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

Supporting Information

Multi-triphenylamine-substituted bis(thiophenyl) benzothiadiazoles as highly efficient solution-processed non-doped red light-emitters for OLED

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Content

Quantum Chemical Calculation

Methods of calculation

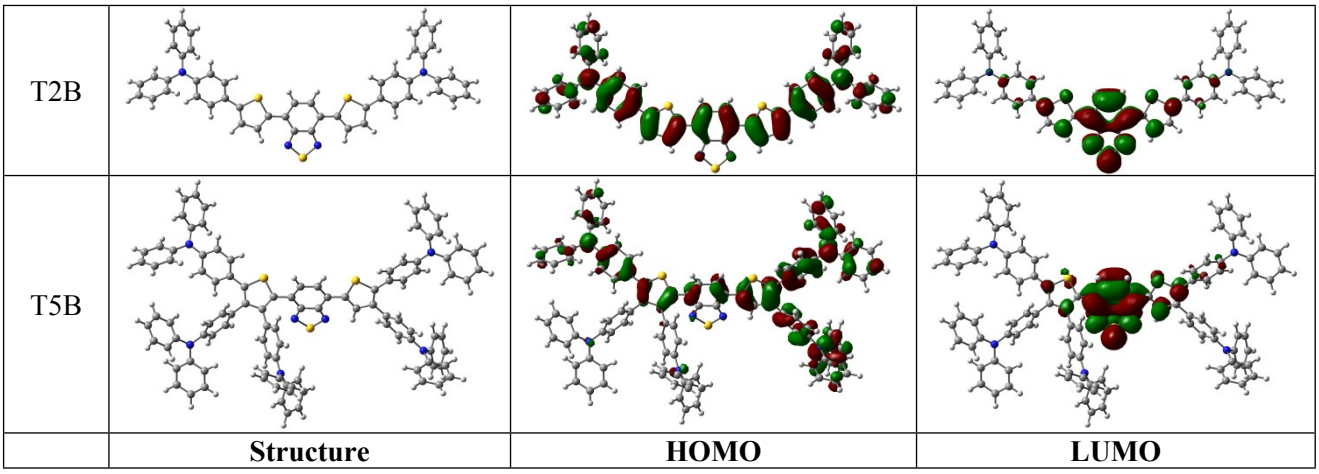
- All calculations were performed by Gaussian 09 code
- CH_2Cl_2 solvent by C-PCM model was applied for all calculations
- Geometry optimizations were done by B3LYP/6-31G(d,p) method
- Excitation energies from ground to excited state were calculated by TD- CAM-B3LYP/6-31G(d,p) method

Table S1 The calculated HOMO, LUMO and HOMO-LUMO energy gap (Δ_{H-L}) of the studied compounds by B3LYP/6-31G(d,p) in CH_2Cl_2 solvent.

Compounds	HOMO	LUMO	Δ_{H-L}	E_{ex} [a] eV (nm)
T2B	-4.82	-2.69	2.13	2.39 (518)
T5B	-4.87	-2.61	2.26	2.70 (459)

[a] Excitation energy were calculated by TD-CAM-B3LYP/6-31G(d,p) method in CH_2Cl_2 solvent.

Fig. S1 HOMO and LUMO orbitals.



