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Supporting Information

Efficient bifunctional materials based on pyrene- and triphenylamine-functionalized dendrimers for electroluminescent devices

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Content:

1. Quantum chemical calculation results **S2**

2. Multiple CV scans **Sx**

3. EL spectra **S9**

4. ^{1}H and ^{13}C NMR spectra **S10**

Quantum chemical calculation results

Table S1 The calculated HOMO, LUMO and HOMO-LUMO energy gap (Δ_{H-L}) of the compounds by B3LYP/6-31G(d,p).

Compounds	HOMO (eV)	LUMO (eV)	Δ_{H-L} (eV)	E_{ex}[a] (eV/nm)
G1PYR	-5.14	-1.67	3.48	3.11 (399)
G2PYR	-5.13	-1.67	3.46	3.11 (399)
G1TPA	-4.86	-0.91	3.96	3.40 (364)
G2TPA	-4.86	-1.18	3.68	3.31 (374)

[a] exciation energies from ground to excited states are calculated by TD-B3LYP/6-31G(d,p) in CH_2Cl_2 solvent

Table S2 The two lowest excitation of from ground to excited states are calculated by TD-B3LYP/6-31G(d,p) in CH_2Cl_2 solvent.

Compounds		E_{ex}[a] (eV/nm)	f	Transition
G1PYR	$S_0 \rightarrow S_1$	3.11 (399)	0.5509	0.69(H→L)+0.11(H-2→L)
	$S_0 \rightarrow S_2$	3.22 (386)	0.2298	0.69(H→L+1)+0.11(H-2→L+1)
G2PYR	$S_0 \rightarrow S_1$	3.11 (399)	0.2200	0.51(H→L)+0.42(H-1→L+1)
	$S_0 \rightarrow S_2$	3.11 (399)	0.8050	0.51(H→L+1)+0.43(H-1→L)
G1TPA	$S_0 \rightarrow S_1$	3.46 (358)	1.2204	0.66(H→L+1)+0.23(H-1→L+2)
	$S_0 \rightarrow S_2$	3.49 (355)	0.0009	0.68(H→L)
G2TPA	$S_0 \rightarrow S_1$	3.31 (374)	0.0089	0.68(H→L+1)+0.19(H-4→L)
	$S_0 \rightarrow S_2$	3.36 (369)	0.0869	0.69(H-1→L)

Multiple CV scans

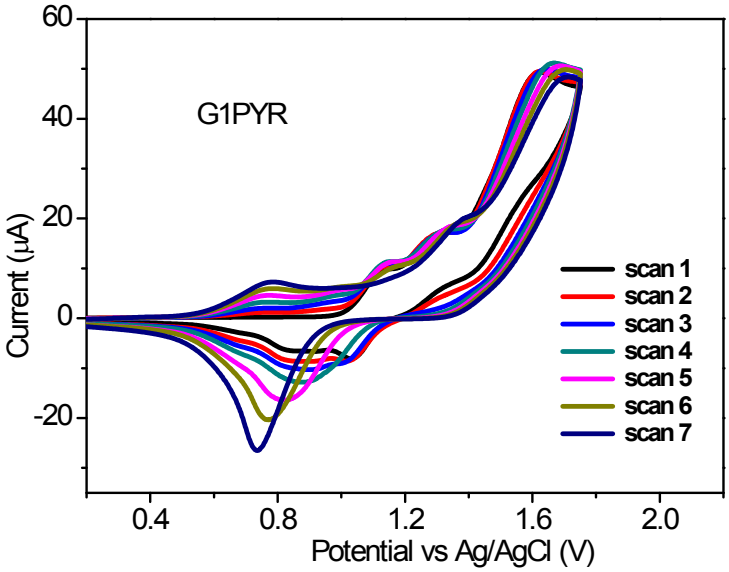


Fig. S1 CV traces measured in CH_2Cl_2/*n*-Bu_4NPF_6 at scan rate of 50 mV s^{-1}

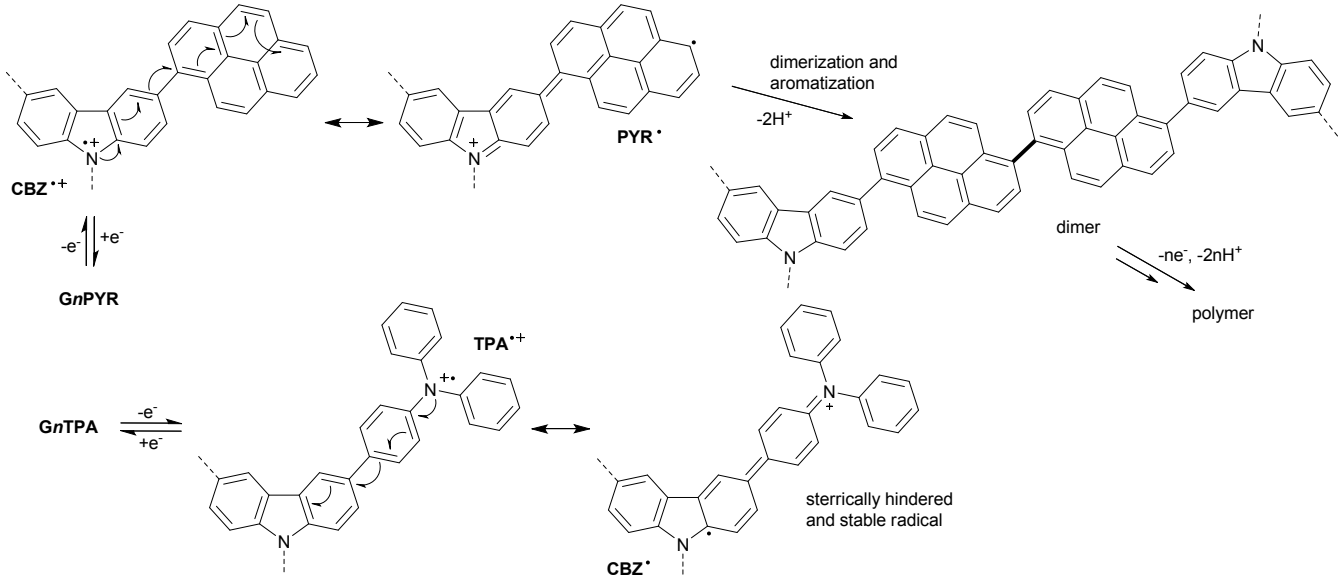
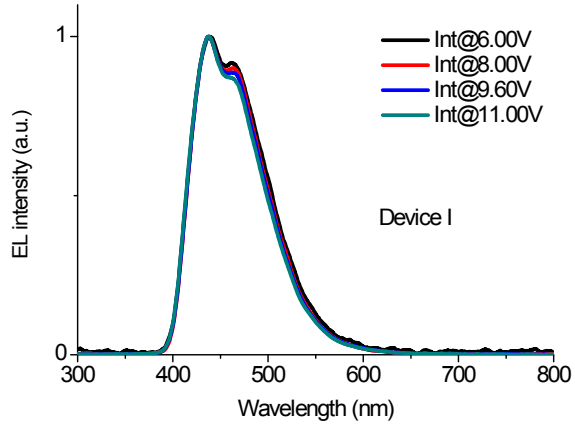


