Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Supporting Information

Synthesis of Donor-Acceptor Molecules Based on Isoxazolones for Nonlinear Optical Properties

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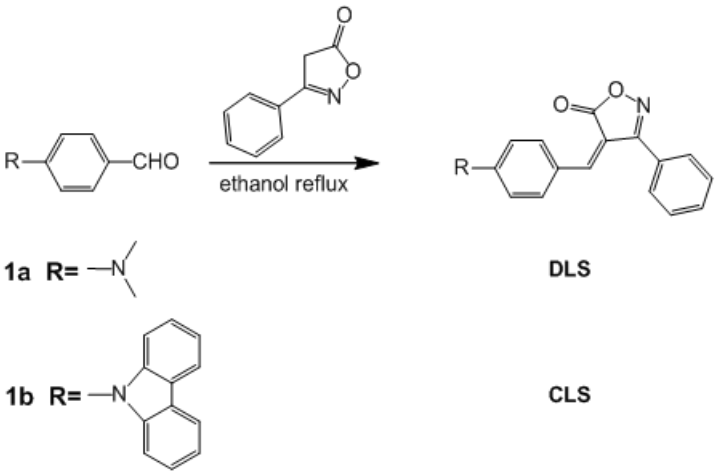
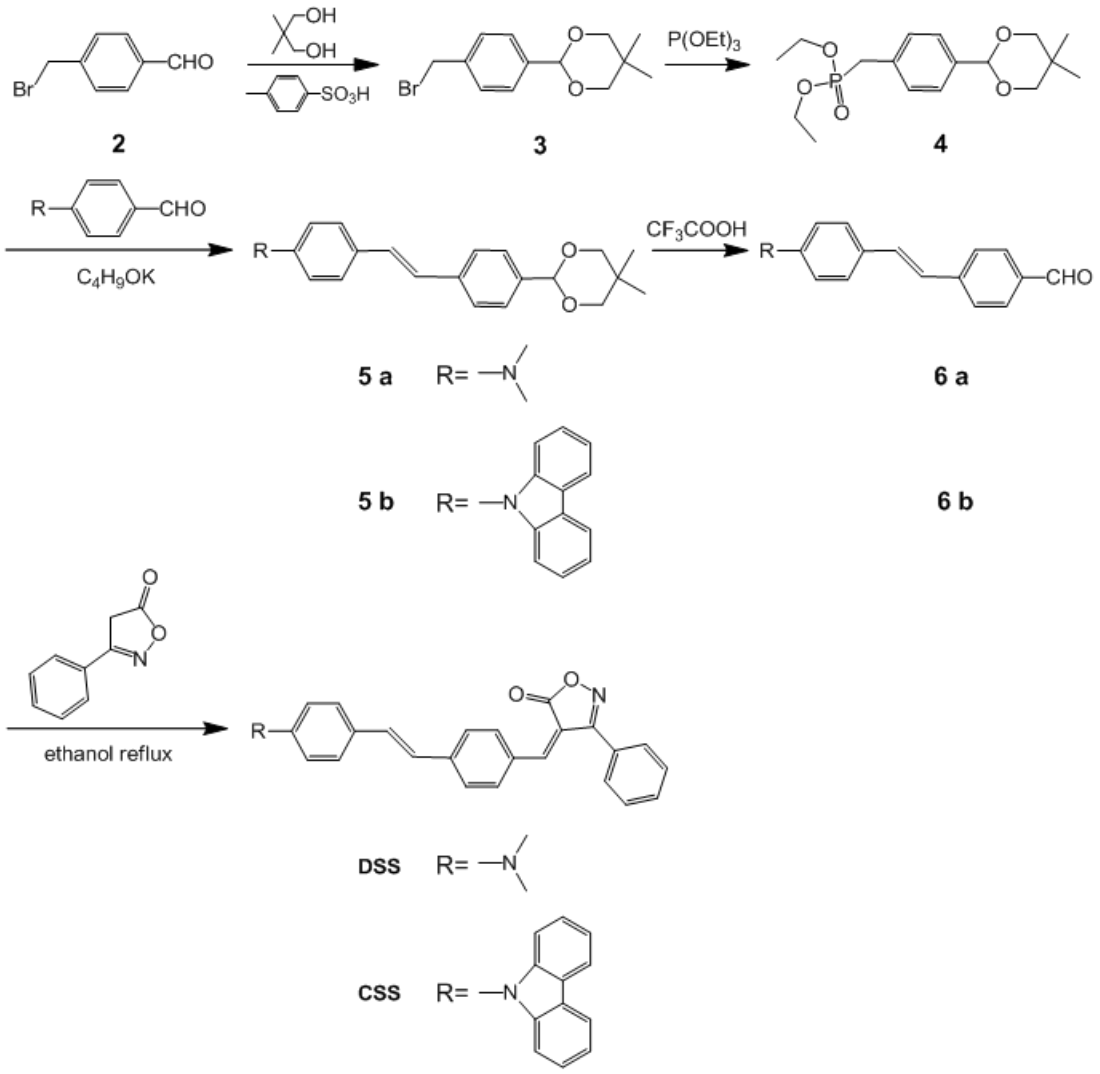
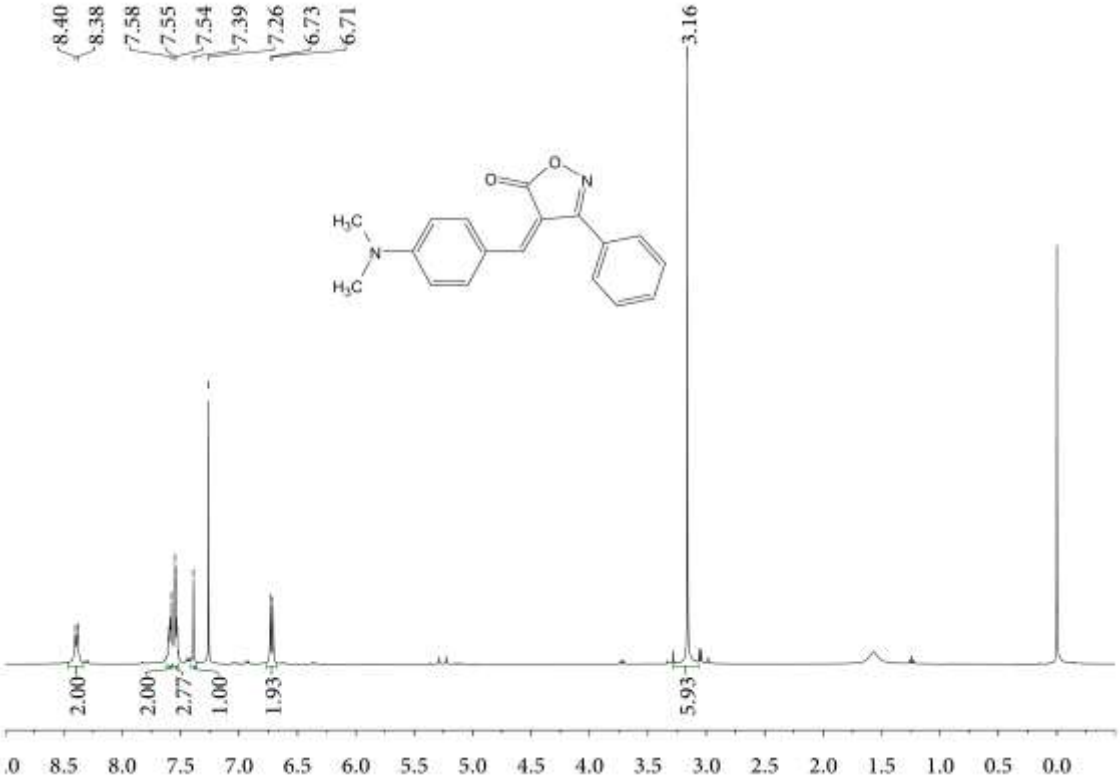
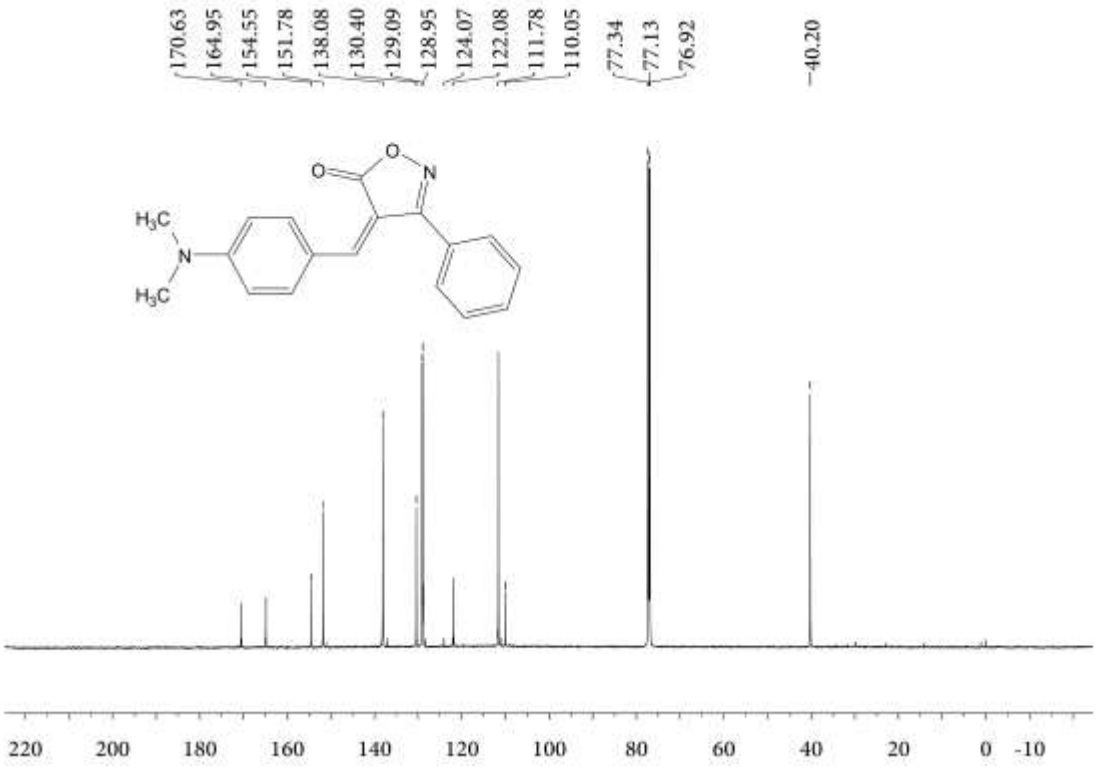
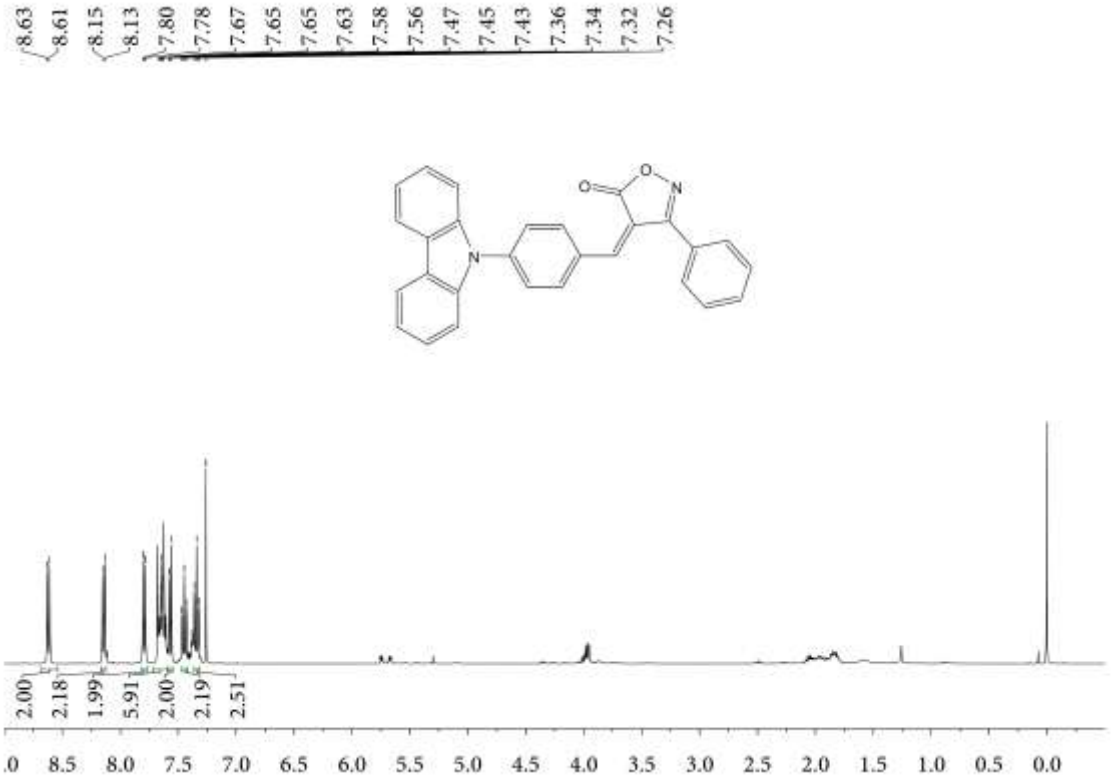
Scheme S1: Synthetic Route of the donor-acceptor compounds