CV plots

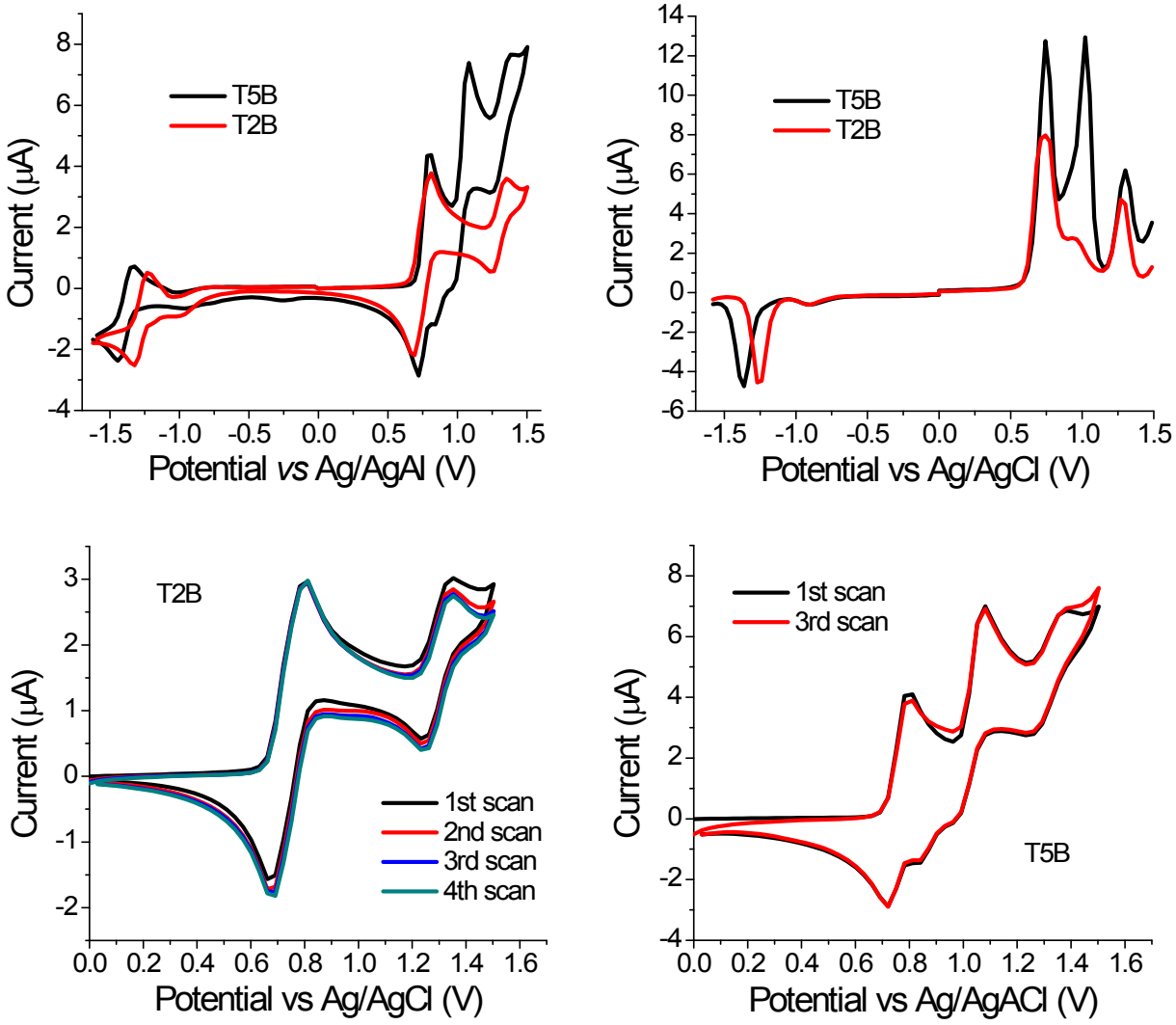


Fig. S2 CV and differential pulse CV traces.

AFM images

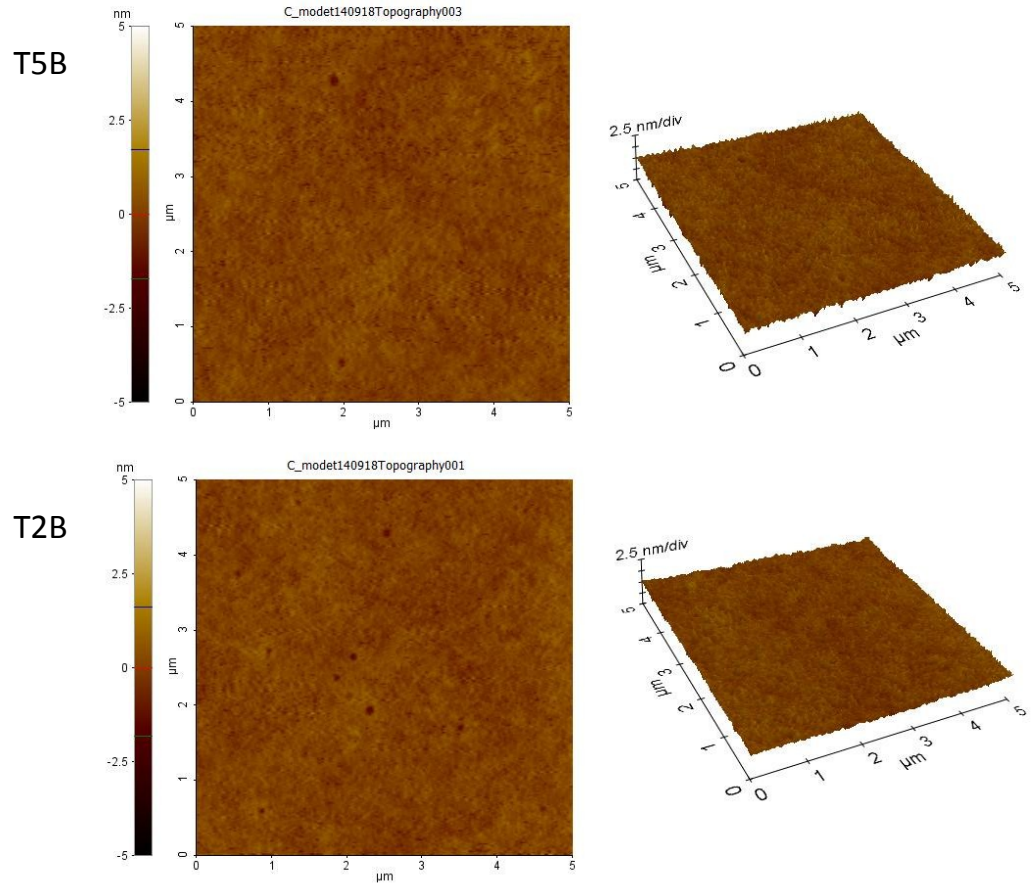


Fig. S3 Tapping mode AFM images of the spin-coated thin films.