Fig. S2 Proposed oxidation and electrochemical coupling reaction of GnPYR and GnTPA under the CV experiments.

EL spectra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Int@11.00V
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Wavelength (nm)
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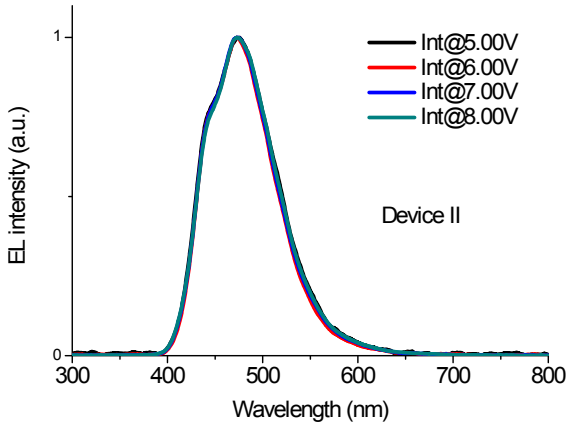
400
500
600
700
800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500
600
700
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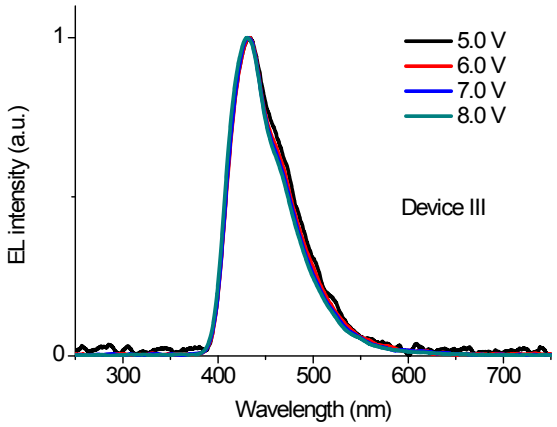
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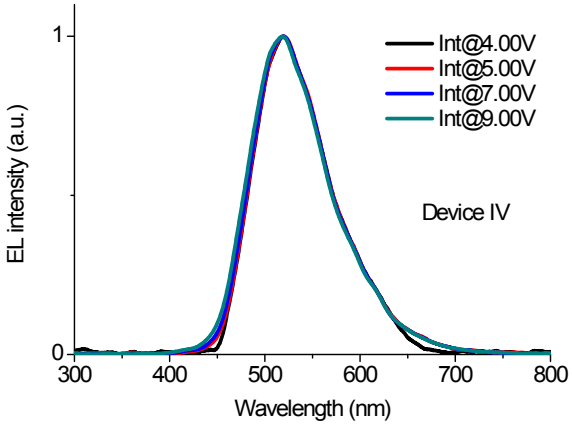
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600
700
800

