Supporting Information for

D-A type luminophores with twisted molecular conformation constructed by phenoxazine and diphenylsulfone showing high contrast mechanofluorochromism

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Table S1. Crystallographic experimental details for **PTZ-DPS** (CCDC 1969955) and **BPTZ-DPS** (CCDC 1969954).

Compound	**PTZ-DPS**	**BPTZ-DPS**
Empirical formula	$C_{28}H_{22}BrNO_3S$	$C_{44}H_{36}N_2O_4S$
Formula weight	532.43	688.81
Temperature/K	293.51(10)	293.50(10)
Crystal system	triclinic	monoclinic
Space group	P-1	P2/c
a/Å	9.9624(5)	13.9869(6)
b/Å	13.4464(7)	5.09616(15)
c/Å	19.3712(10)	24.4610(8)
α/°	87.677(4)	90
β/°	76.294(5)	104.972(4)
γ/°	73.020(5)	90
Volume/Å^3	2410.0(2)	1684.38(11)
Z	43.384	2
ρ_{calc}g/cm^3	1.467	1.358
μ/mm^{-1}	3.384	1.248
F(000)	1088.0	724.0
Crystal size/mm^3	0.13 × 0.11 × 0.07	0.19 × 0.15 × 0.12
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	20.088 to 133.198	7.482 to 133.188
Index ranges	-11 ≤ h ≤ 9, -15 ≤ k ≤ 14, -23 ≤ l ≤ 20	-16 ≤ h ≤ 16, -6 ≤ k ≤ 3, -29 ≤ l ≤ 28
Reflections collected	15163	5537
Independent reflections	8403 [R_{int} = 0.0284, R_{sigma} = 0.0399]	2963 [R_{int} = 0.0163, R_{sigma} = 0.0221]
Data/restraints/parameters	8403/0/615	2963/0/232
Goodness-of-fit on F^2	1.021	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0472, wR_2 = 0.1251	R_1 = 0.0405, wR_2 = 0.1054
Final R indexes [all data]	R_1 = 0.0629, wR_2 = 0.1391	R_1 = 0.0500, wR_2 = 0.1140
Largest diff. peak/hole / e Å^{-3}	0.33/-0.65	0.17/-0.29

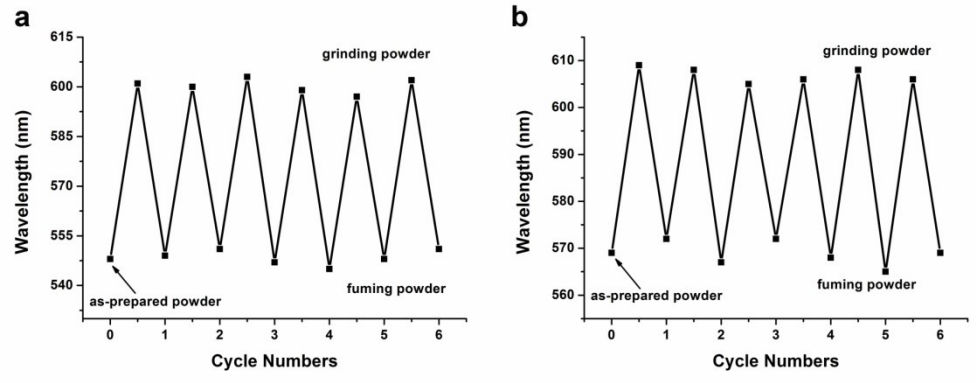

Fig. S1 Maximum emission wavelengths of **PXZ-DPS** (a) and **BPXZ-DPS** (b) upon repeating treated by grinding and fuming with DCM.