OLED EL spectra

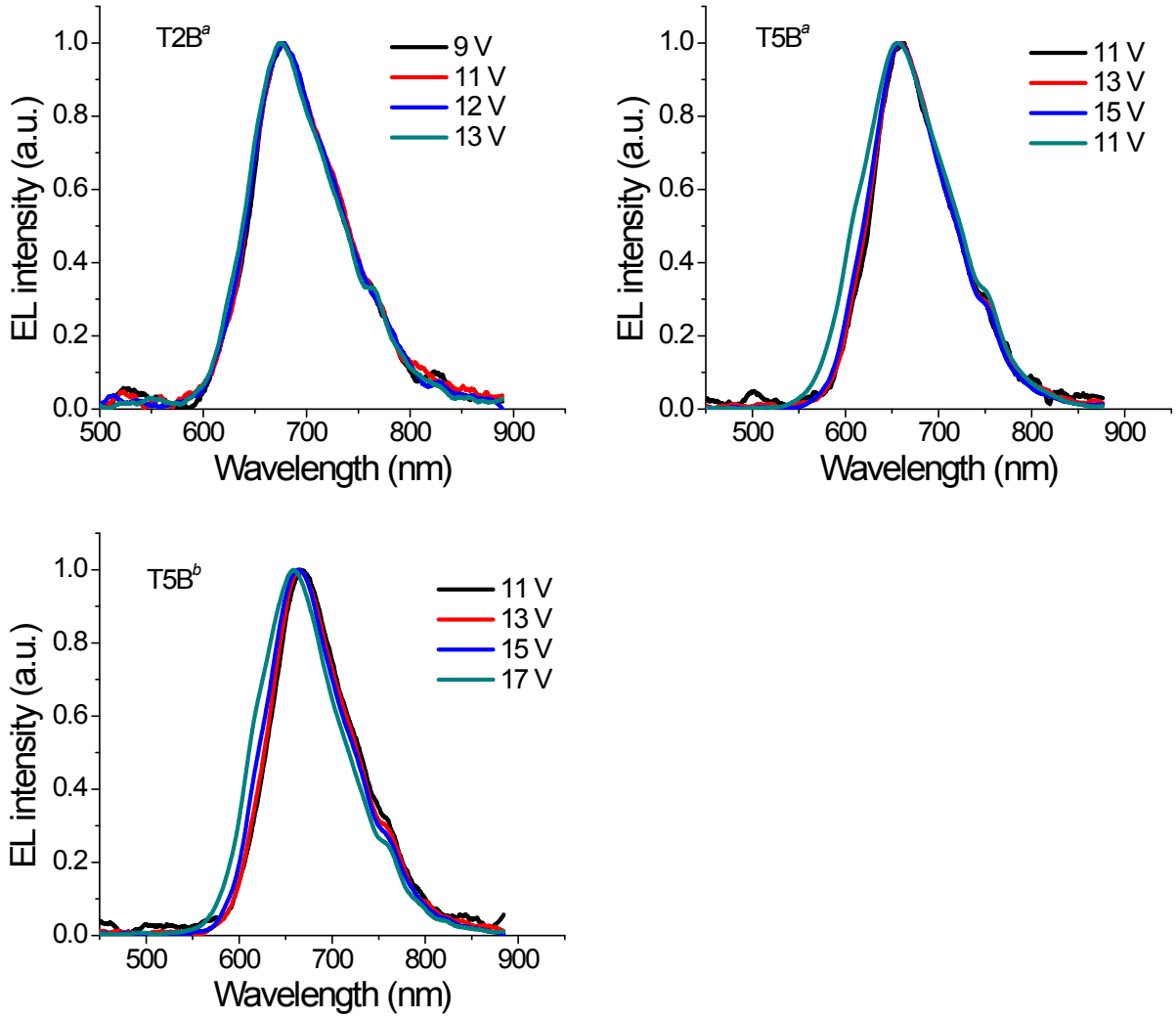
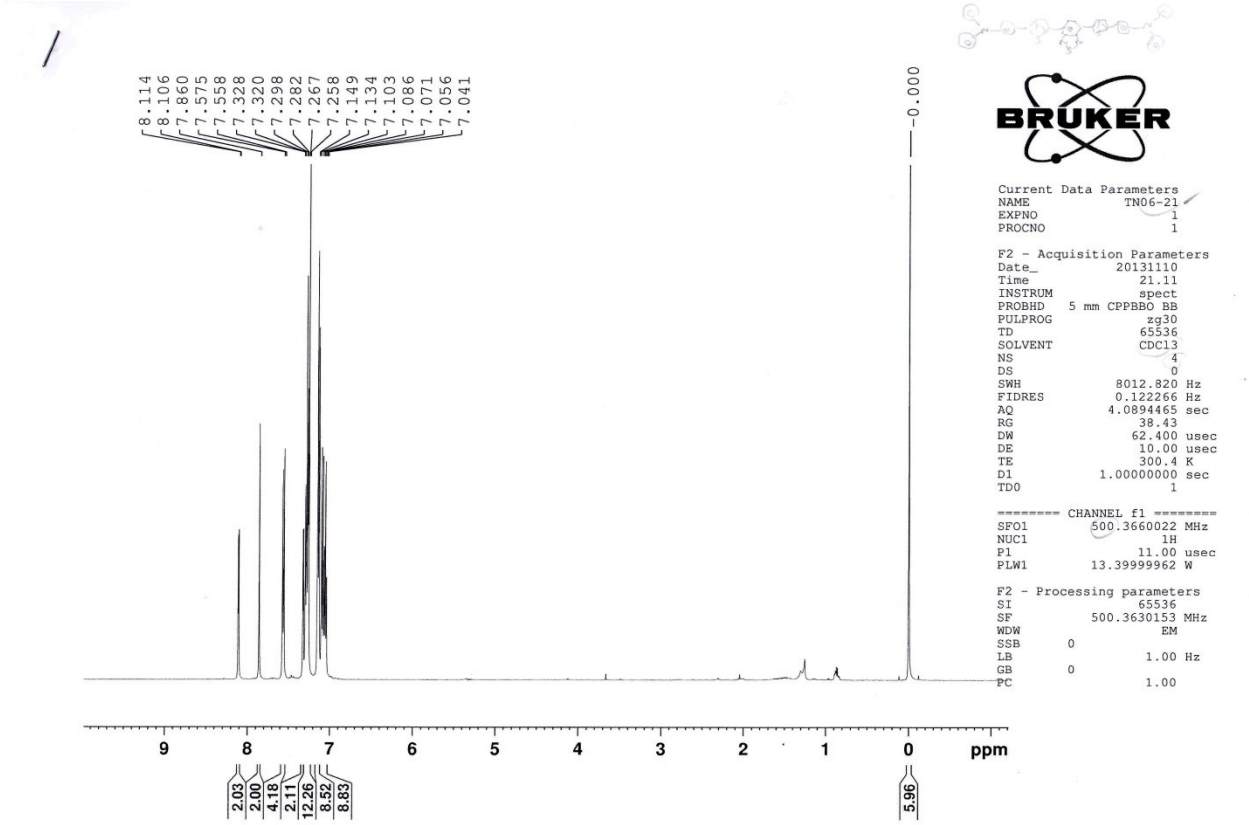
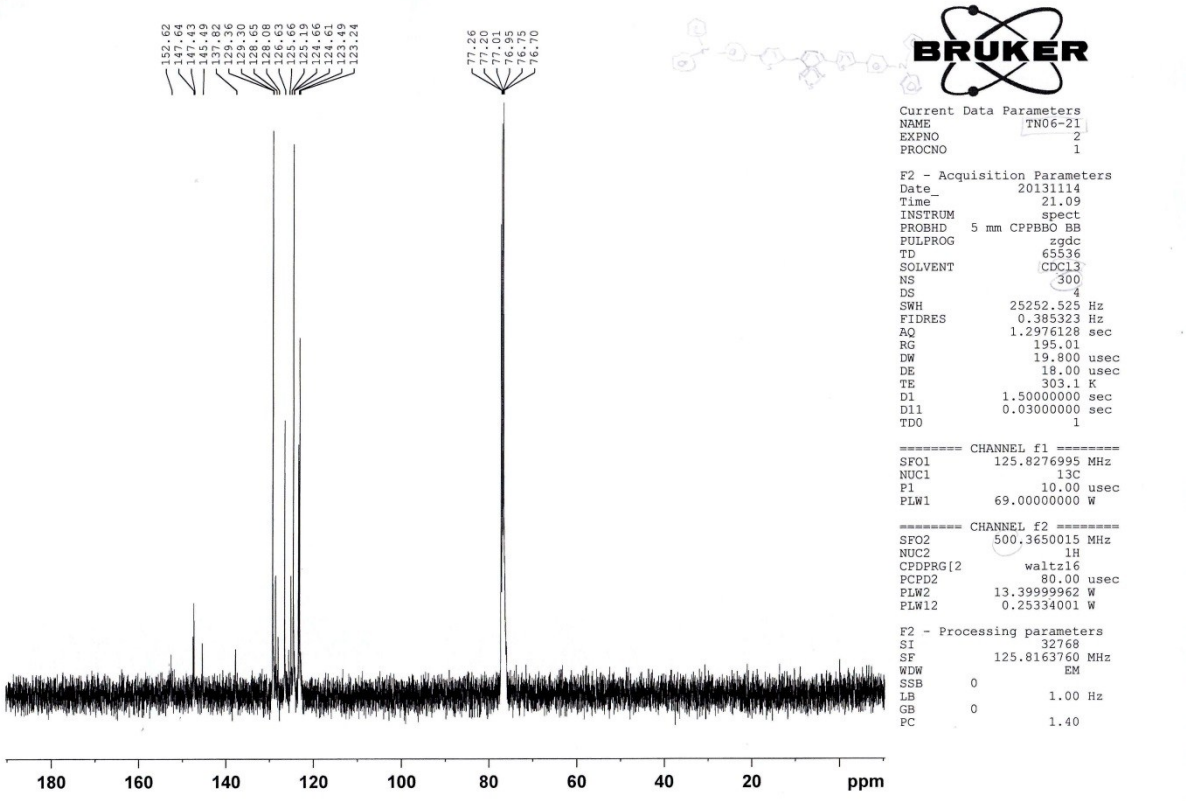