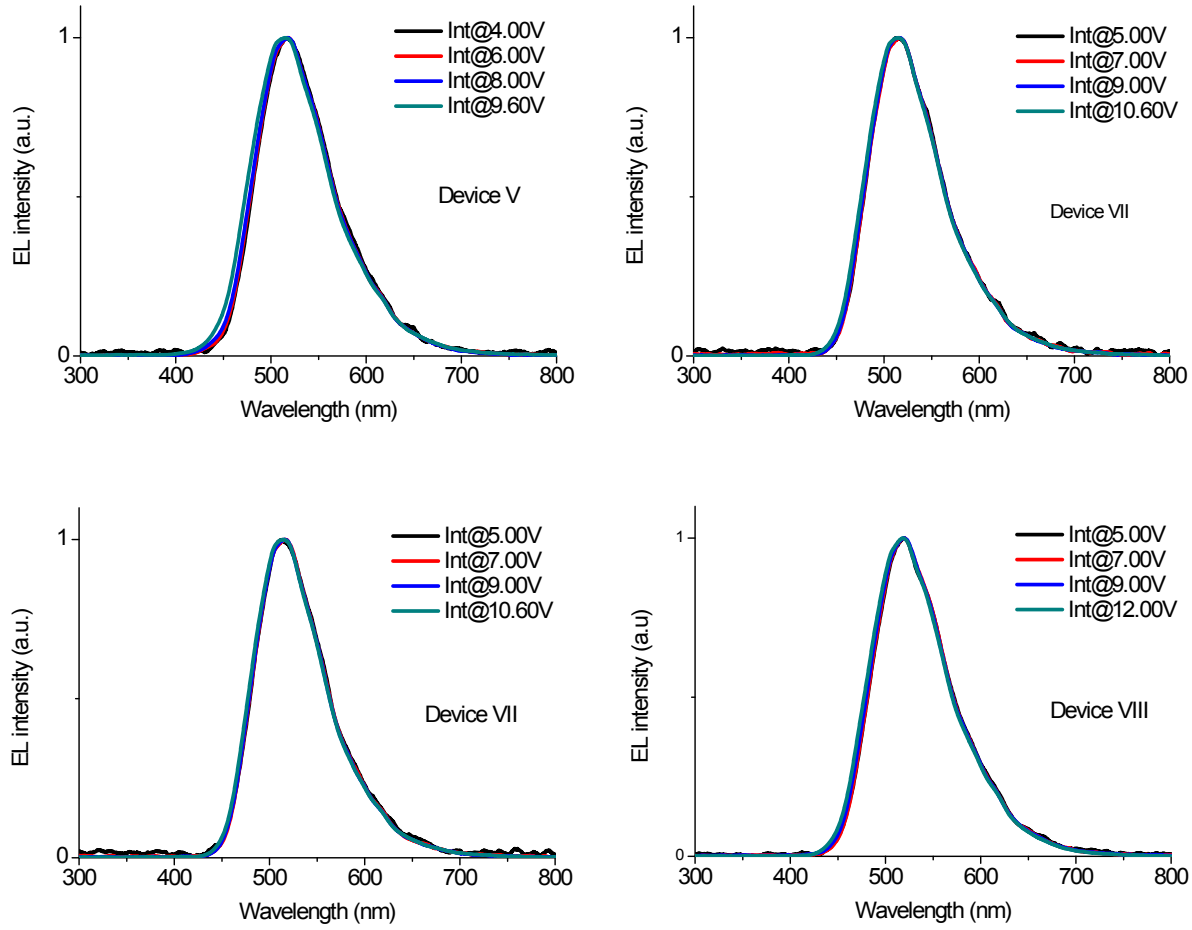
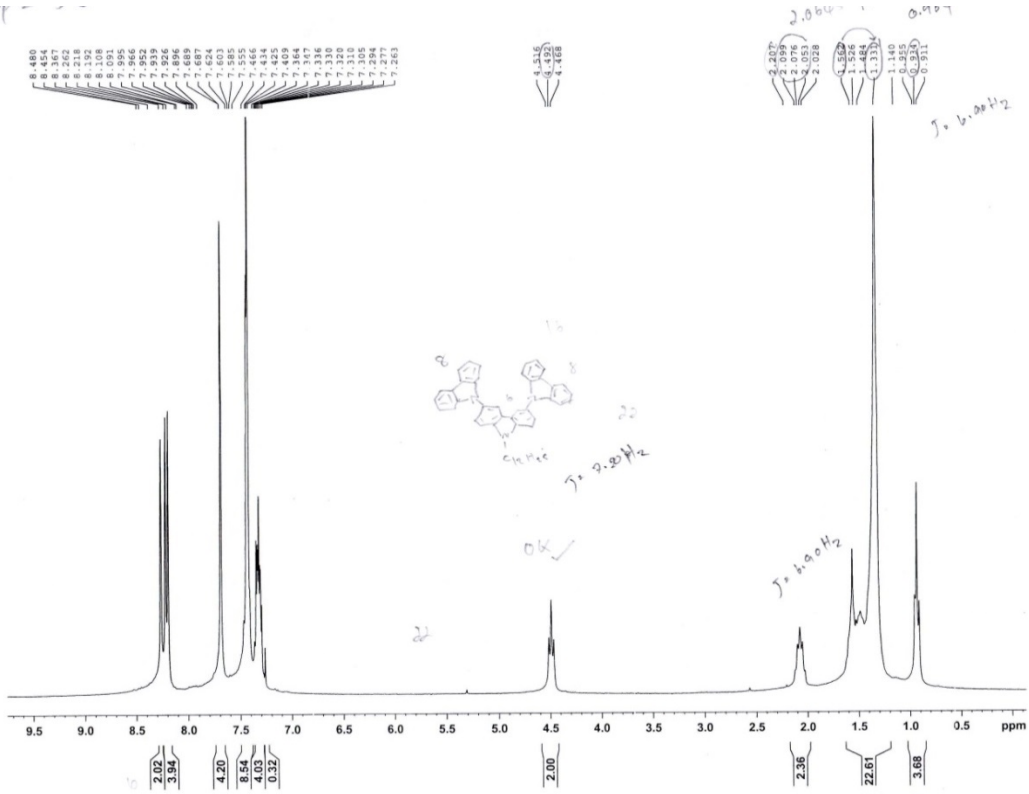


Fig. S3 EL spectra of the OELDs at different applied voltages

[1]H-NMR and [13]C-NMR spectra

Compound 2



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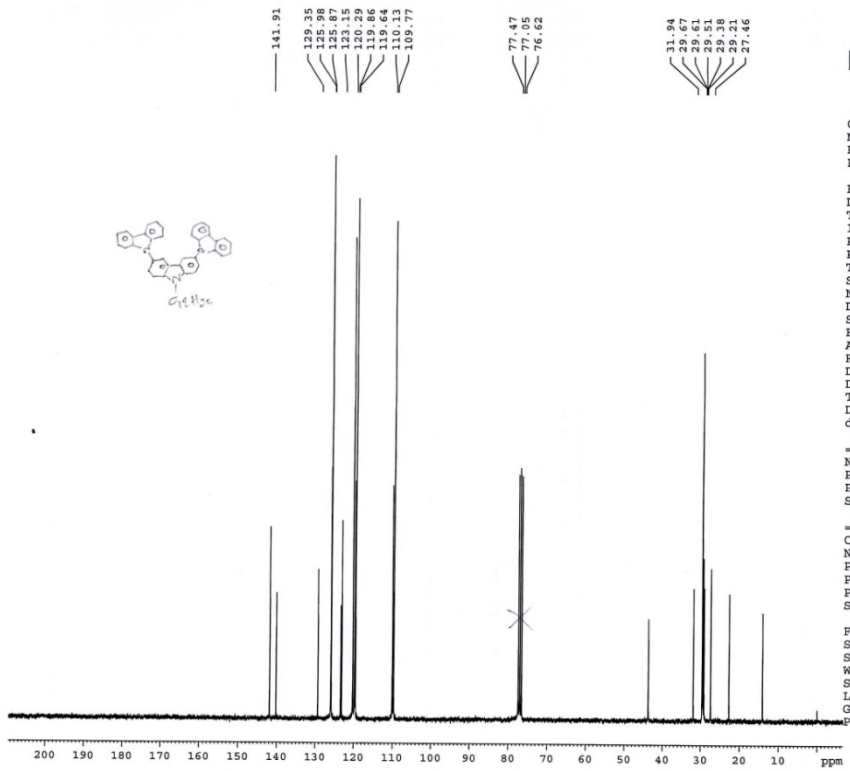

BRUKER

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PROCNO                      1