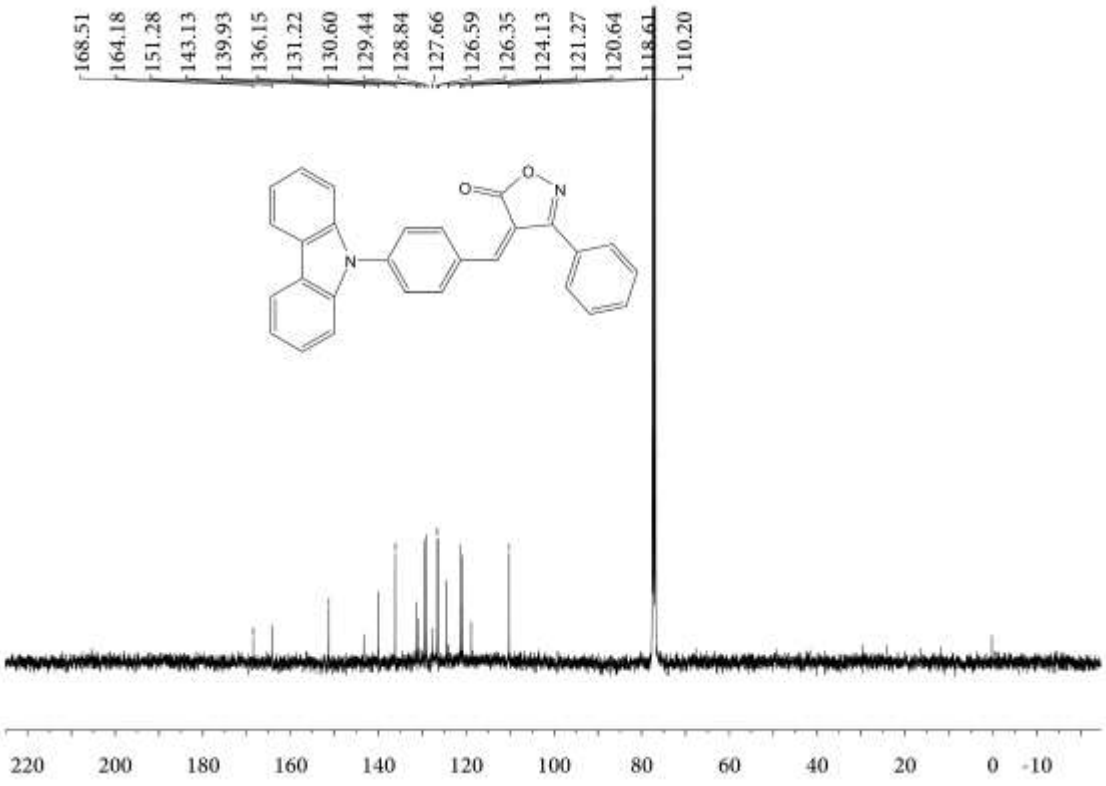


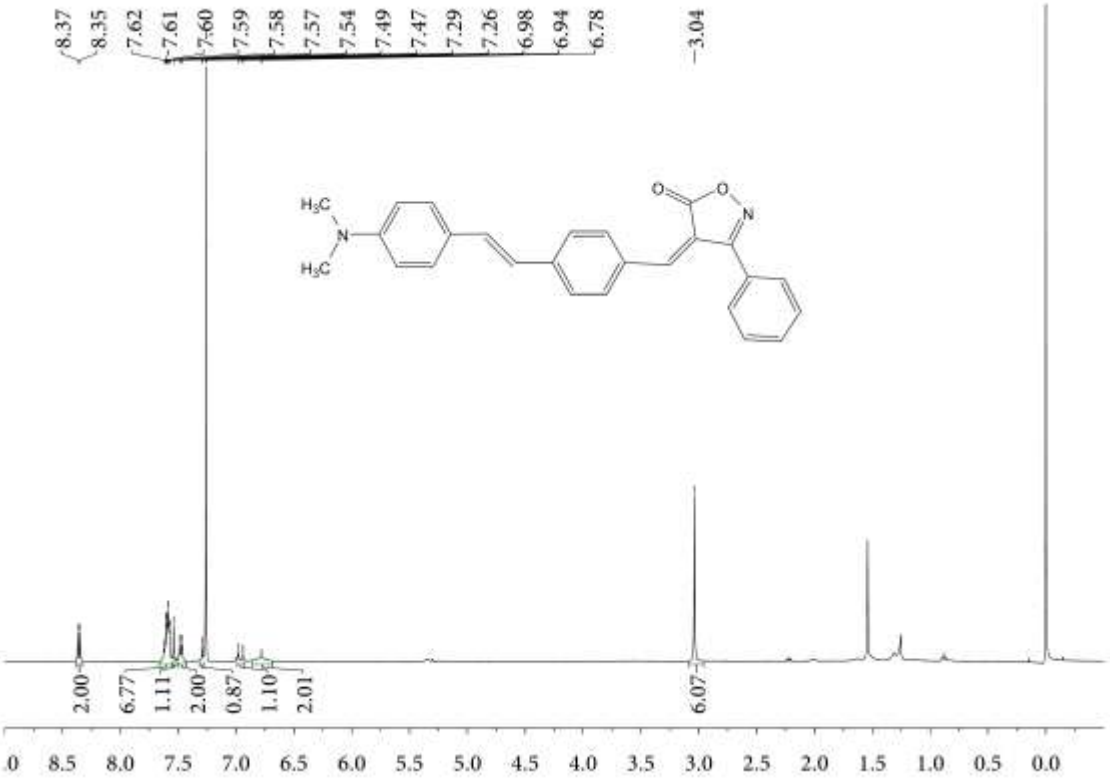


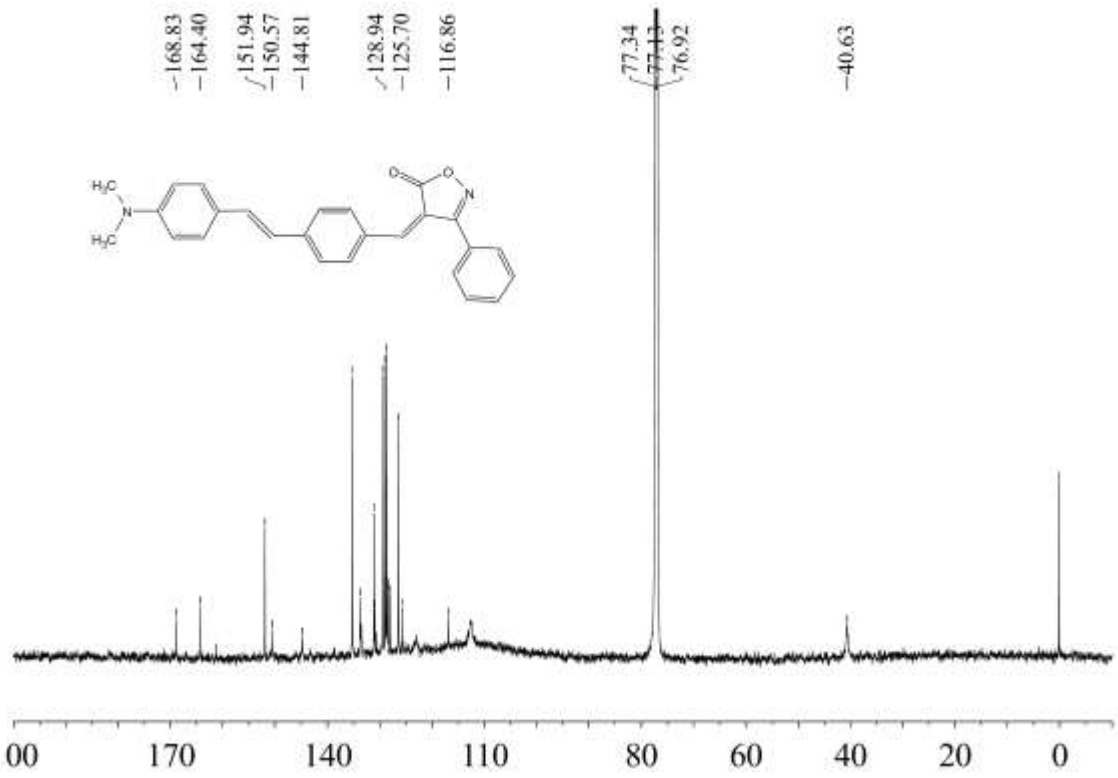


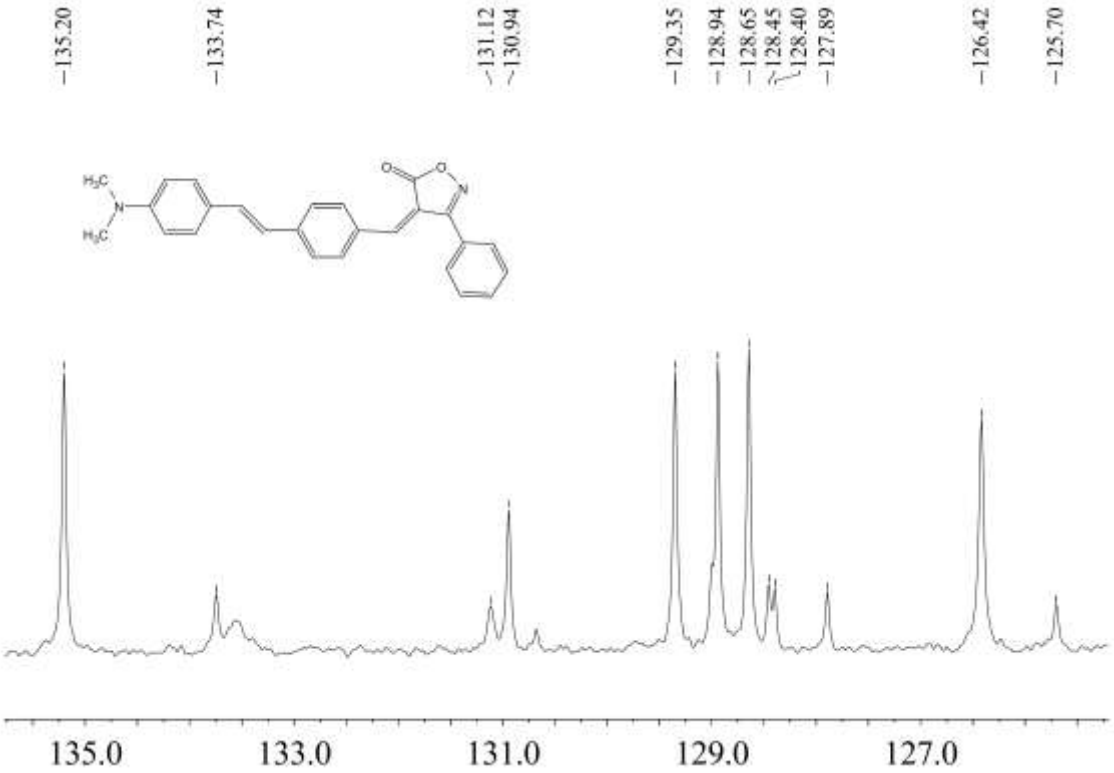


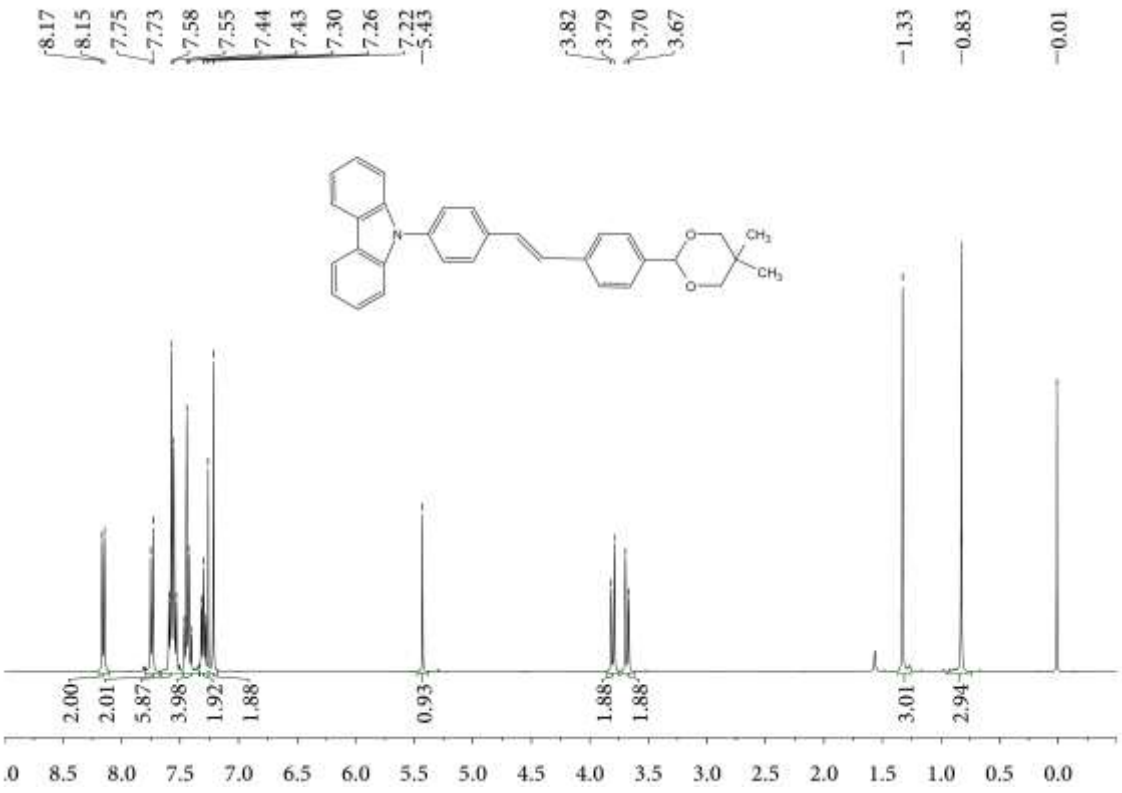


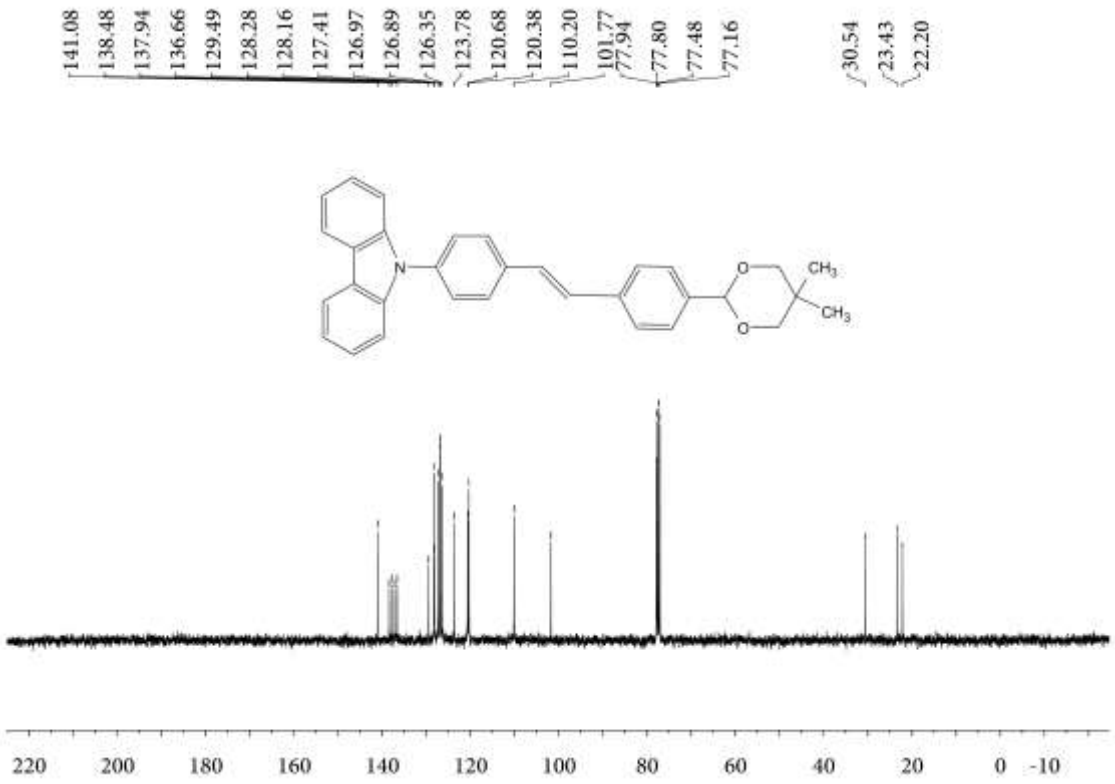


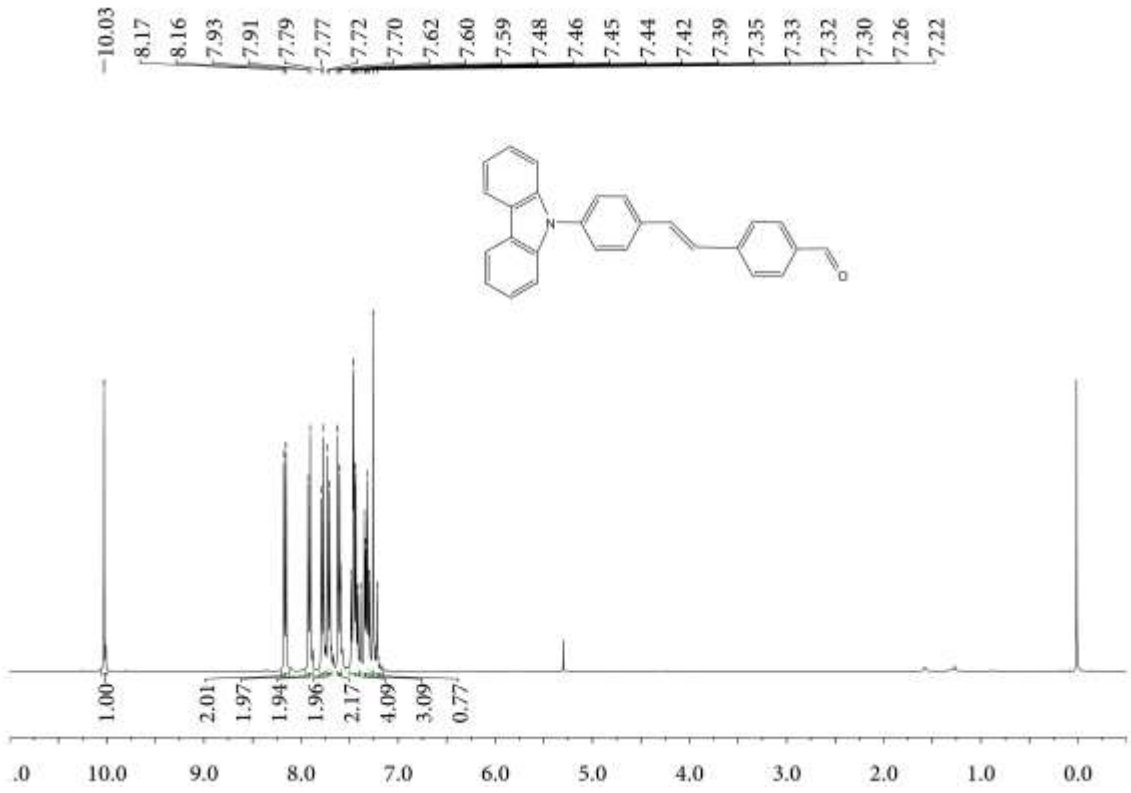