Fig. S4 EL spectra of the OELDs at different applied voltages.

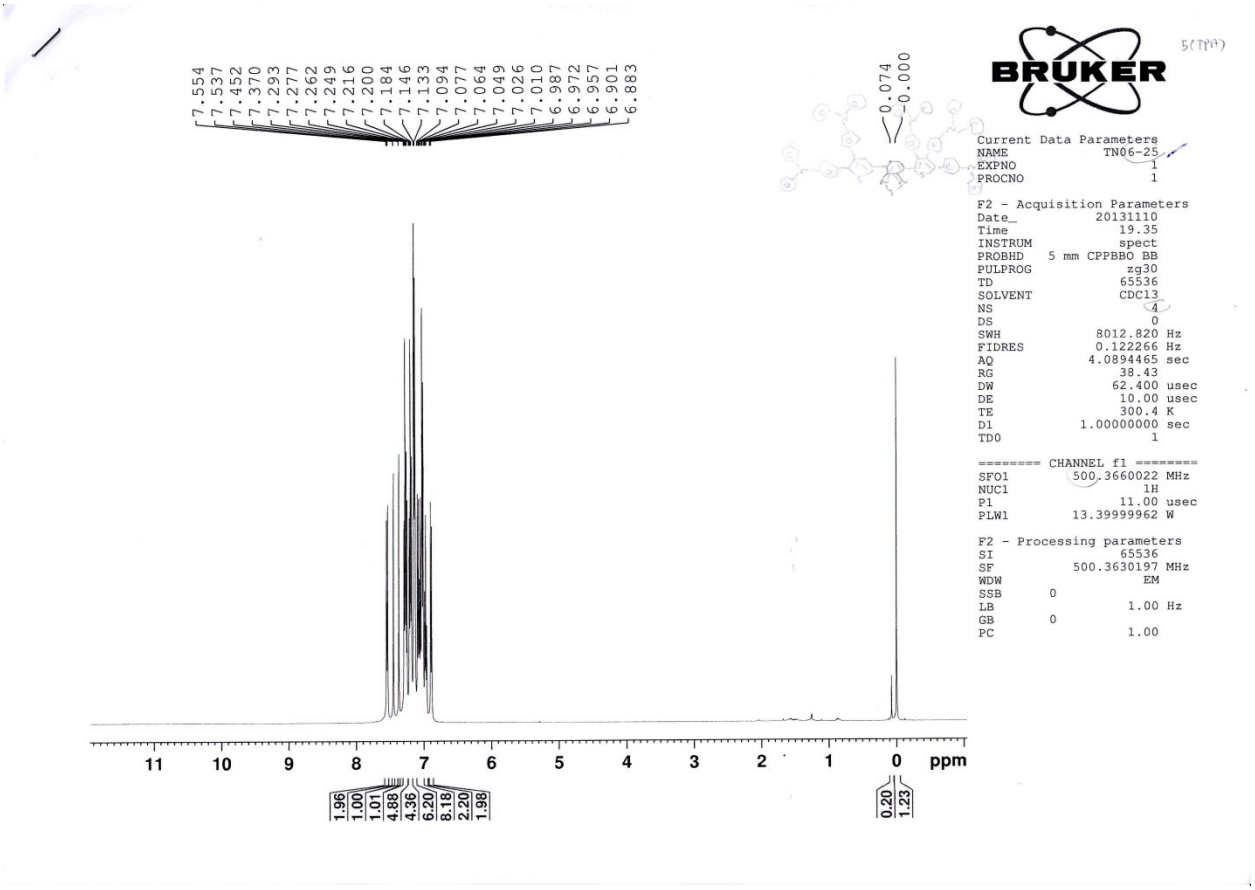
^{1}H and ^{13}C NMR spectra and MALDI-TOF