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TE                   300.0 K
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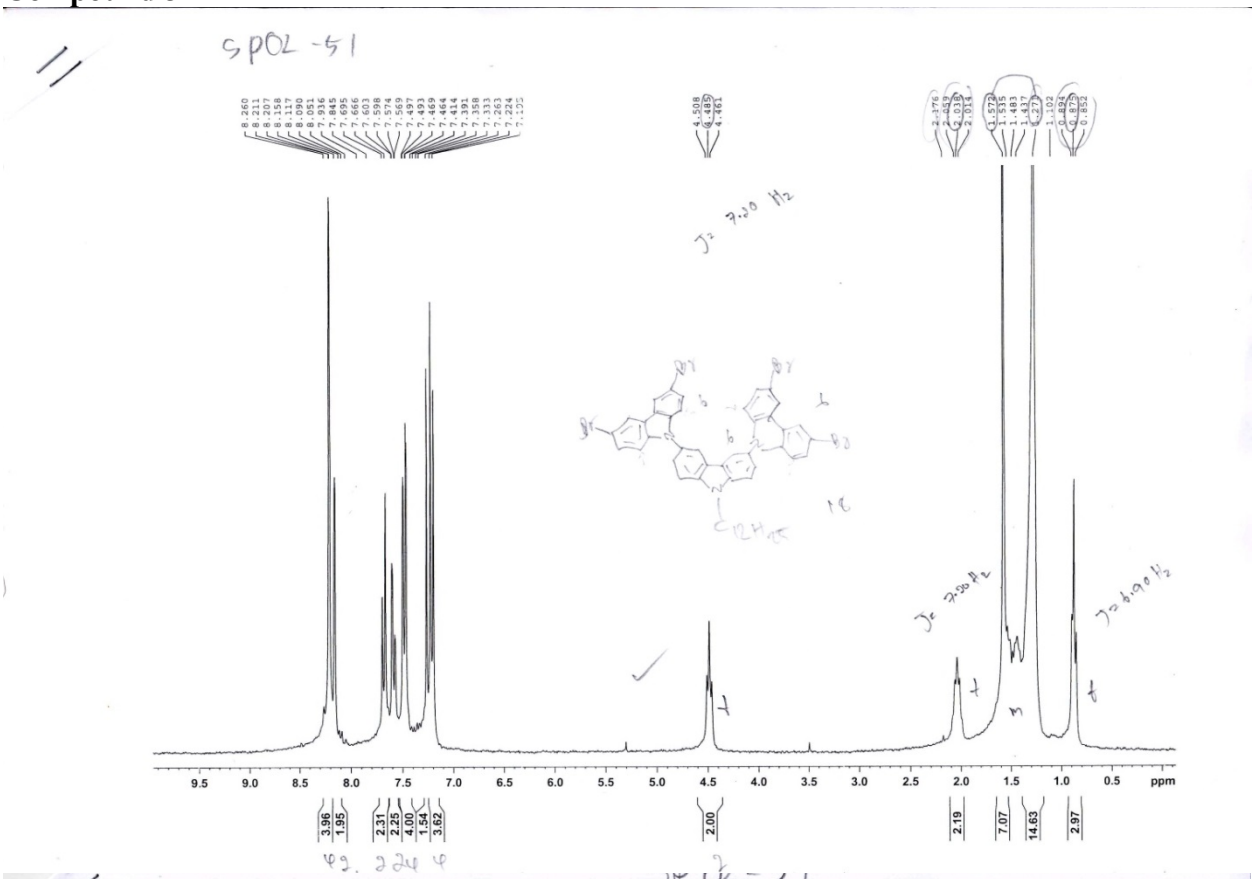
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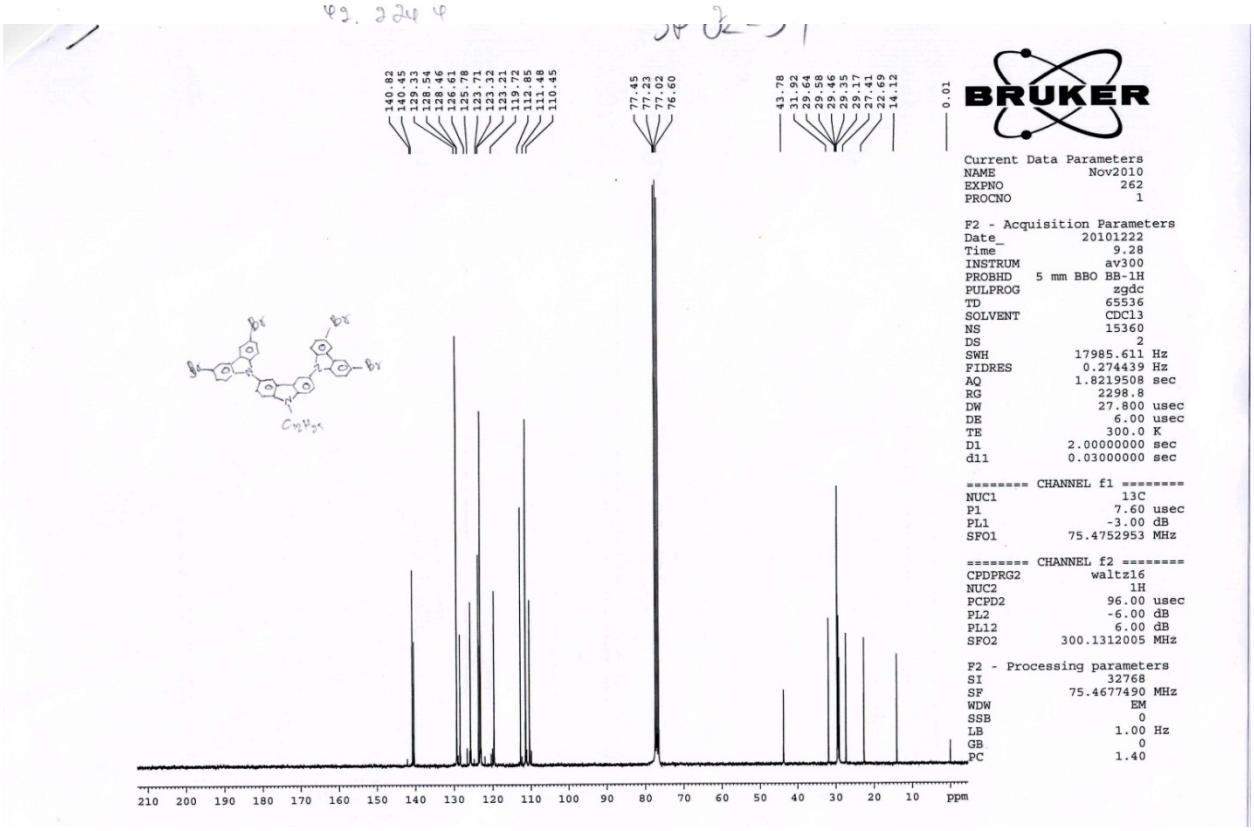
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d11 0.03000000 sec
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P1 7.60 usec
