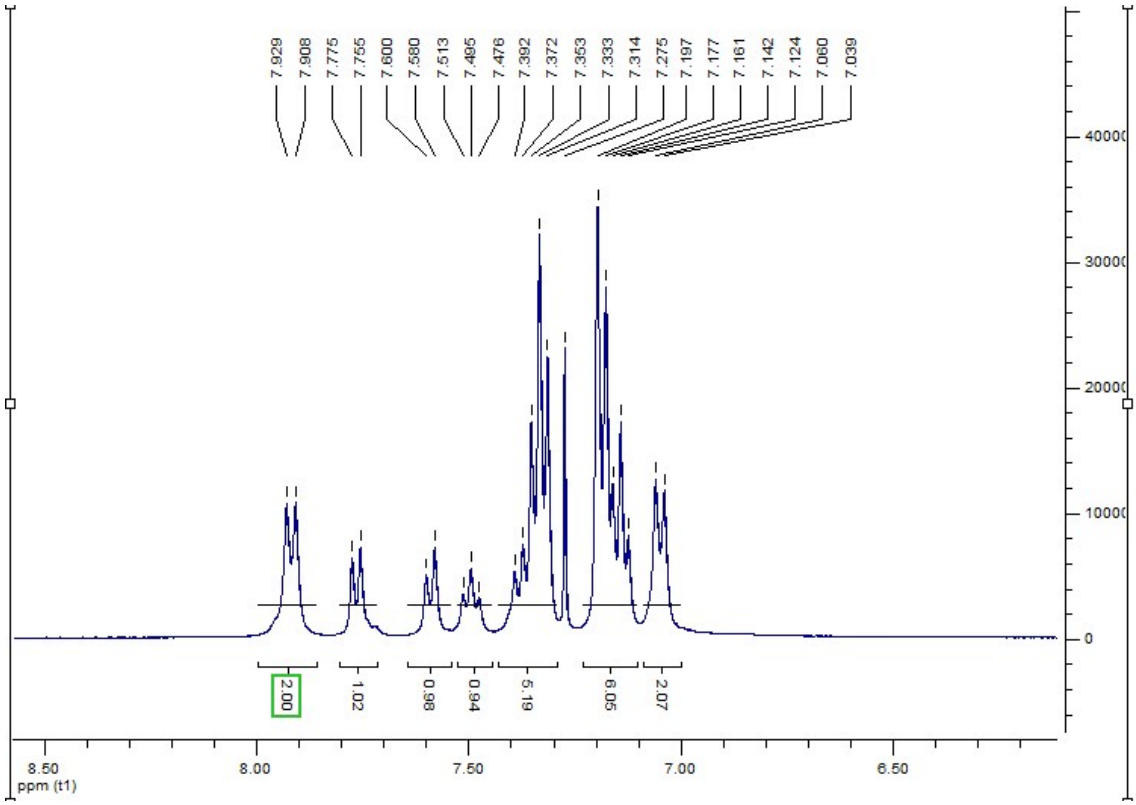

Fig. S10 ^{1}H NMR (400 MHz) spectrum of compound **3**.

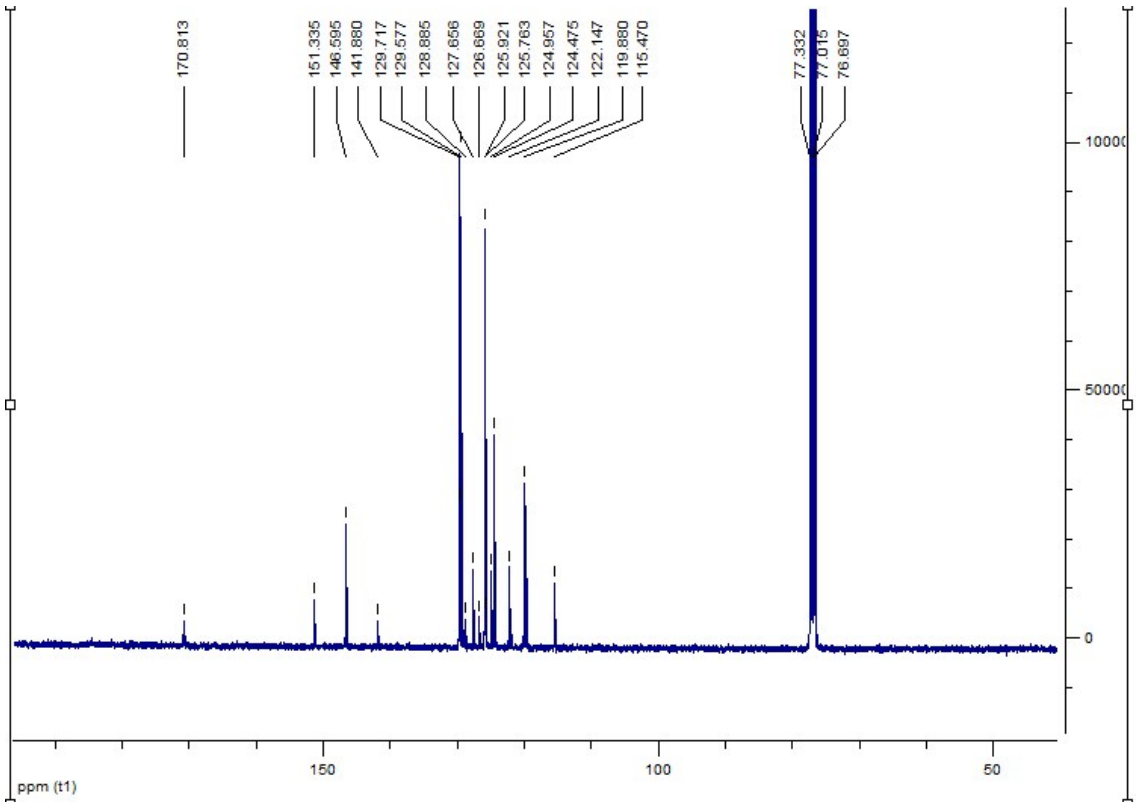

Fig. S11 ^{13}C NMR (100 MHz) spectrum of compound **3**.