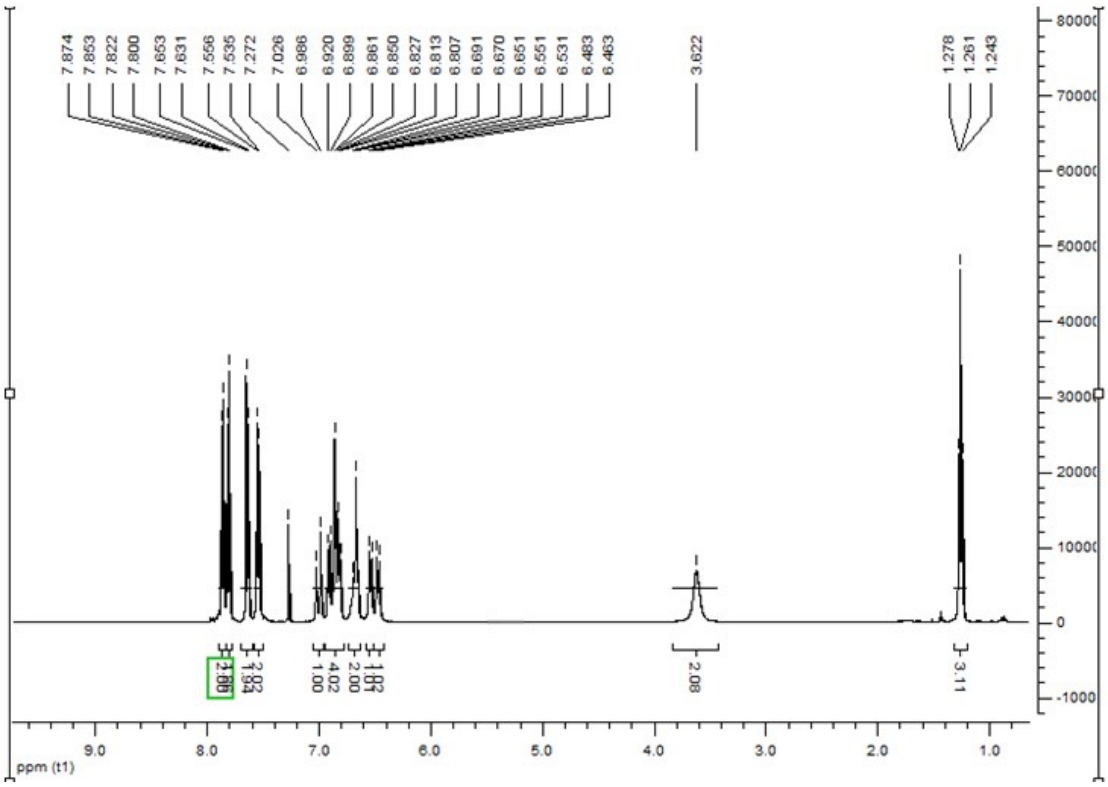

Fig. S2 ^{1}H NMR (400 MHz) spectrum of **PXZ-DPS**.