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PCPD2 96.00 usec
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PL12 6.00 dB
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F2 - Processing parameters
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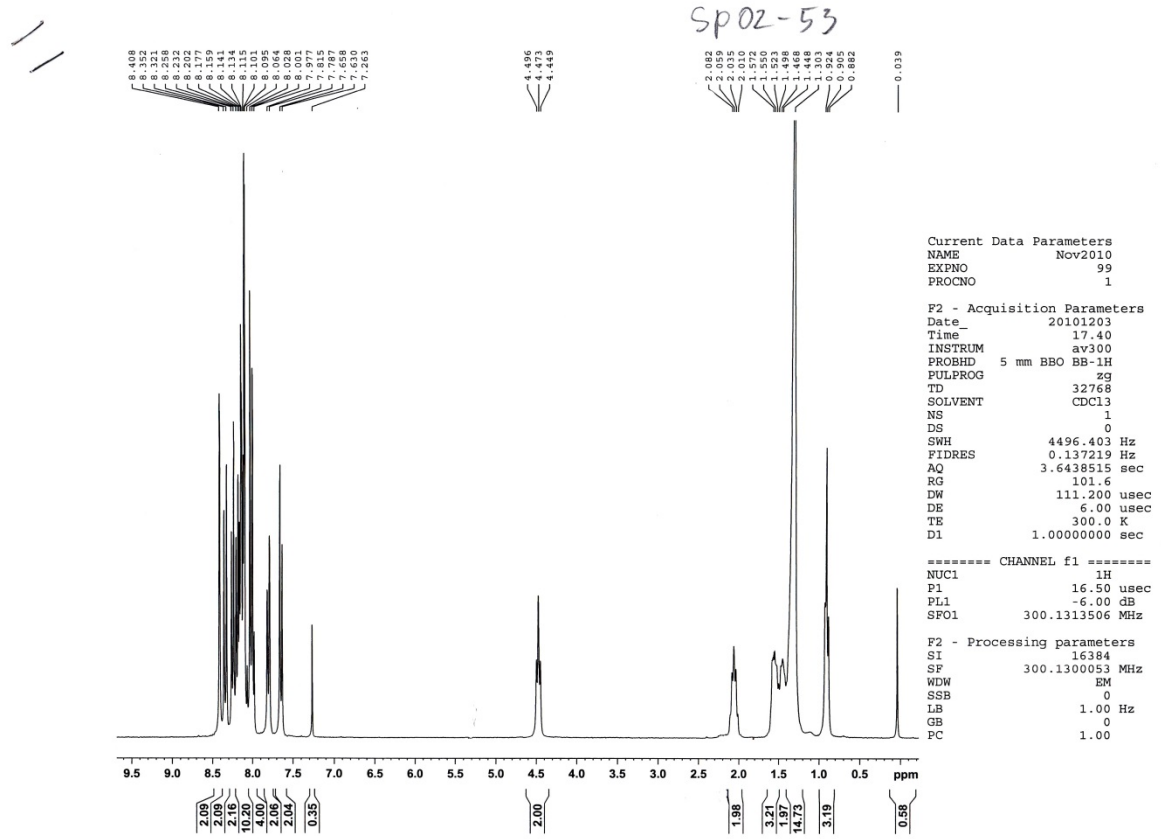
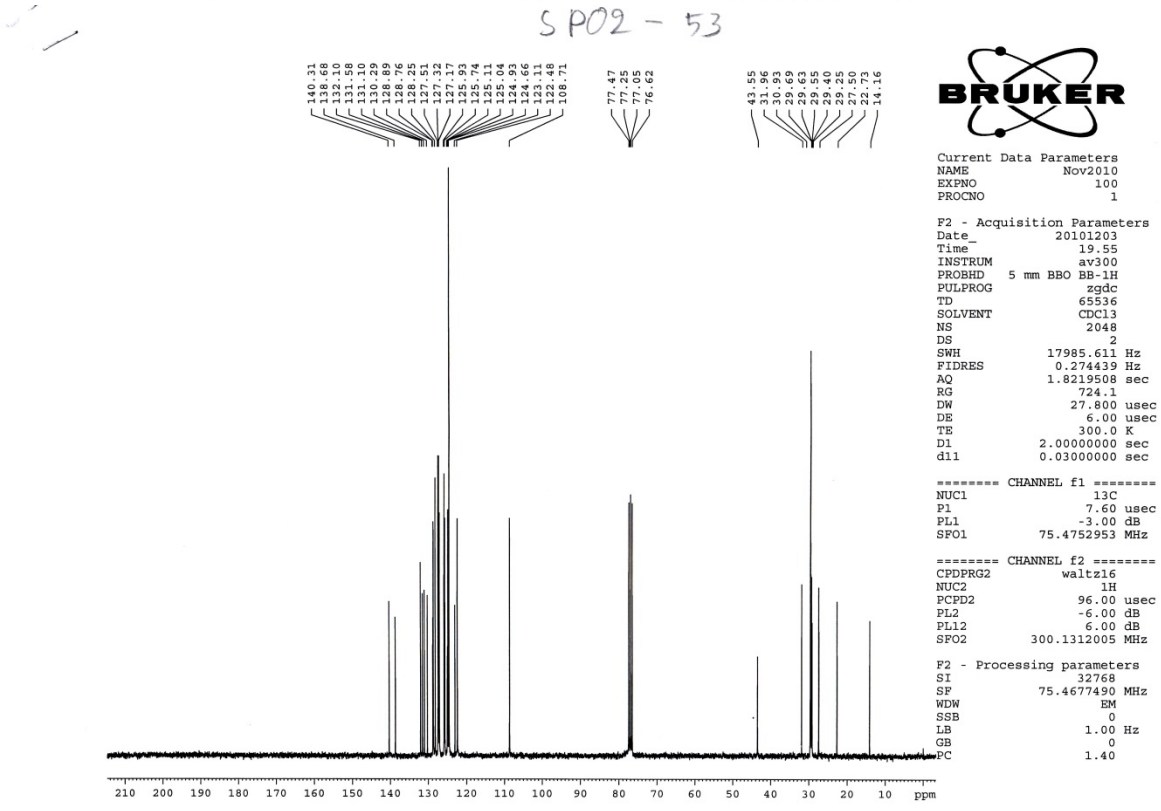
Compound G1PYR