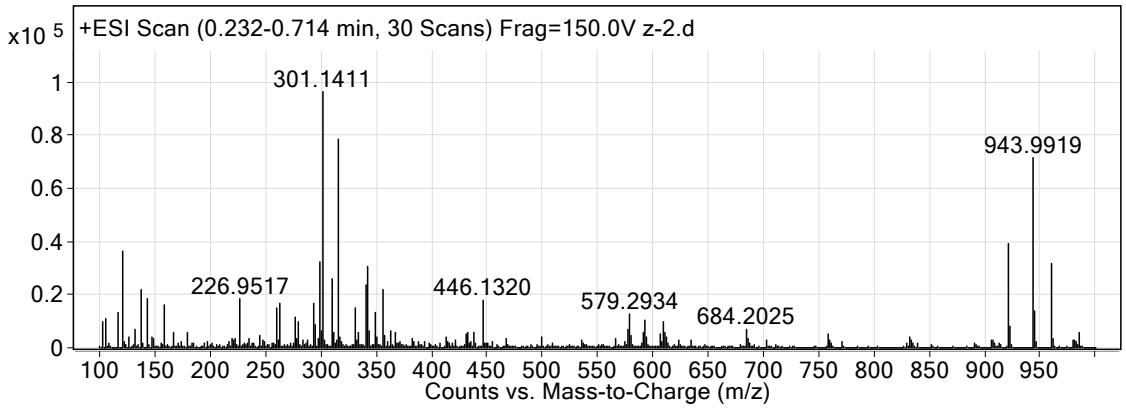

Fig. S12 TOF LC/MS spectrum of compound **3**.

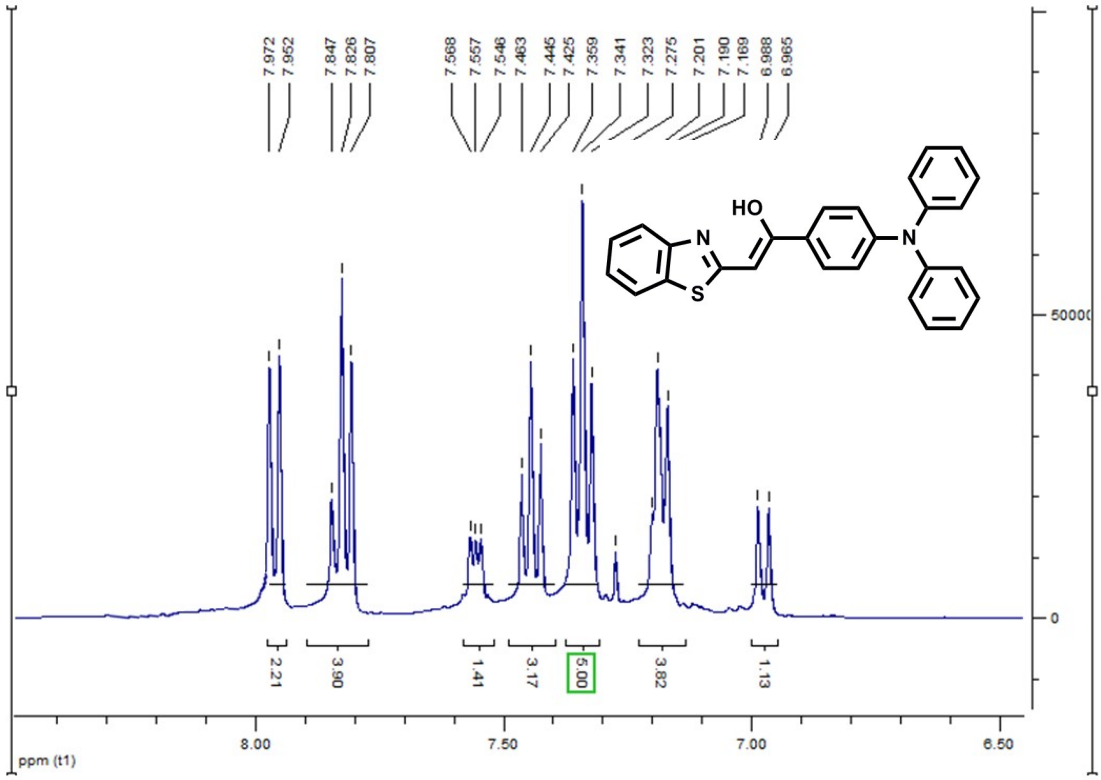

Fig. S13 ^{1}H NMR (400 MHz) spectrum of compound **4**.