T2B





T5B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7.094
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7.064
7.049
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7.010
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6.972
6.957
6.901
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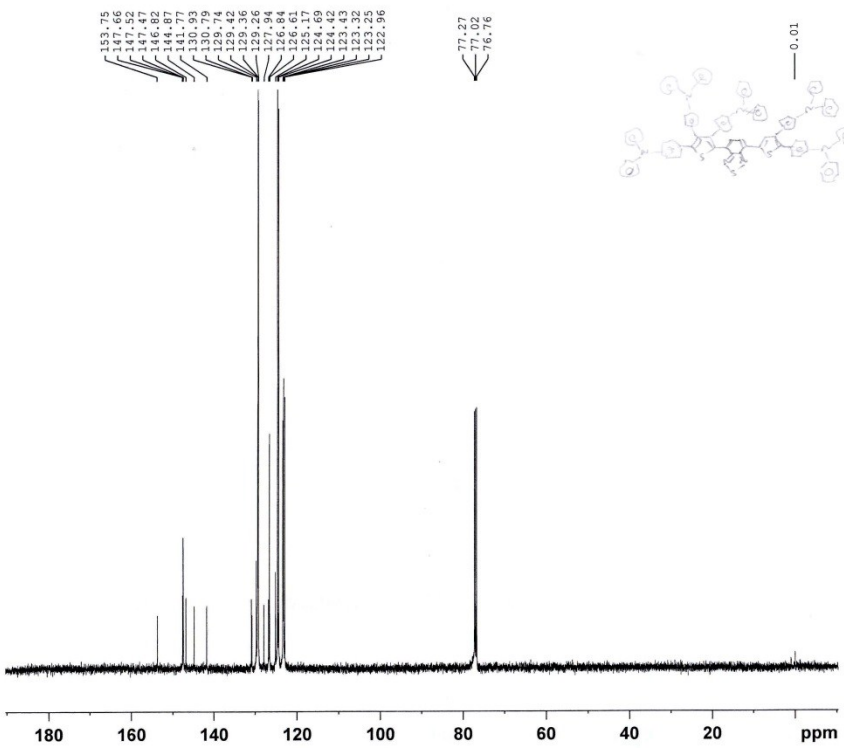