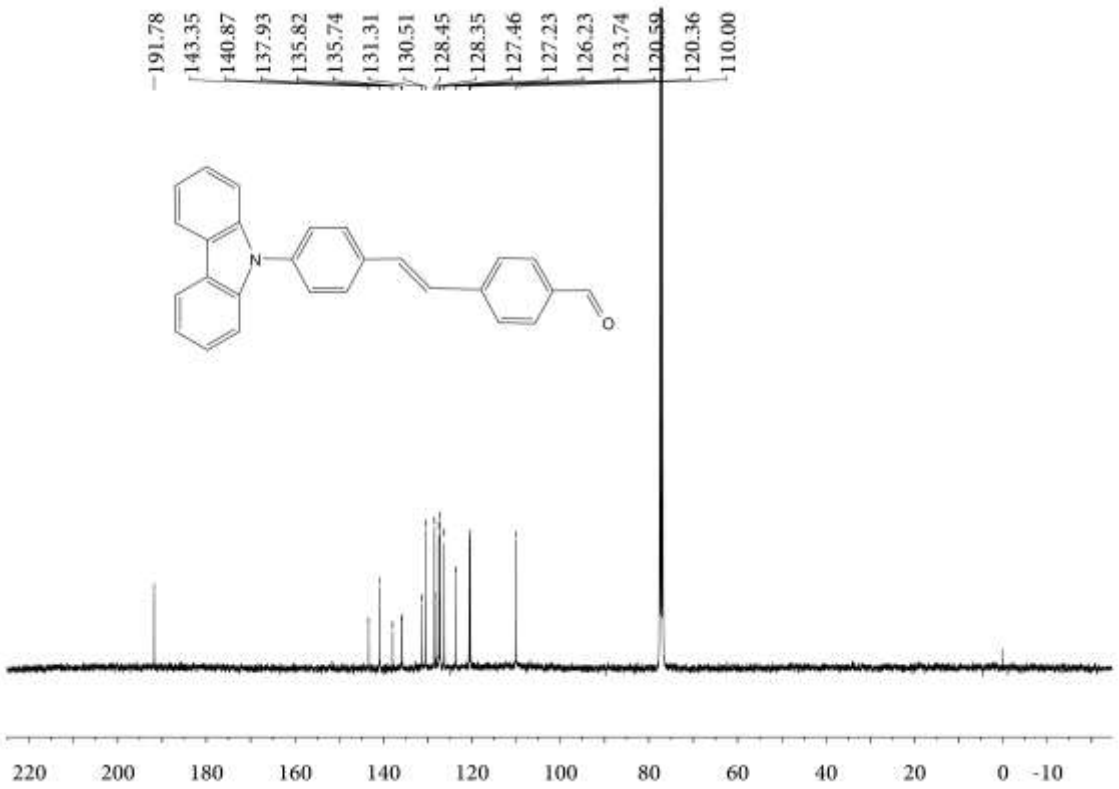


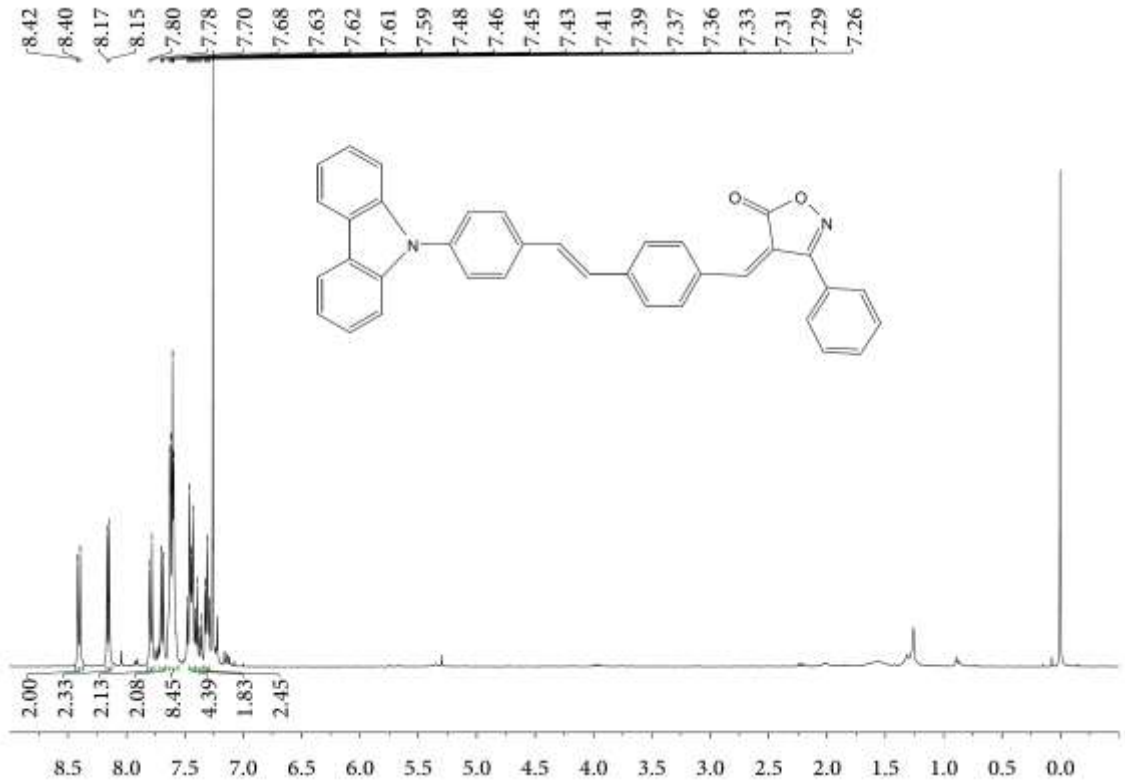


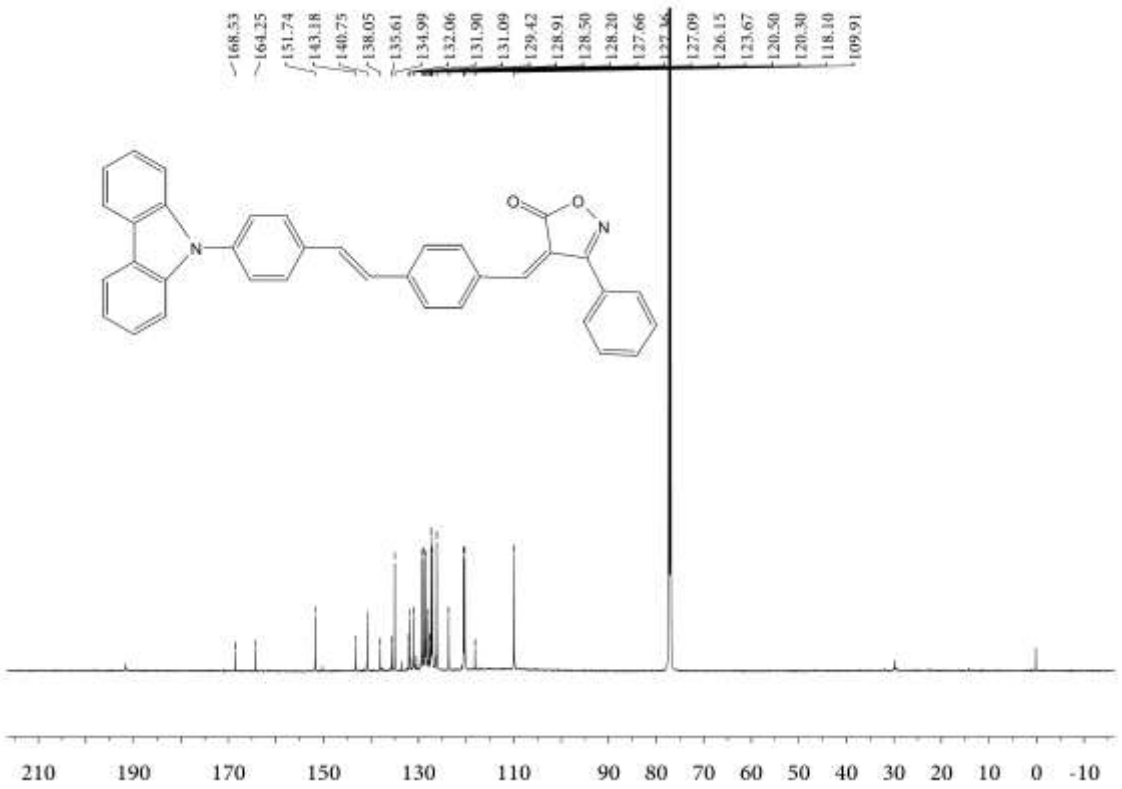












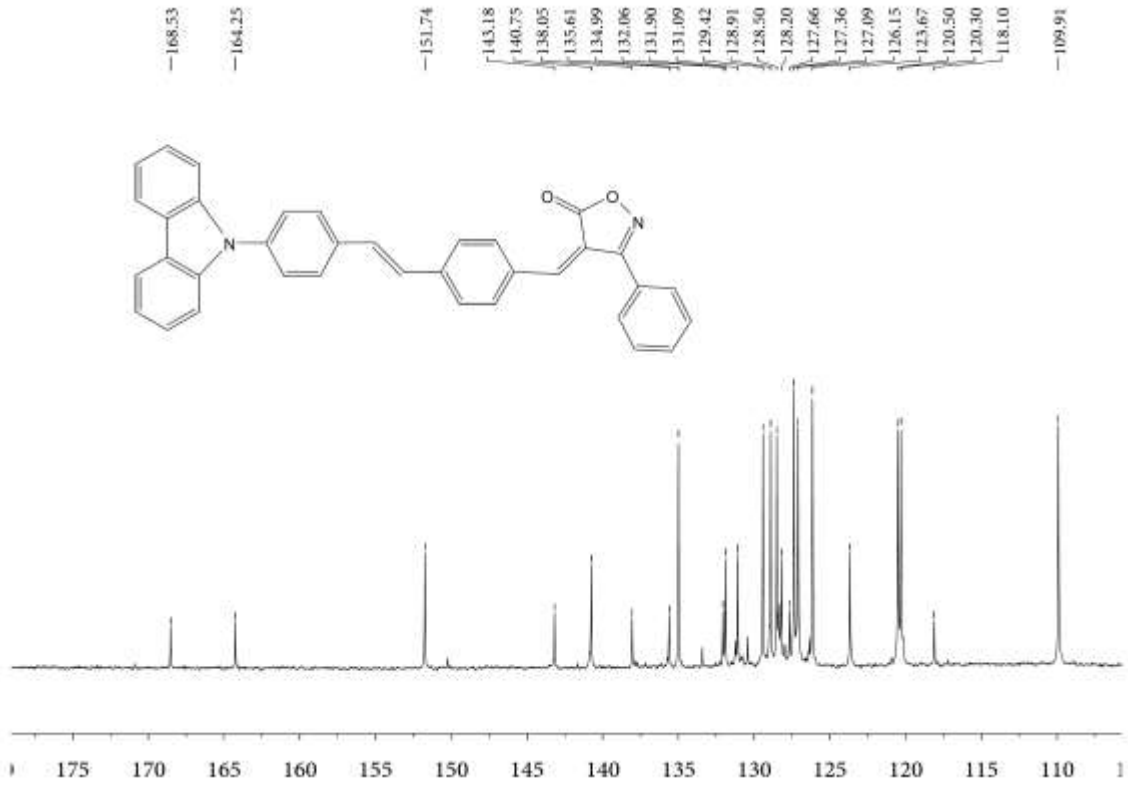


Table S1. Crystallographic data for **DLS**, **DSS** and **CSS**

	DLS	**DSS**	**CSS**