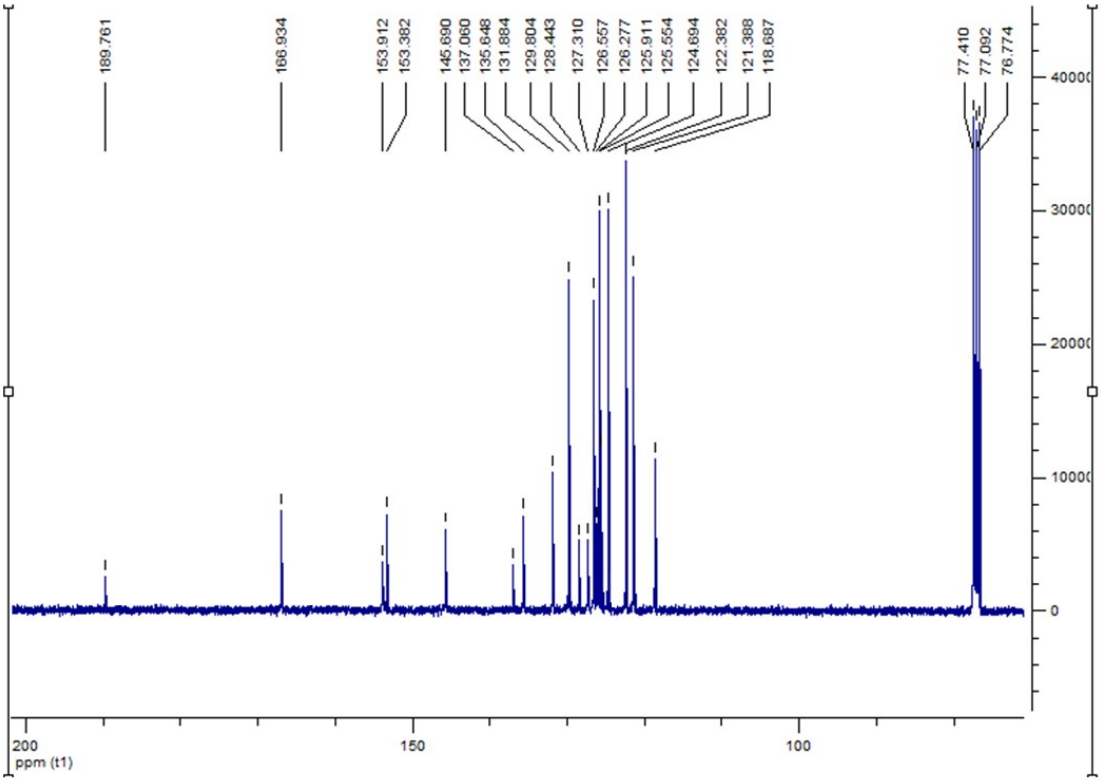

Fig. S14 ^{13}C NMR (100 MHz) spectrum of compound **4**.

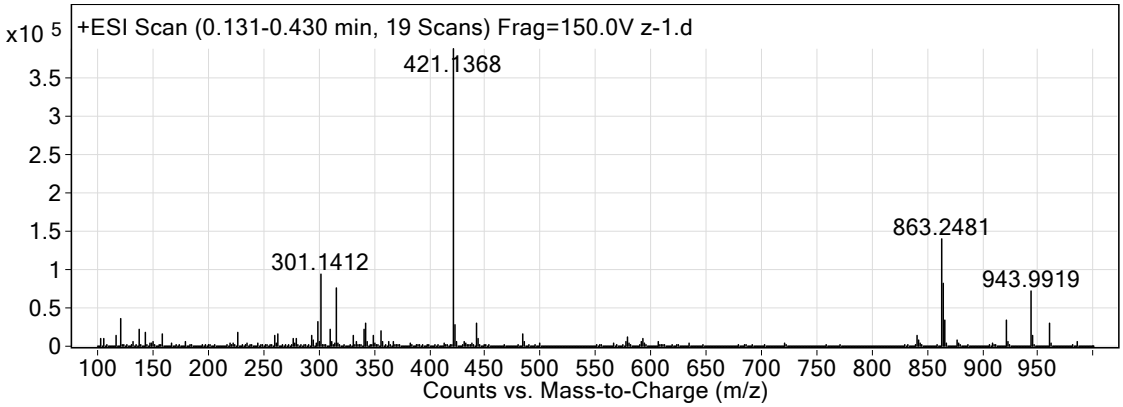

Fig. S15 TOF LC/MS spectrum of compound **4**.

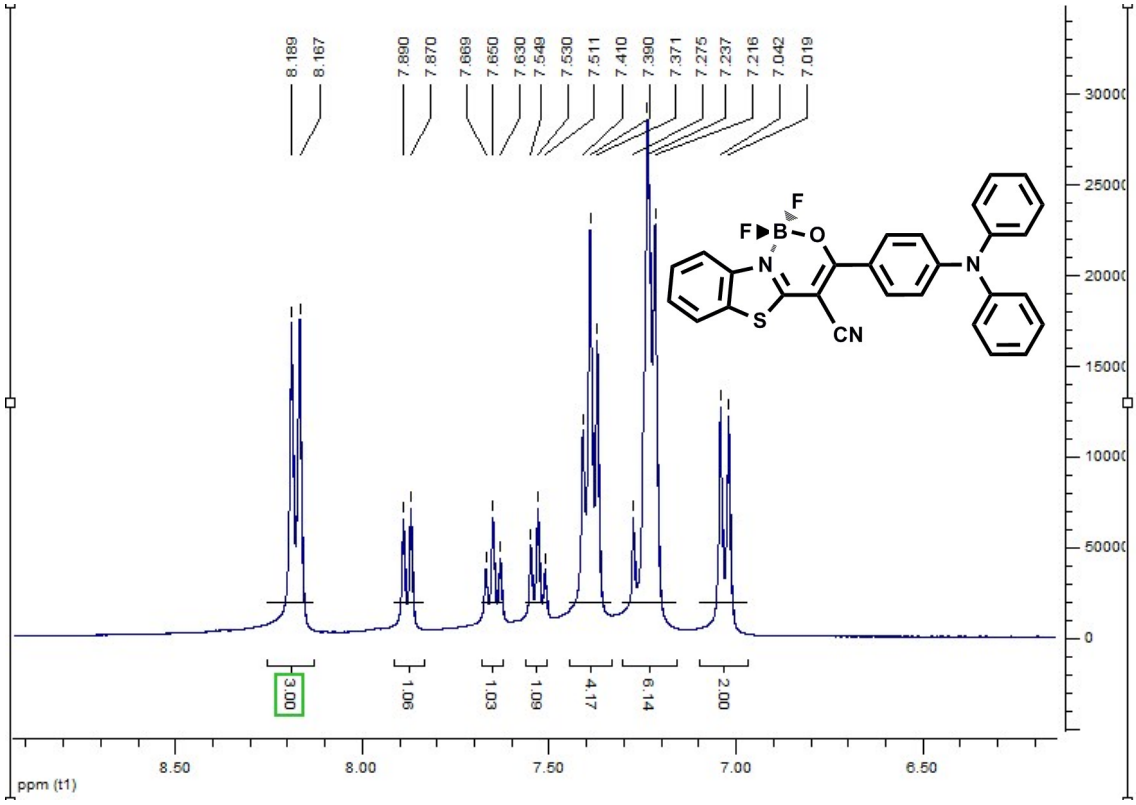

Fig. S16 ^{1}H NMR (400 MHz) spectrum of compound **BF_2-TT-CN**.