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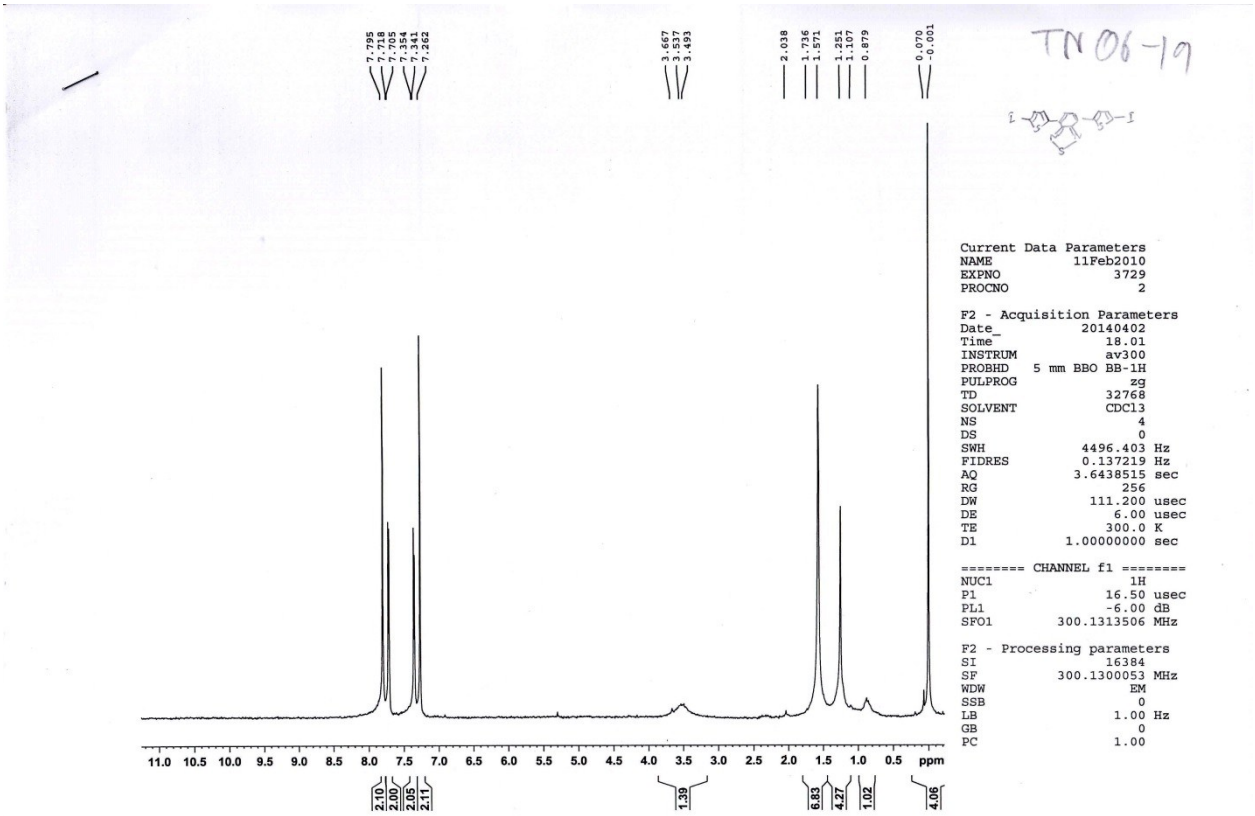
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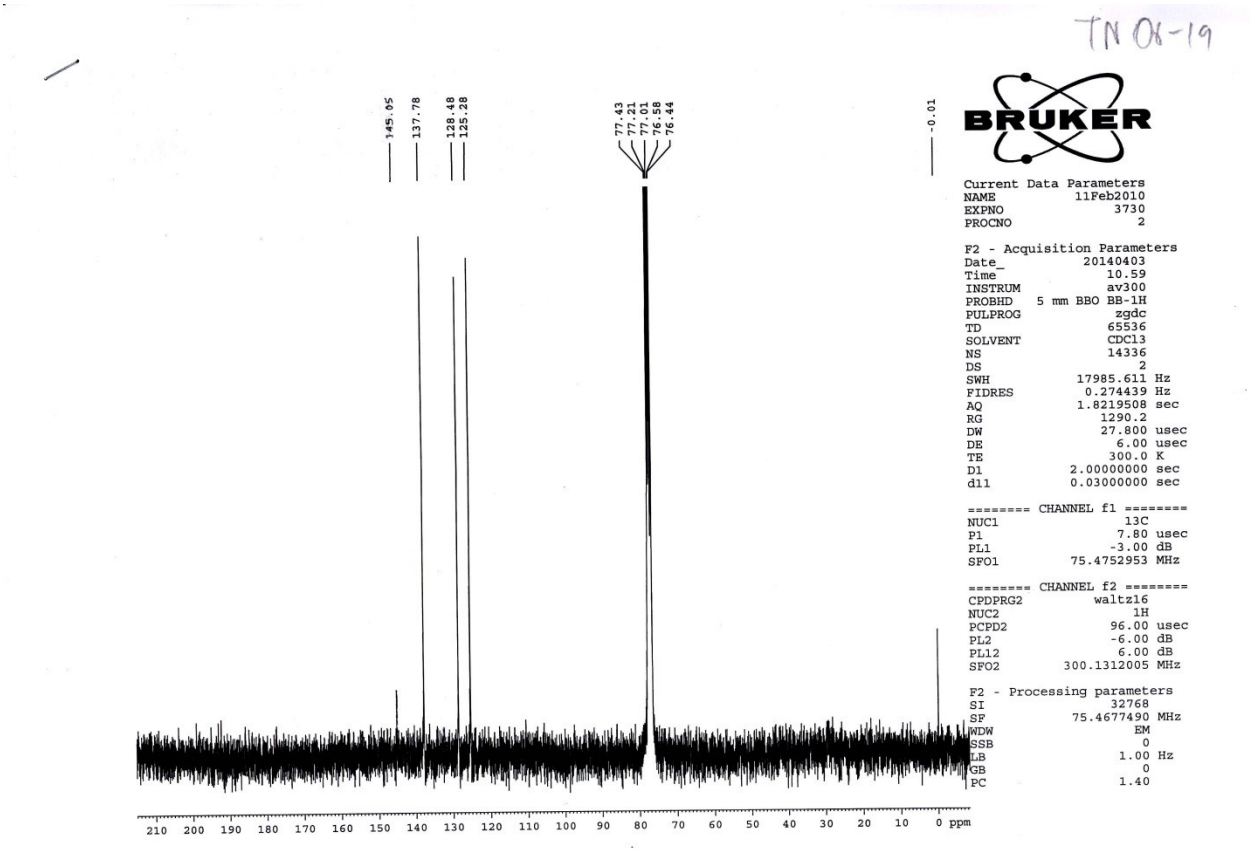
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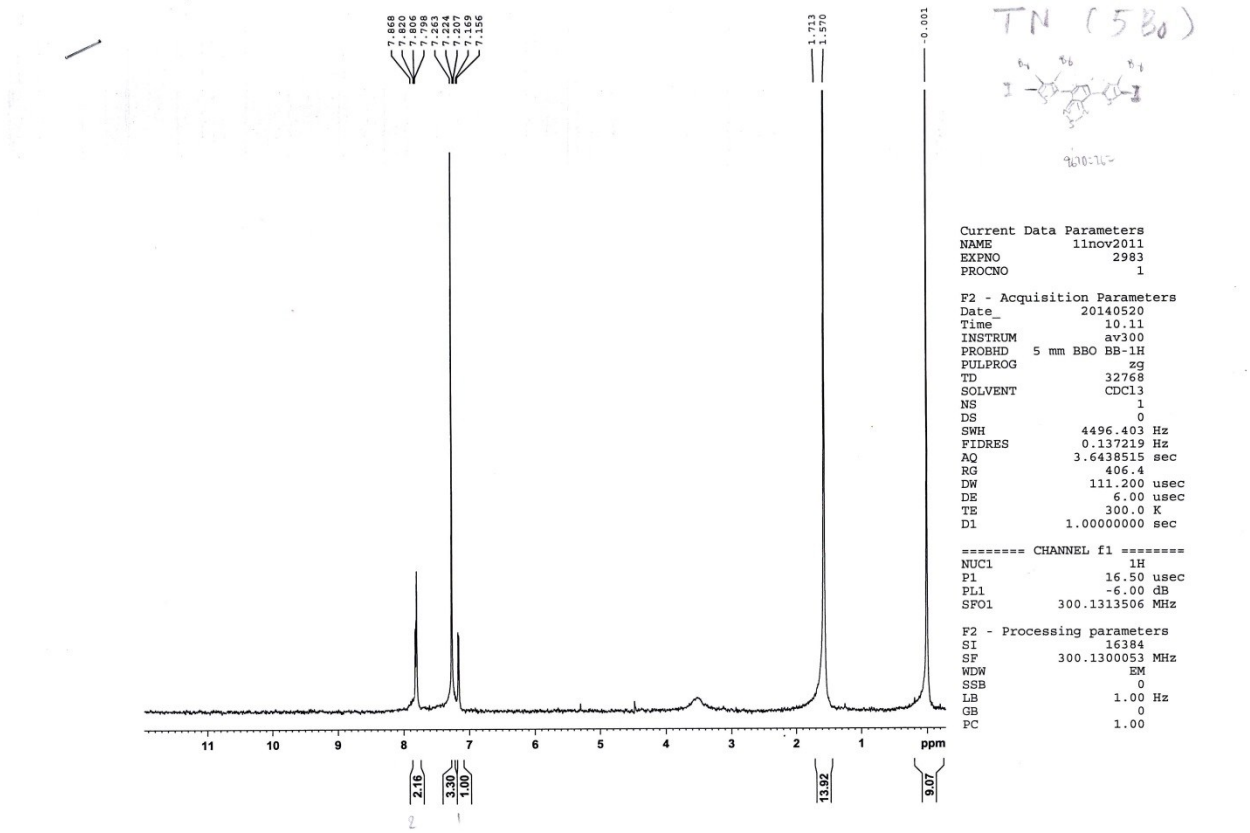
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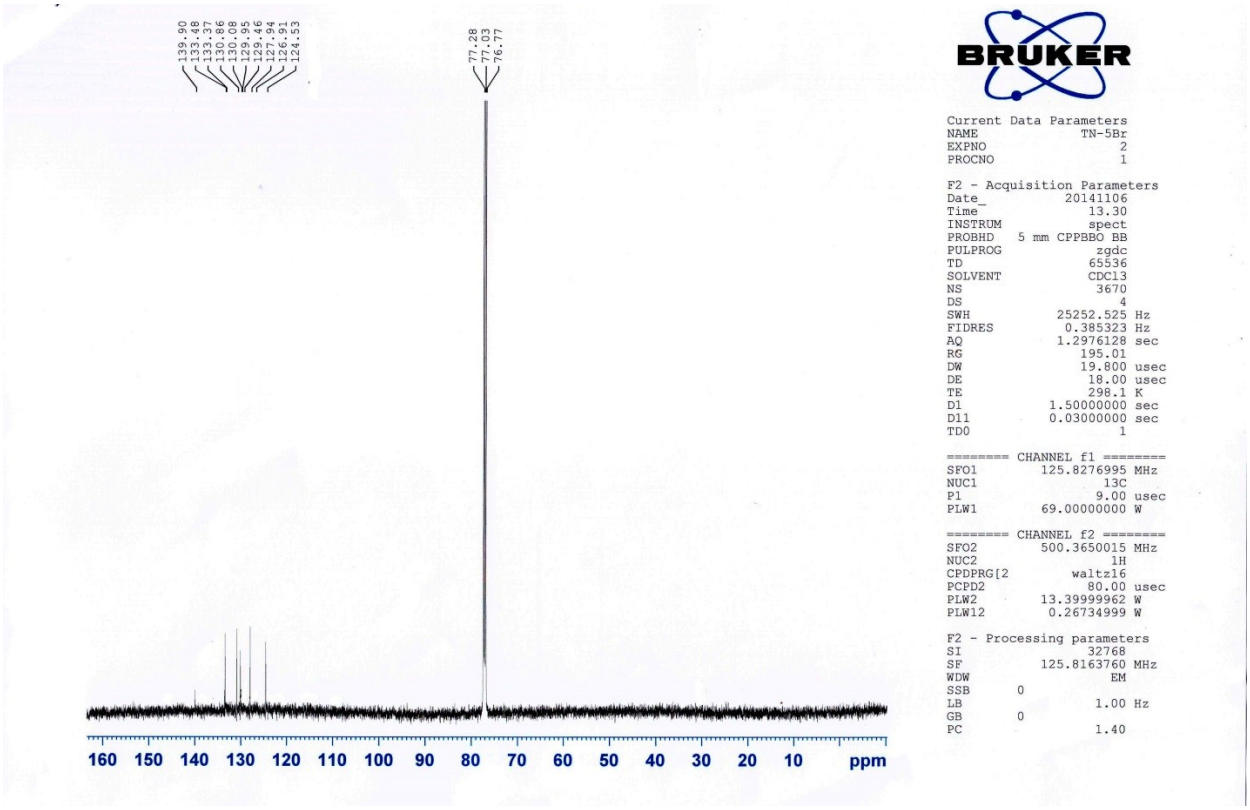
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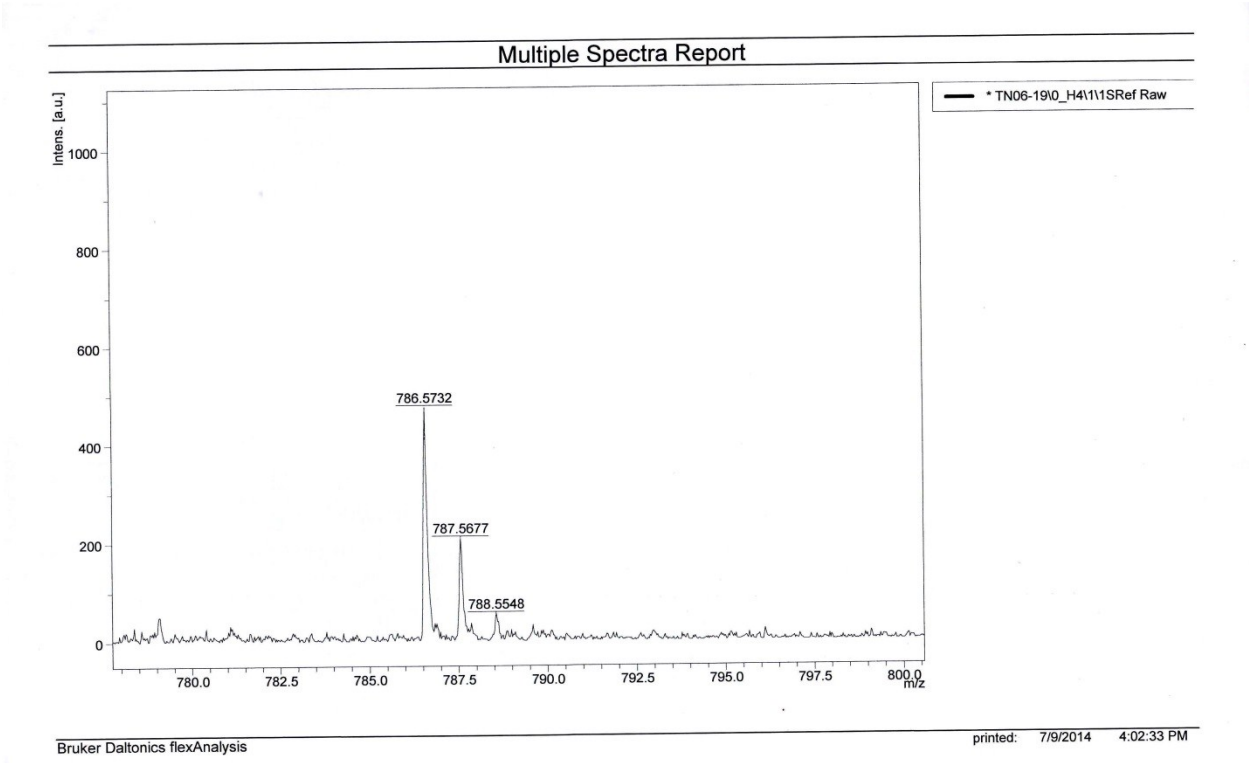
Compound 3