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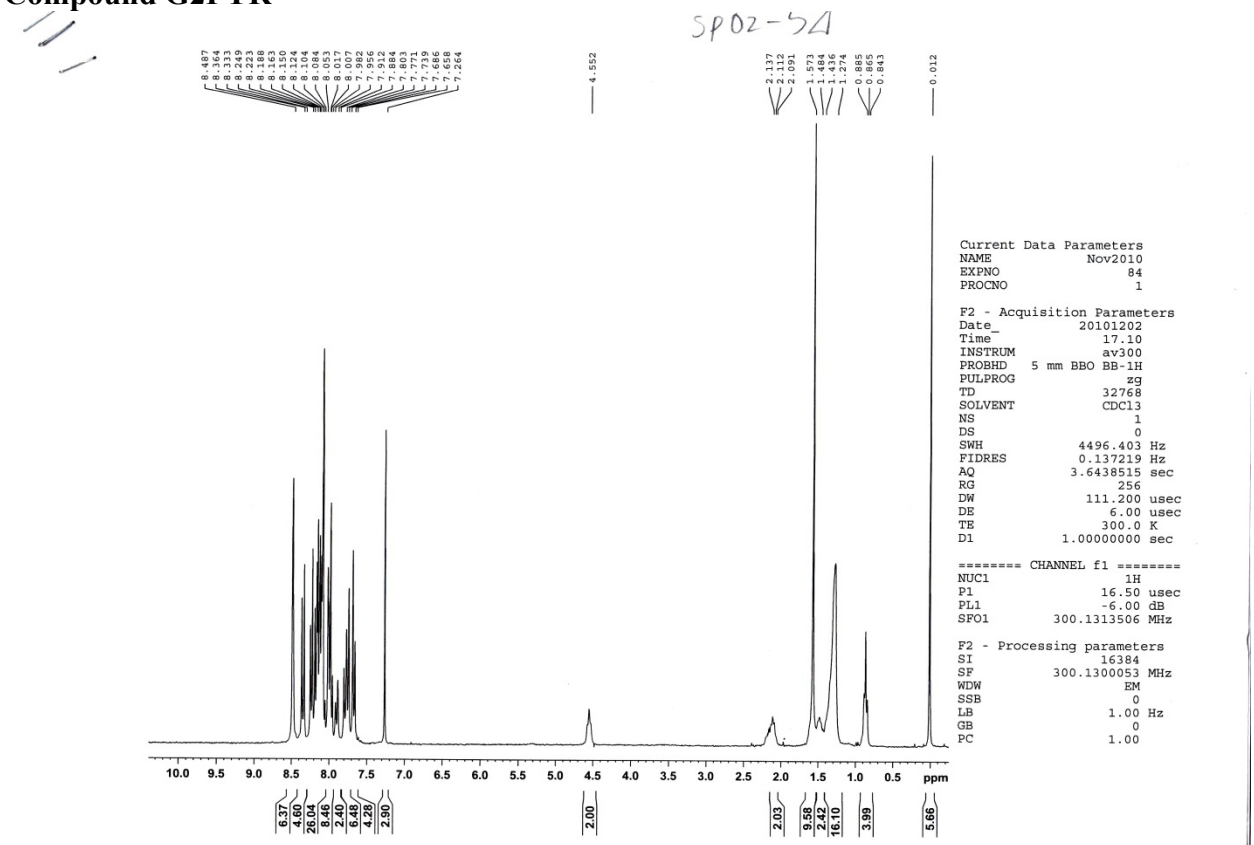