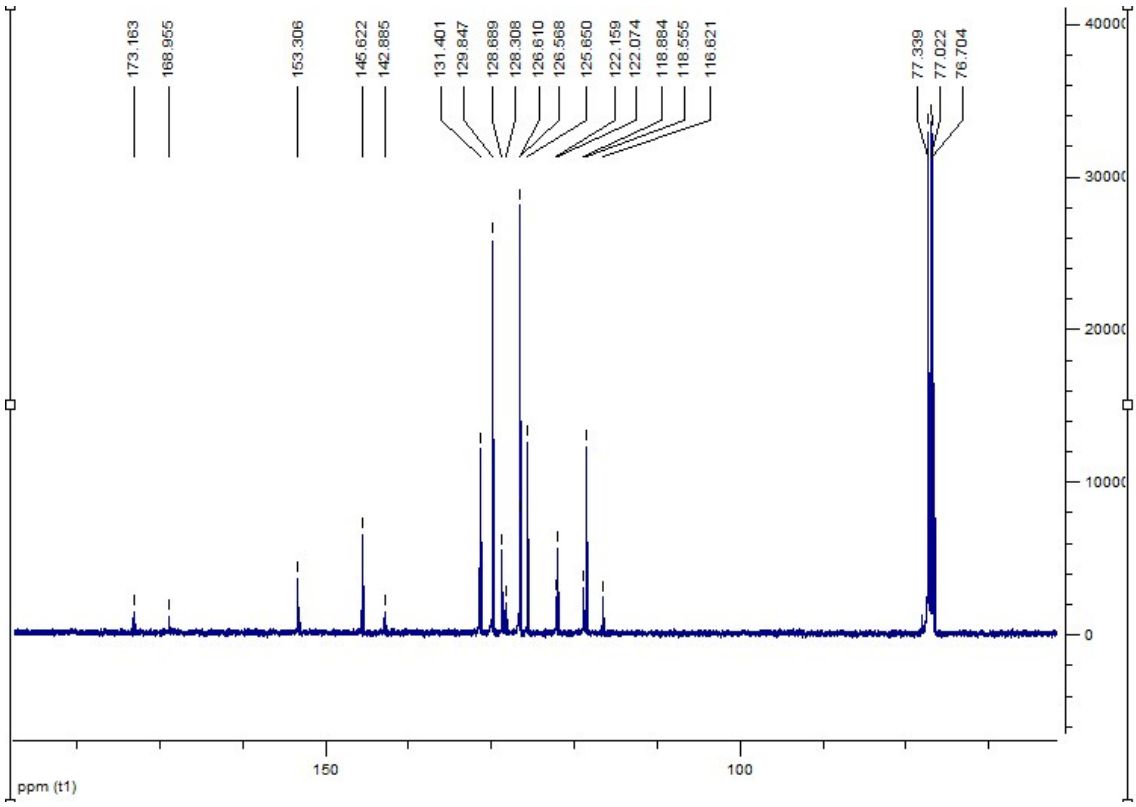

Fig. S17 ^{13}C NMR (100 MHz) spectrum of compound **BF_2-TT-CN**.

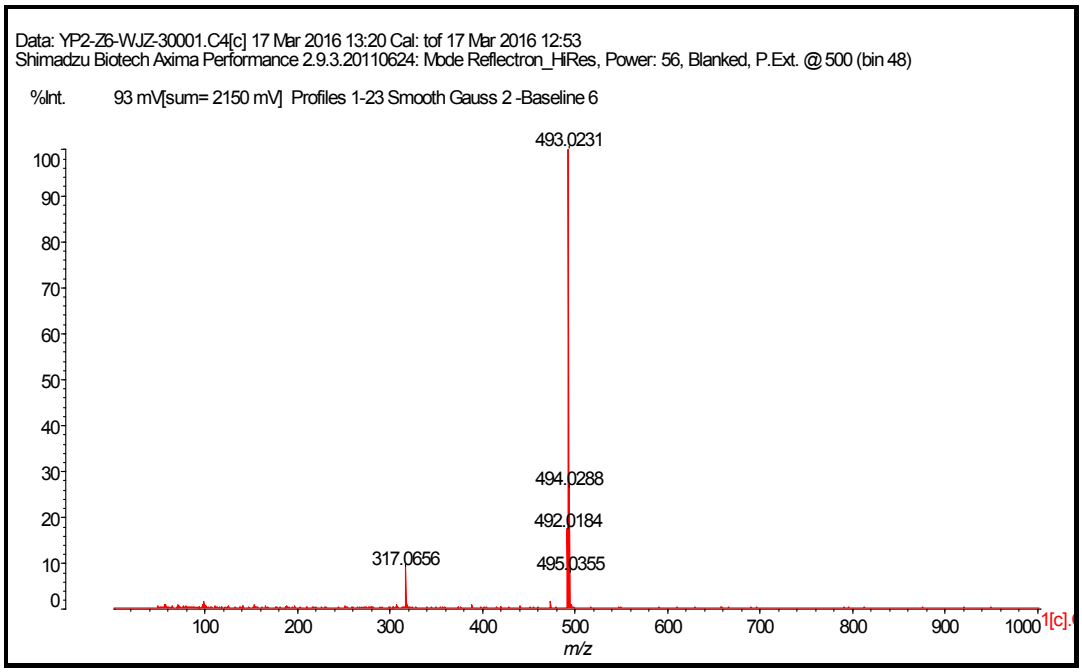

Fig. S18 MALDI/TOF MS spectrum of compound **BF_2-TT-CN**.