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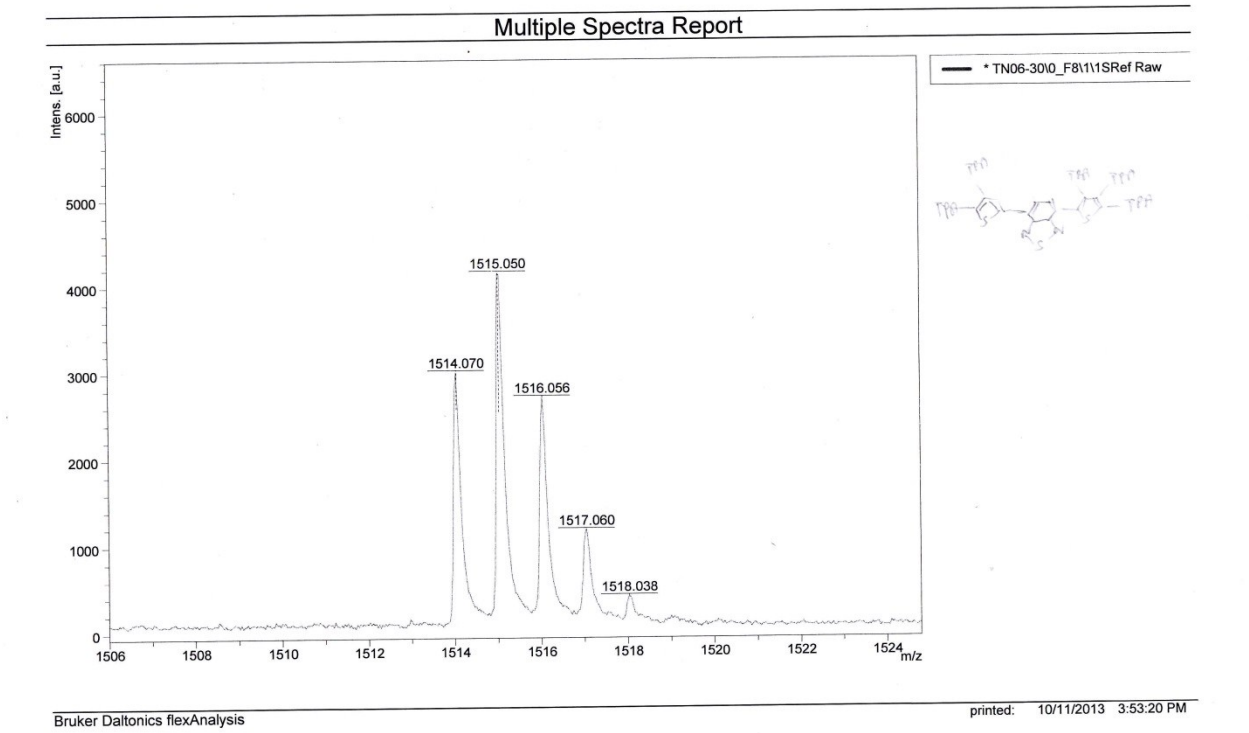