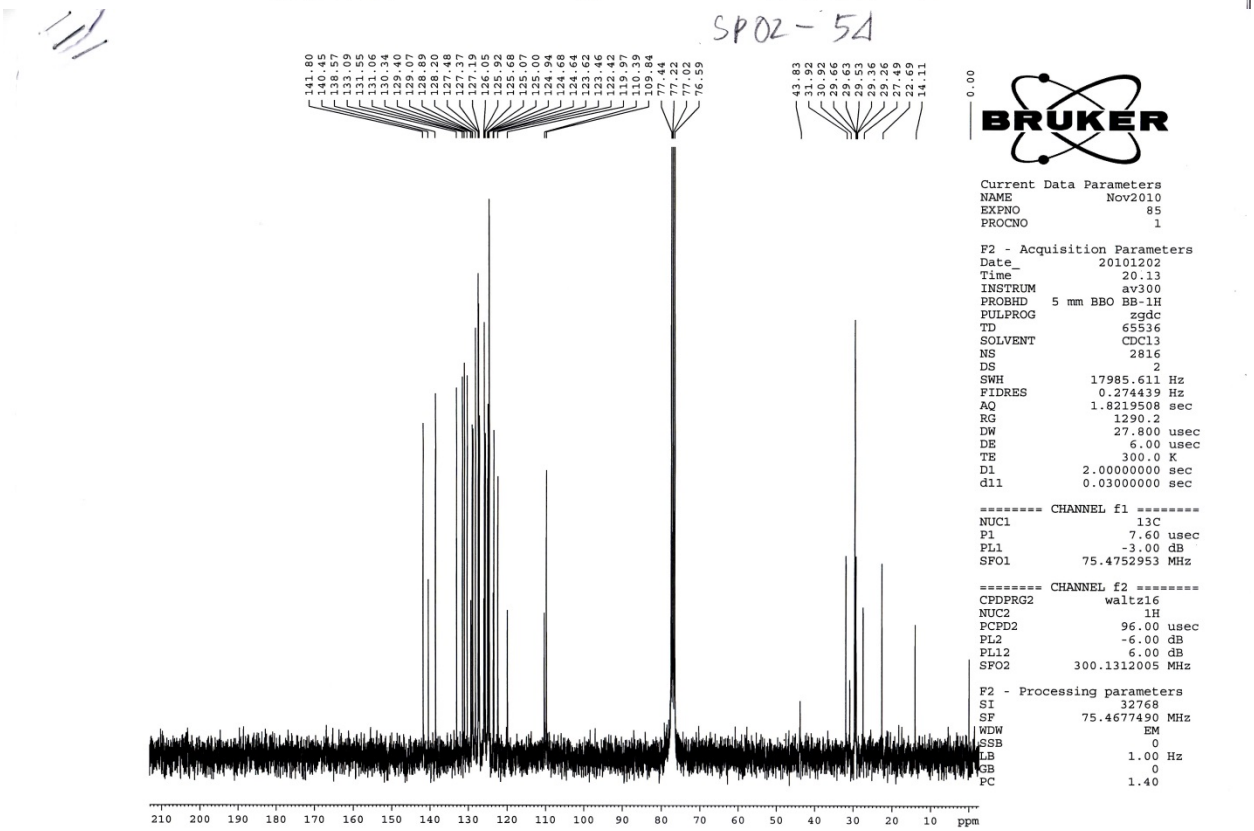

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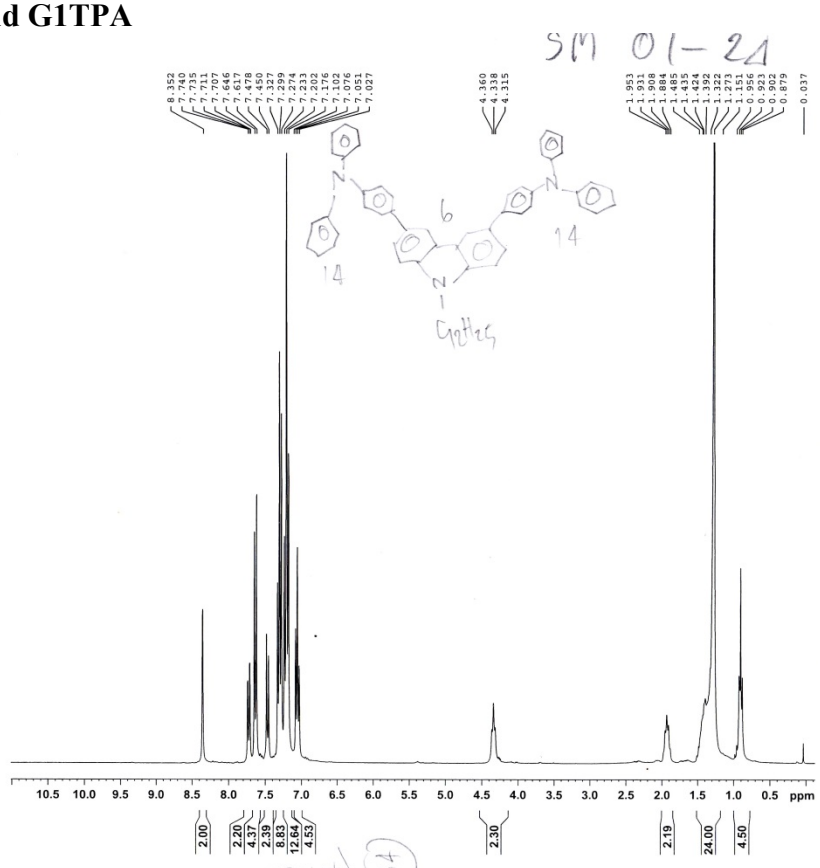