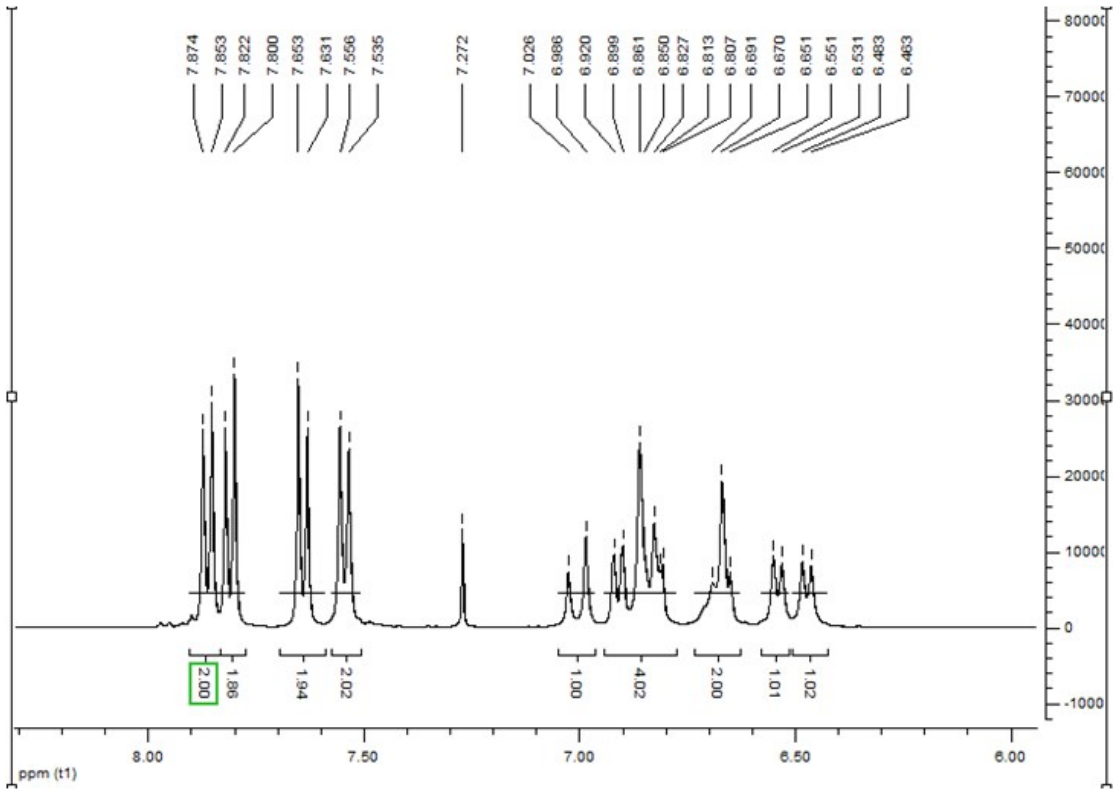

Fig. S3 ^{1}H NMR (400 MHz) spectrum of **PXZ-DPS**.

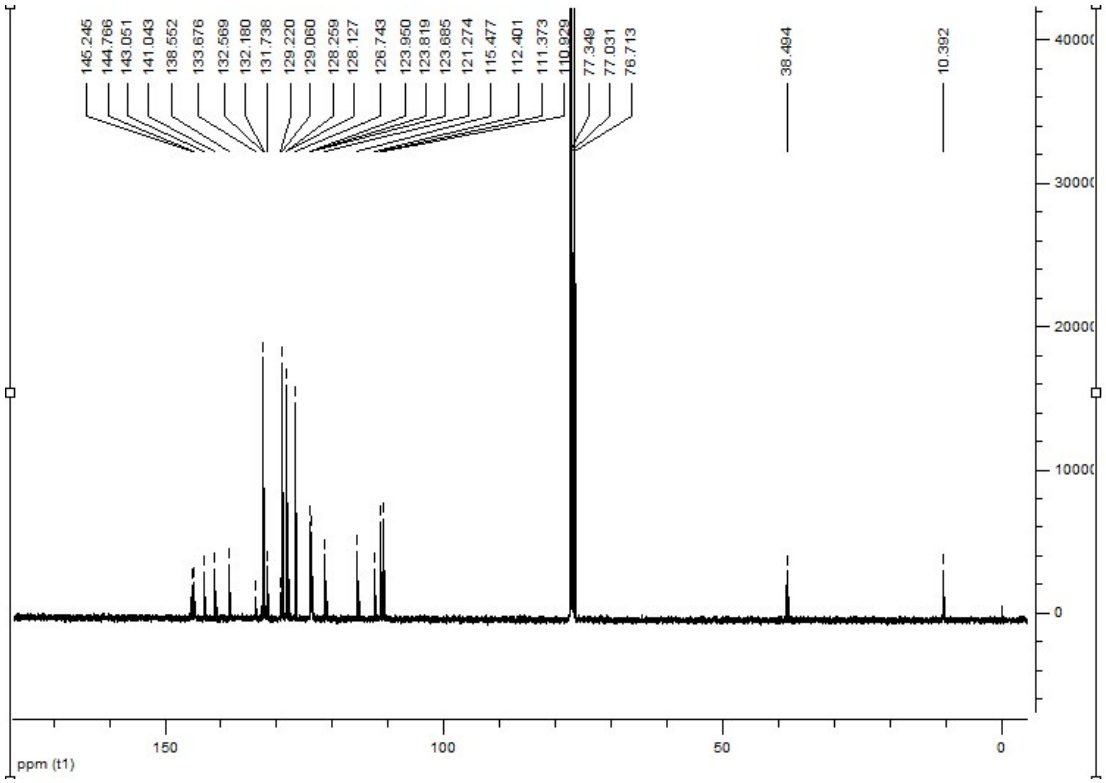

Fig. S4 ^{13}C NMR (100 MHz) spectrum of **PXZ-DPS**.