empirical formula	$C_{18}H_{16}N_2O_2$	$C_{26}H_{22}N_2O_2$	$C_{36}H_{24}N_2O_2$
fw	292.33	394.46	516.18
cryst syst	monoclinic	orthorhombic	monoclinic
cryst description/color	plate/orange	prism/dark red	rod/orange
space group	C c	$P\,2_1\,2_1\,2_1$	$P\,2_1/n$
a (Å)	21.092(13)	5.844(4)	16.6077(15)
b (Å)	6.521(3)	7.720(5)	8.2169(8)
c (Å)	12.149(7)	44.76(3)	20.0522(2)
α(deg)	90	90.00	90.00
β(deg)	119.587(8)	90.00	109.011(11)
γ(deg)	90	90.00	90.00
vol ($Å^3$)	1453.2(14)	2019(2)	2587.15
F(000)	616.00	832.00	1080.00
ρcalcul ($mg\cdot m^{-3}$)	1.336	1.297	1.326
θ range (°)	3.32 to 27.50	2.97 to 26.37	3.38 to 65.07
temp (K)	173(2)	173(2)	173(2)
Z	4	4	4
R_1, wR_2 (all data)	0.0556, 0.1356	0.0942, 0.1635	0.0718, 0.1649
GOF	0.996	0.993	0.996

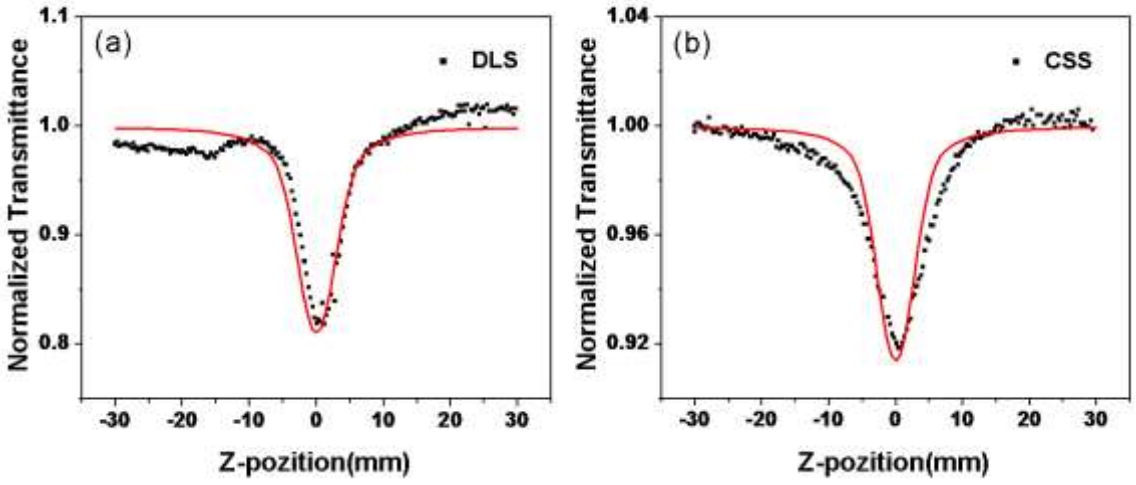


Fig. S1 Normalized open-aperture *Z*-scan curves of **DLS** (a) and **CSS** (b).The solid lines are the fitting curves.