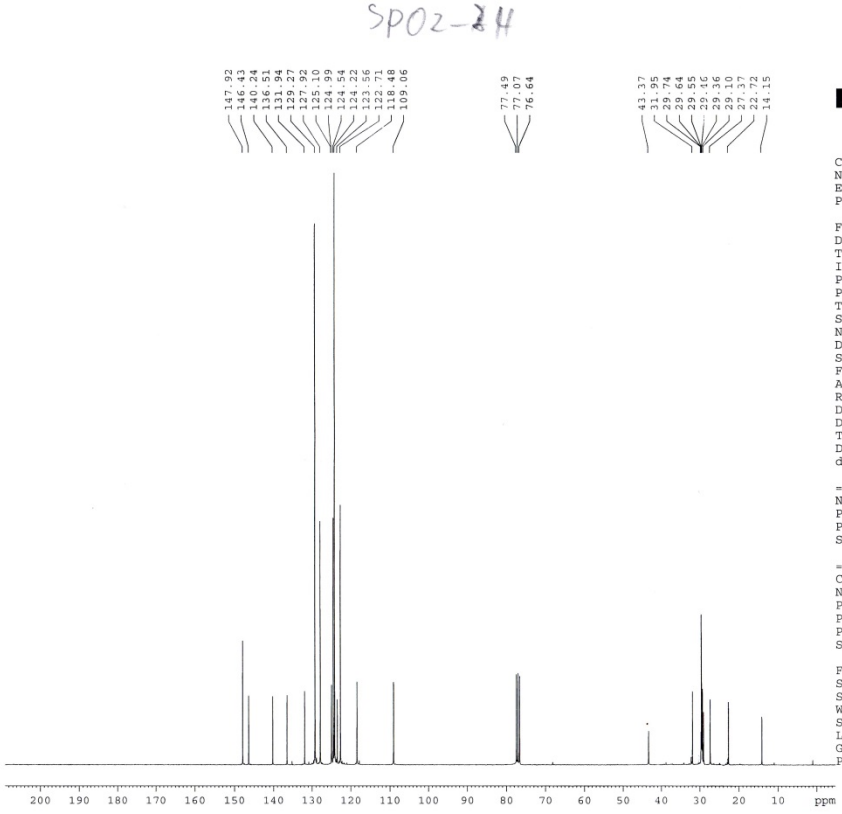
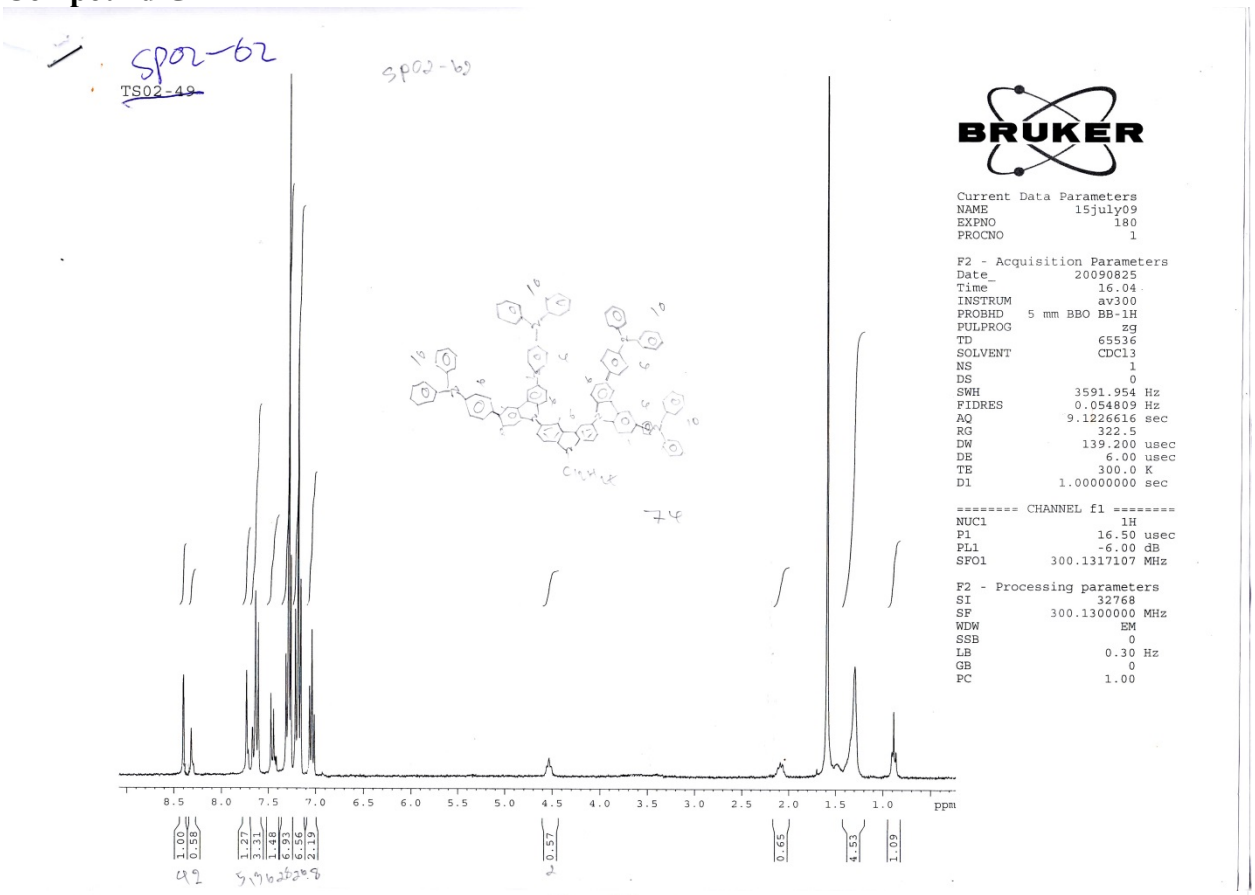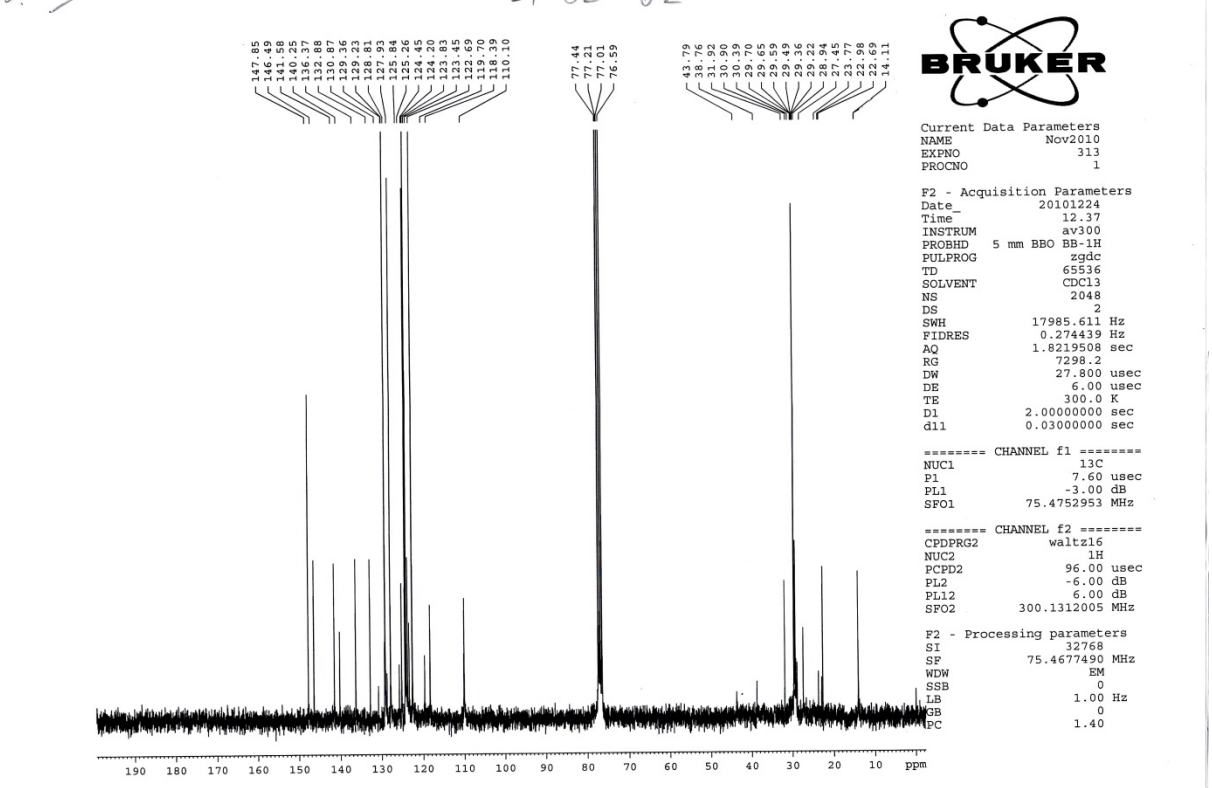
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