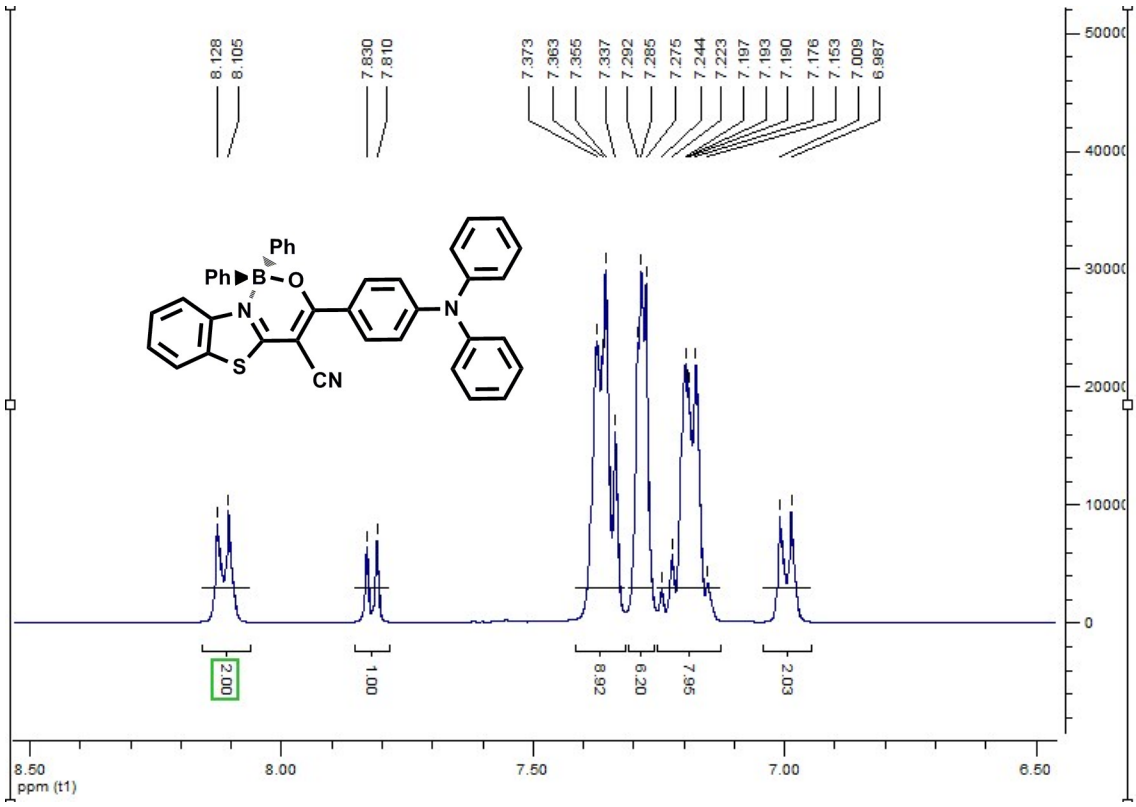

Fig. S19 ^{1}H NMR (400 MHz) spectrum of compound **BPh_2-TT-CN**.

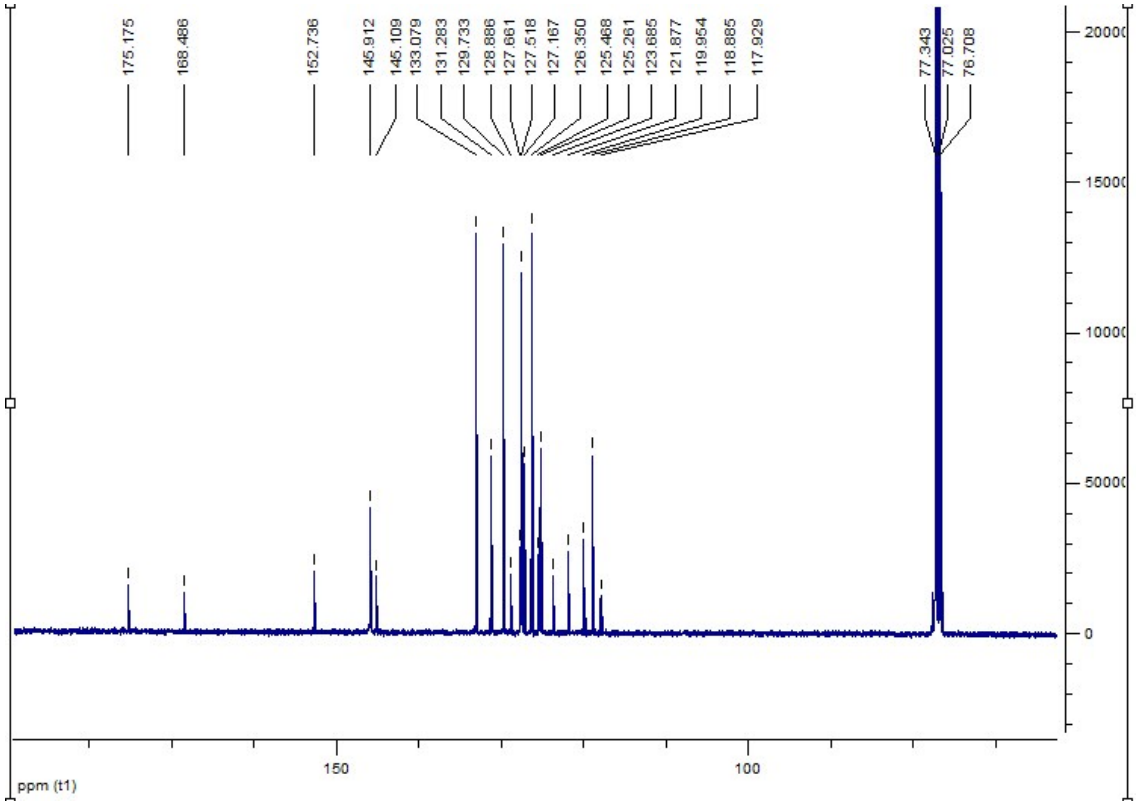

Fig. S20 ^{13}C NMR (100 MHz) spectrum of compound **BPh_2-TT-CN**.