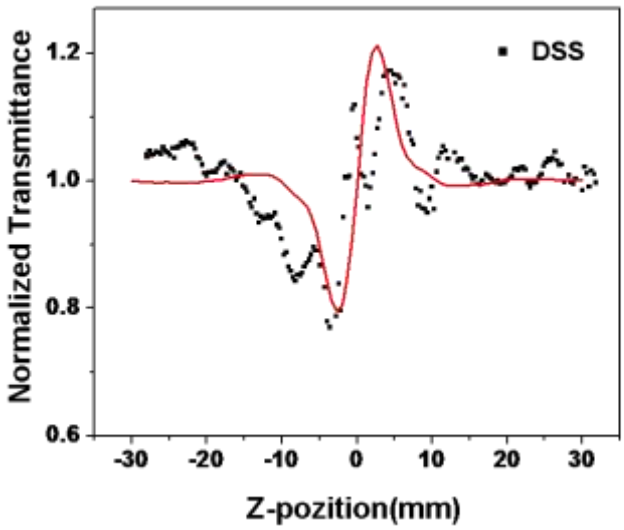


Fig. S2 Normalized closed-aperture *Z*-scan curves of **DSS** .The solid lines are the fitting curves.

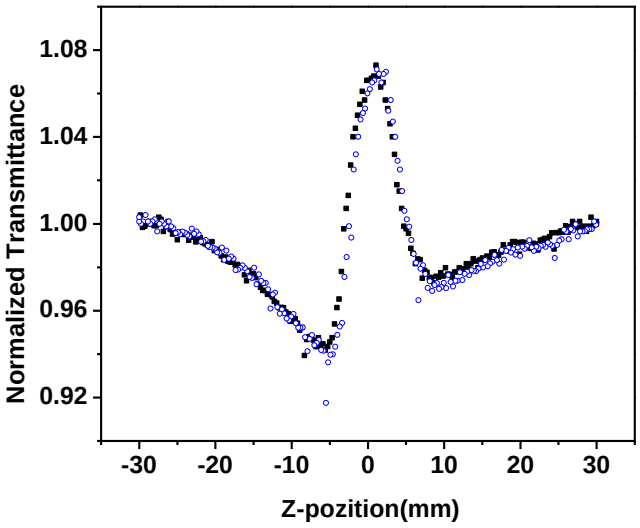


Fig. S3 Normalized open-aperture *Z*-scan curve of **DSS**.