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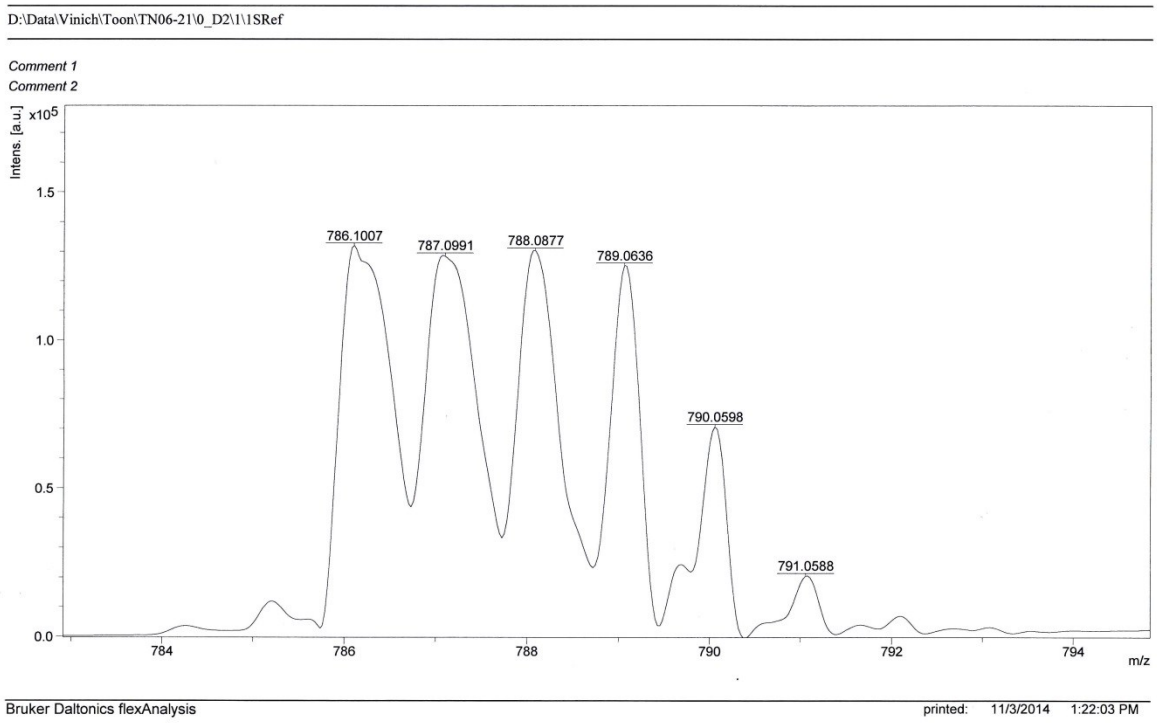
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