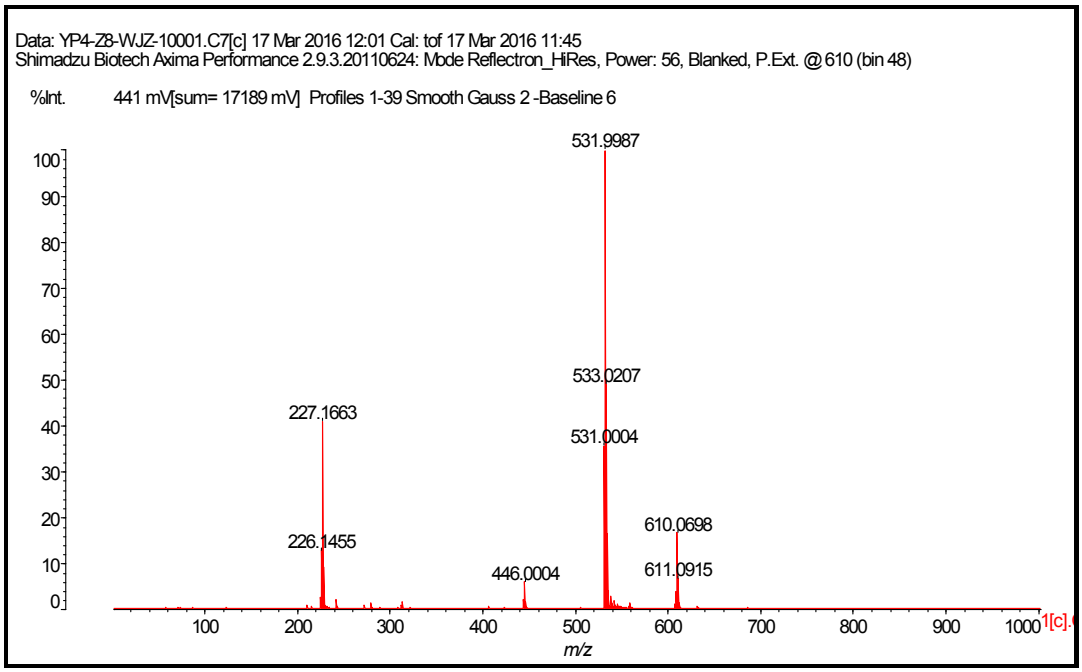

Fig. S21 MALDI/TOF MS spectrum of compound **BPh_2-TT-CN**.

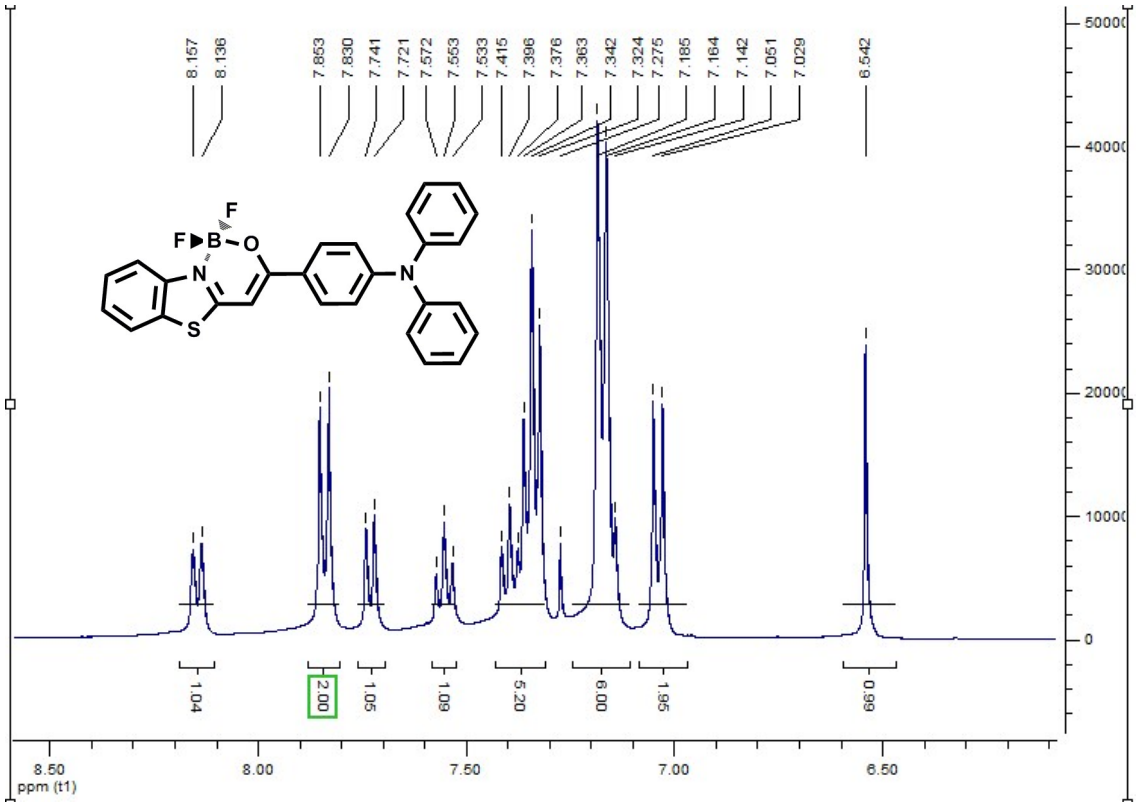

Fig. S22 ^{1}H NMR (400 MHz) spectrum of compound **BF_2-TT**.