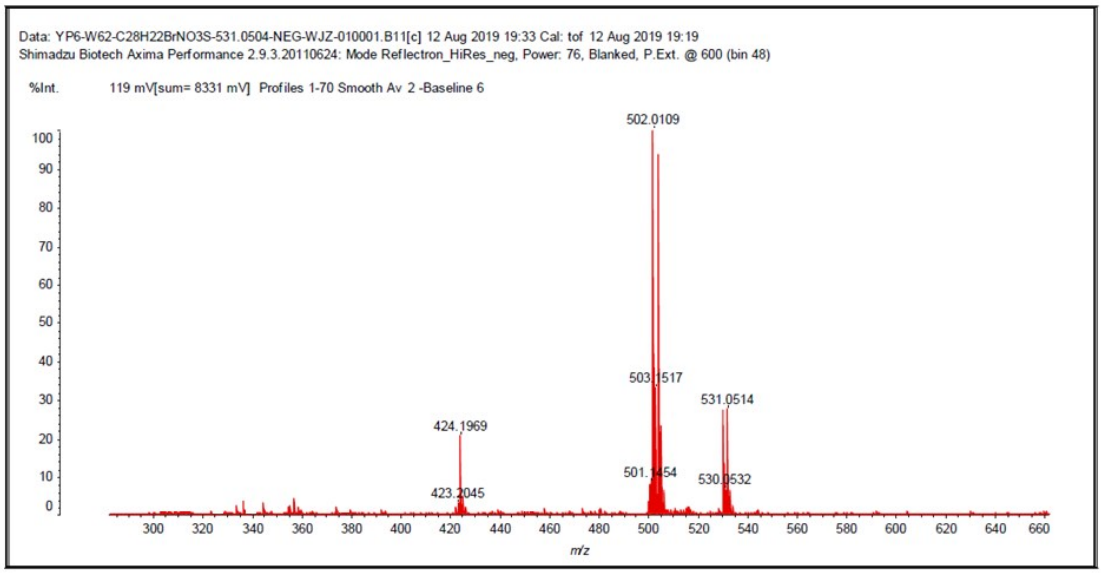

Fig. S5 MALDI/TOF MS spectrum of **PXZ-DPS**.

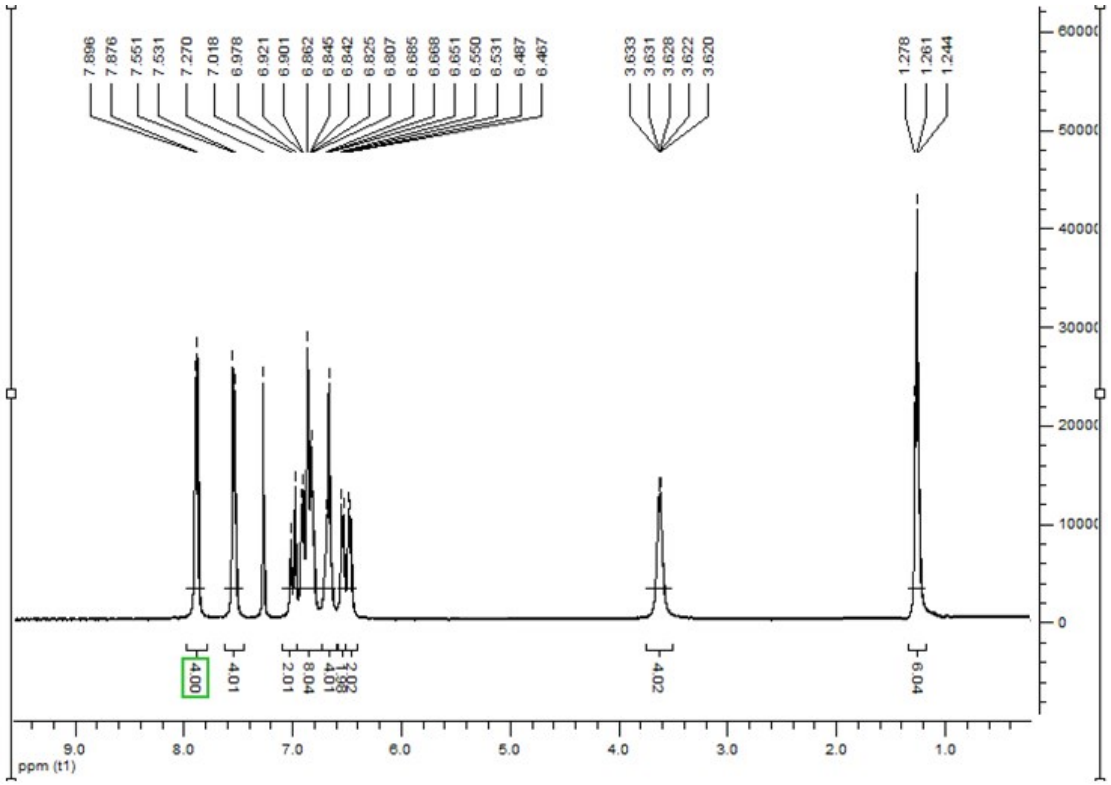

Fig. S6 ^{1}H NMR (400 MHz) spectrum of **BPXZ-DPS**.