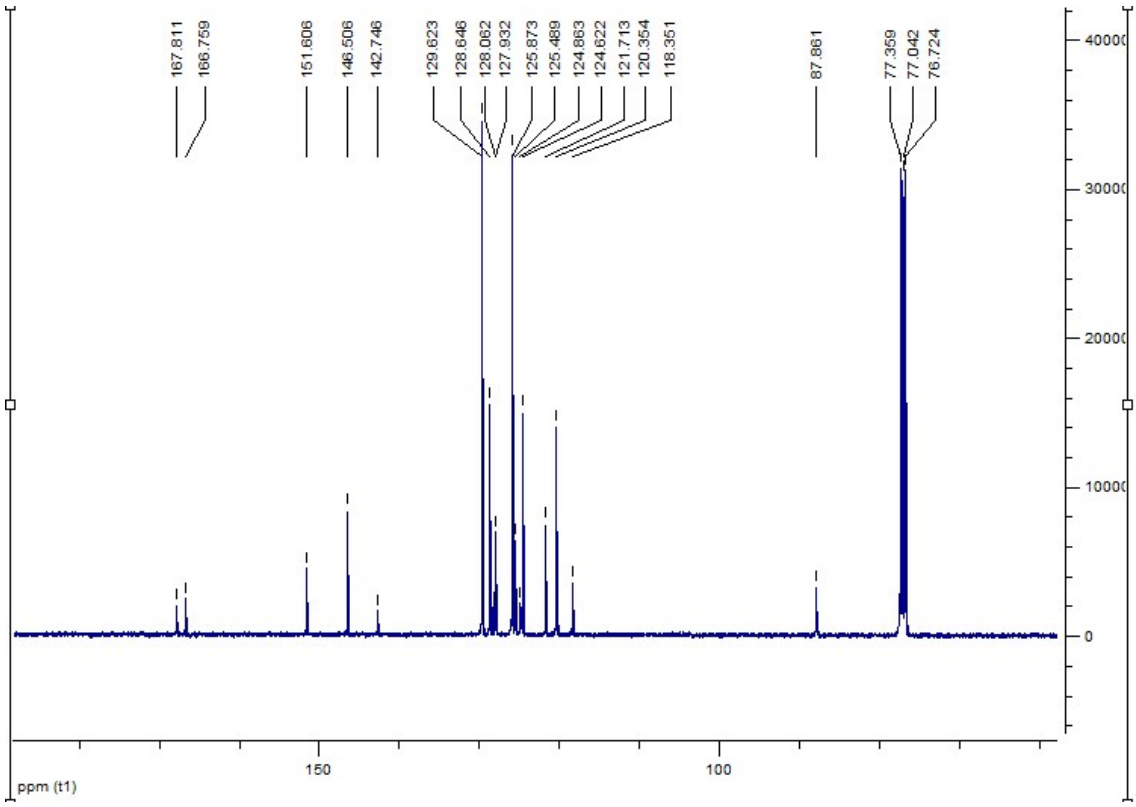

Fig. S23 ^{13}C NMR (100 MHz) spectrum of compound **BF_2-TT**.

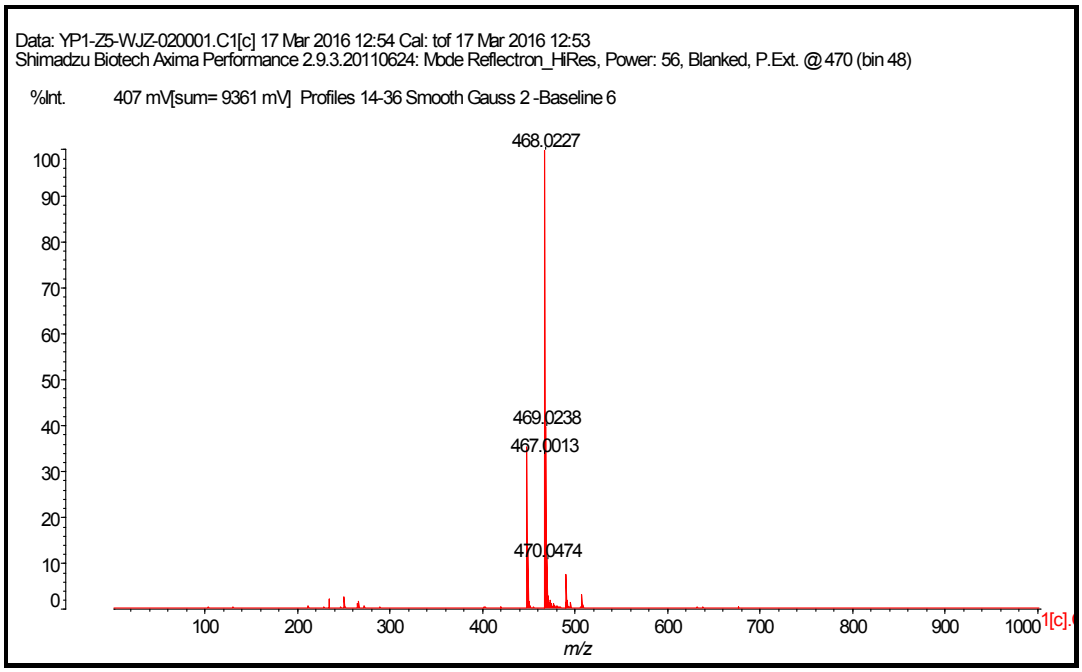

Fig. S24 MALDI/TOF MS spectrum of compound **BF_2-TT**.

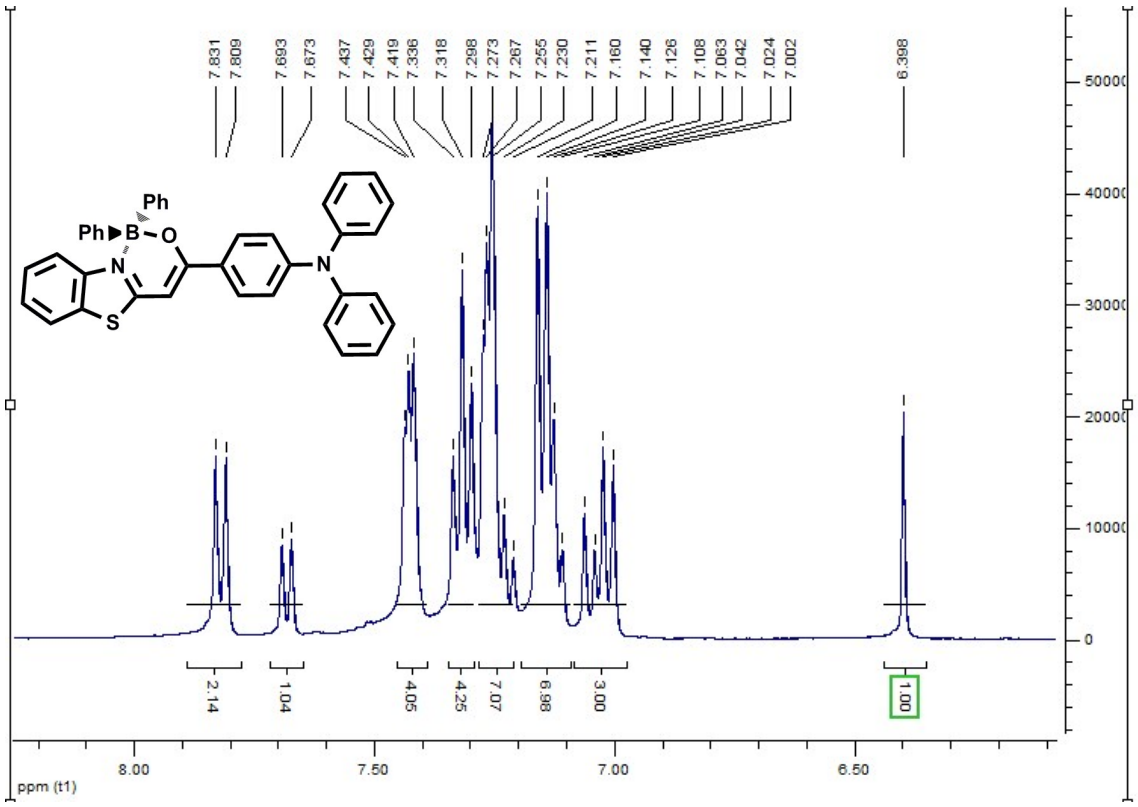

Fig. S25 ^{1}H NMR (400 MHz) spectrum of compound **BPh_2-TT**.