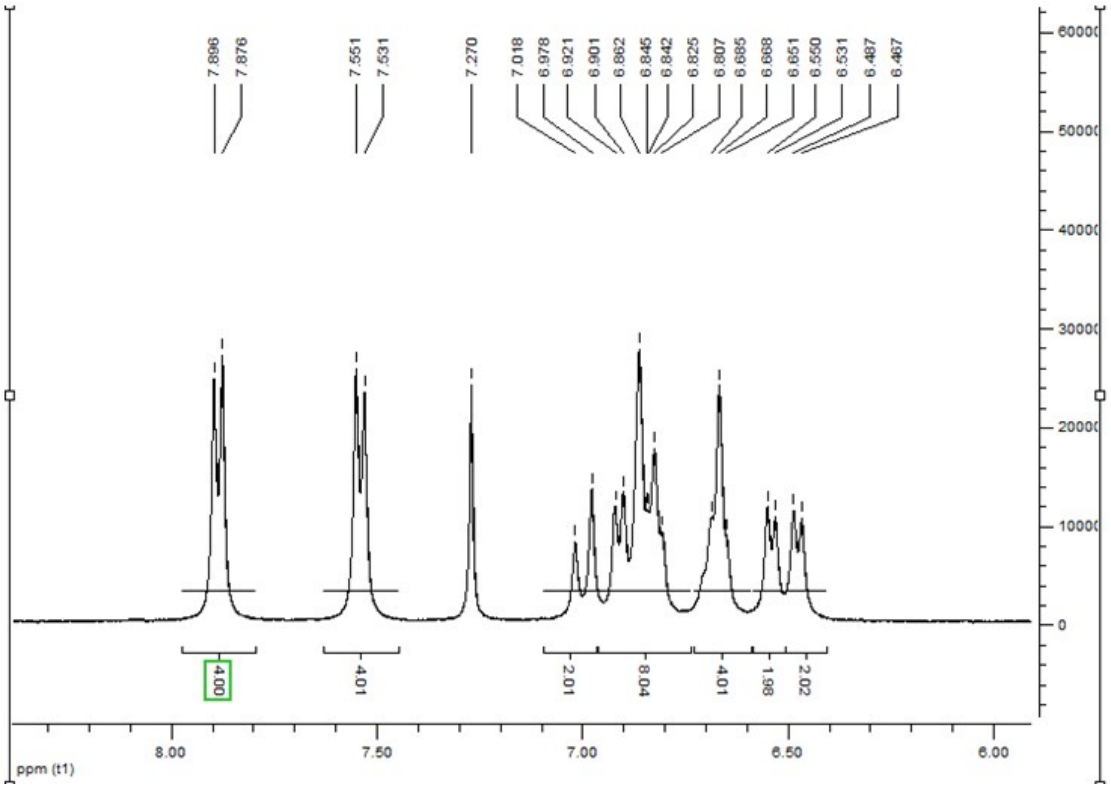

Fig. S7 ^{1}H NMR (400 MHz) spectrum of **BPXZ-DPS**.

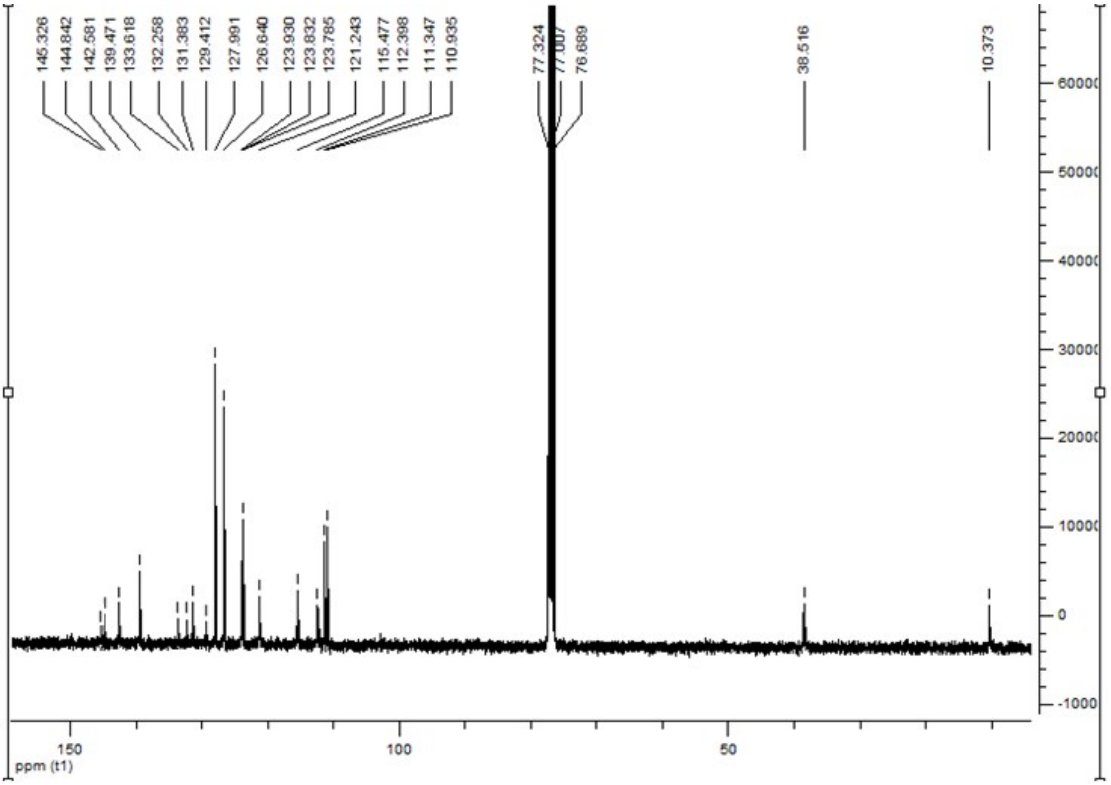

Fig. S8 ^{13}C NMR (100 MHz) spectrum of **BPXZ-DPS**.

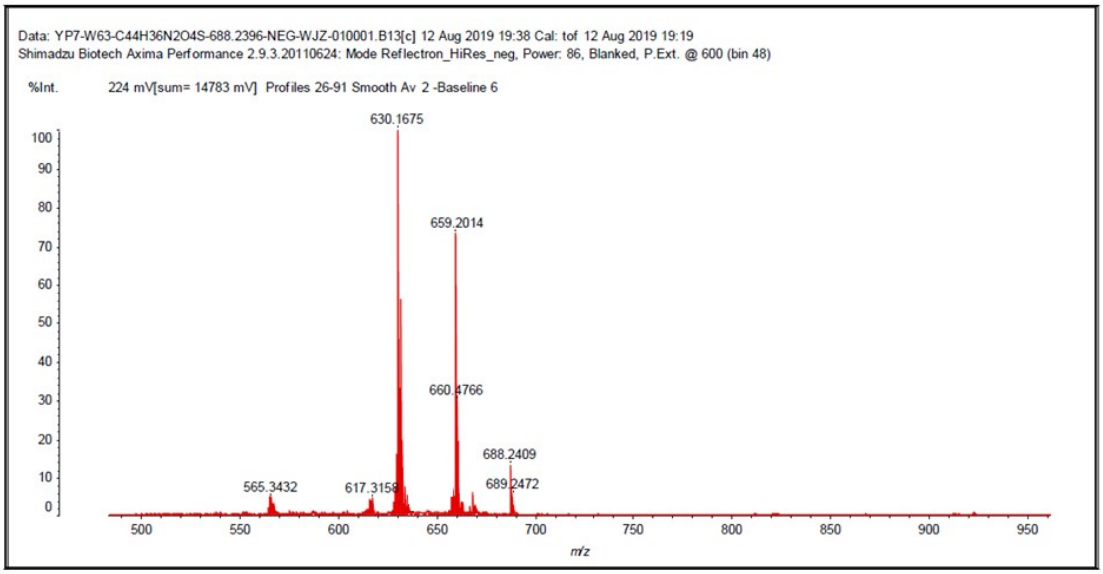

Fig. S9 MALDI/TOF MS spectrum of **BPXZ-DPS**.