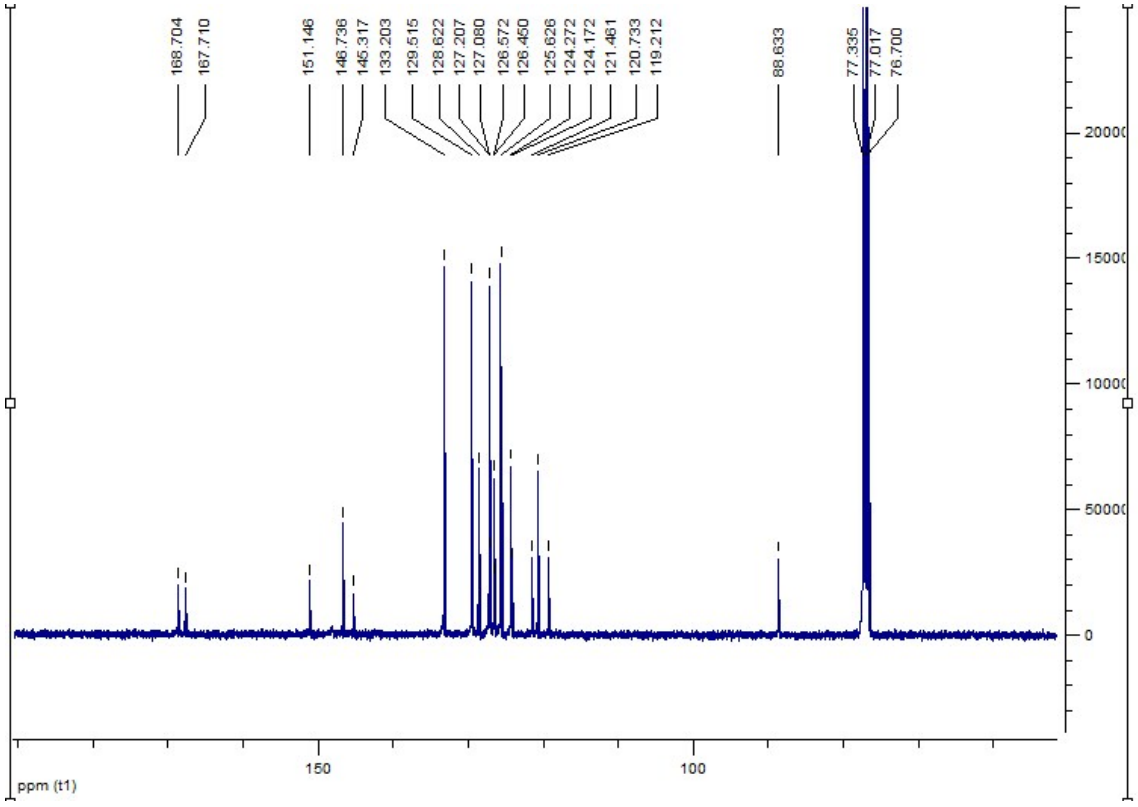

Fig. S26 ^{13}C NMR (100 MHz) spectrum of compound **BPh_2-TT**.

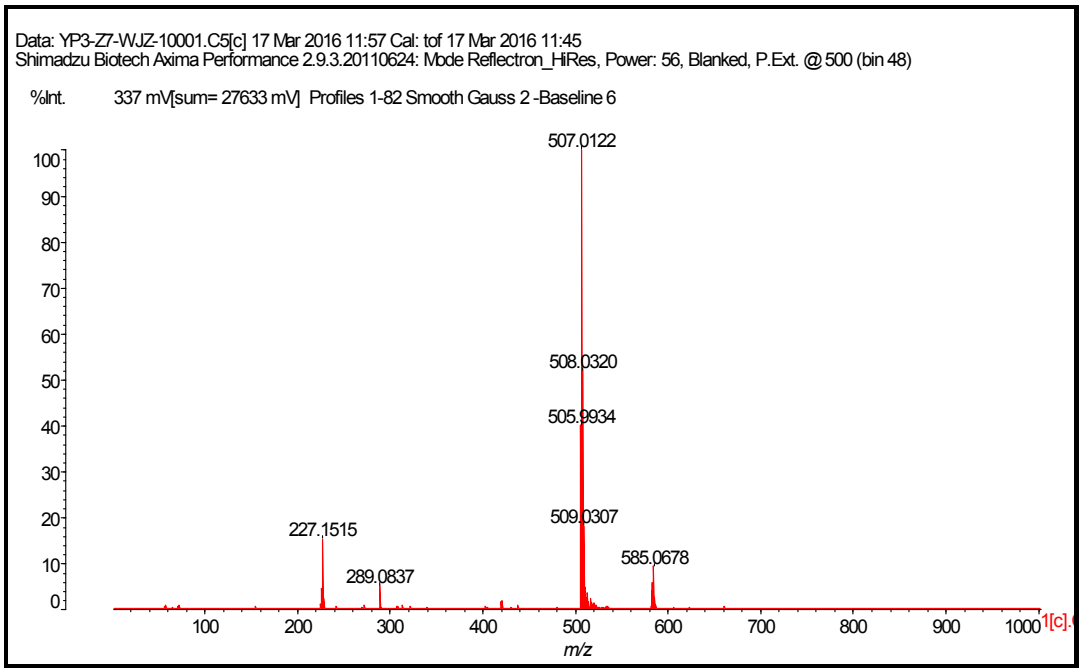

Fig. S27 MALDI/TOF MS spectrum of compound **BPh_2-TT**.