

Supporting Information

Bibridged bianchoring metal free dyes based on Phenoxazine and Triphenyl amine as donors for dye sensitized solar cell applications

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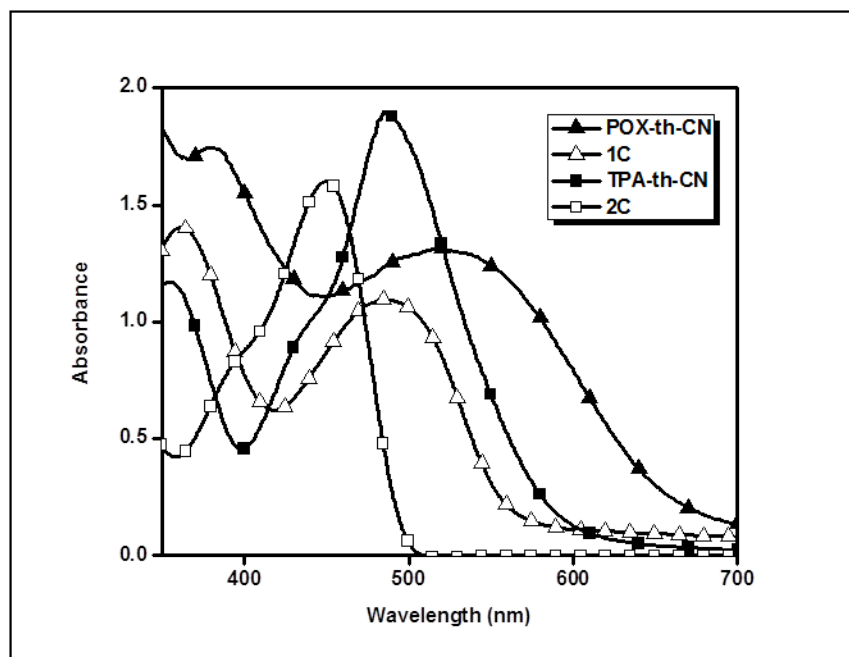


Fig. S1 Absorption spectra of POX-th-CN, TPA-th-CN dyes and their preliminary compounds for conforming ICT property, recorded in DMF (3×10^{-4} M).

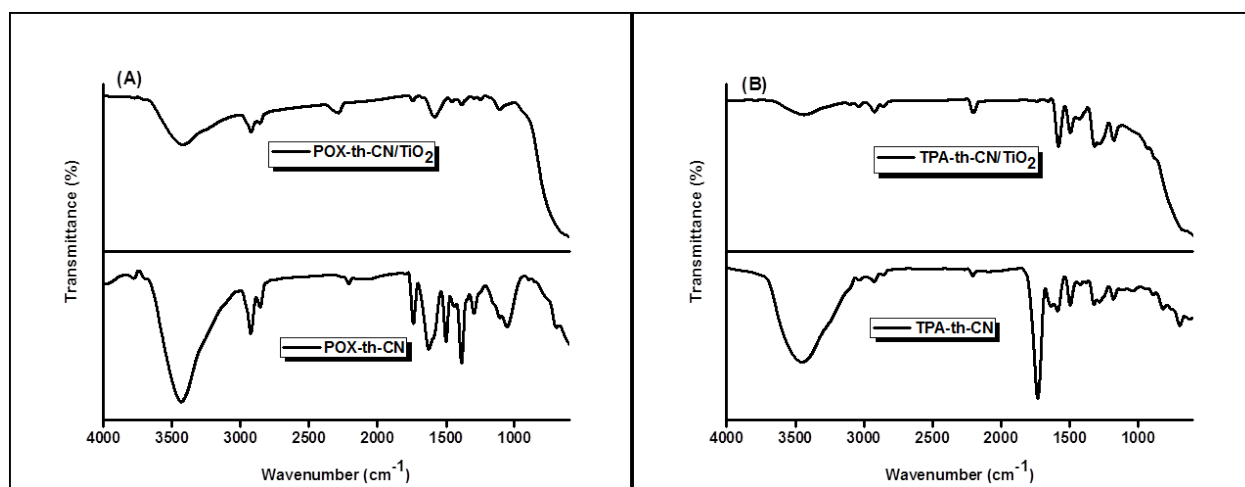


Fig. S2 ATR-FT-IR spectra of neat dyes (bottom) and dye adsorbed TiO_2 films (top): (A) POX-th-CN, (B) TPA-th-CN.

$$E_{\text{HOMO}} \text{ (eV)} = -e [E_{\text{onset}}^{\text{ox}} \text{ V (vs Fc/Fc}^+) + 4.8 \text{ V}] \quad (1)$$

where,

the potential of Fc was measured to be 0.45 V against Ag/AgCl_(aq) electrode.

$$E_{\text{HOMO}} \text{ (eV) (POX-th-CN)} = -e [(0.79-0.45) \text{ V} + 4.8 \text{ V}]$$

$$E_{\text{HOMO}} \text{ (eV) (POX-th-CN)} = -5.14 \text{ eV}$$

$$E_{\text{HOMO}} \text{ (eV) (TPA-th-CN)} = -e [(1.10-0.45) \text{ V} + 4.8 \text{ V}]$$

$$E_{\text{HOMO}} \text{ (eV) (TPA-th-CN)} = -5.45 \text{ eV}$$

$$E_{\text{LUMO}} \text{ (eV)} = E_{0-0} \text{ (eV)} + E_{\text{HOMO}} \text{ (eV)} \quad (2)$$

where,

E_{0-0} is the intersection between the absorption and emission spectra of the sensitizers.

$$E_{\text{LUMO}} \text{ (eV) (POX-th-CN)} = 2.03 \text{ (eV)} - 5.14 \text{ (eV)}$$

$$E_{\text{LUMO}} \text{ (eV) (POX-th-CN)} = -3.11 \text{ (eV)}$$

$$E_{\text{LUMO}} \text{ (eV) (TPA-th-CN)} = 2.19 \text{ (eV)} - 5.45 \text{ (eV)}$$

$$E_{\text{LUMO}} \text{ (eV) (TPA-th-CN)} = -3.26 \text{ (eV)}$$

Cartesian Coordinates of (2E,2'E)-3,3'-(5,5'-(1E,1'E)-2,2'-(10-hexyl-10H-phenoxazine-3,7-diyl)bis(1-cyanoethene-2,1-diyl)bis(thiophene-5,2-diyl))bis(2-cyanoacrylic acid) (POX-th-CN)

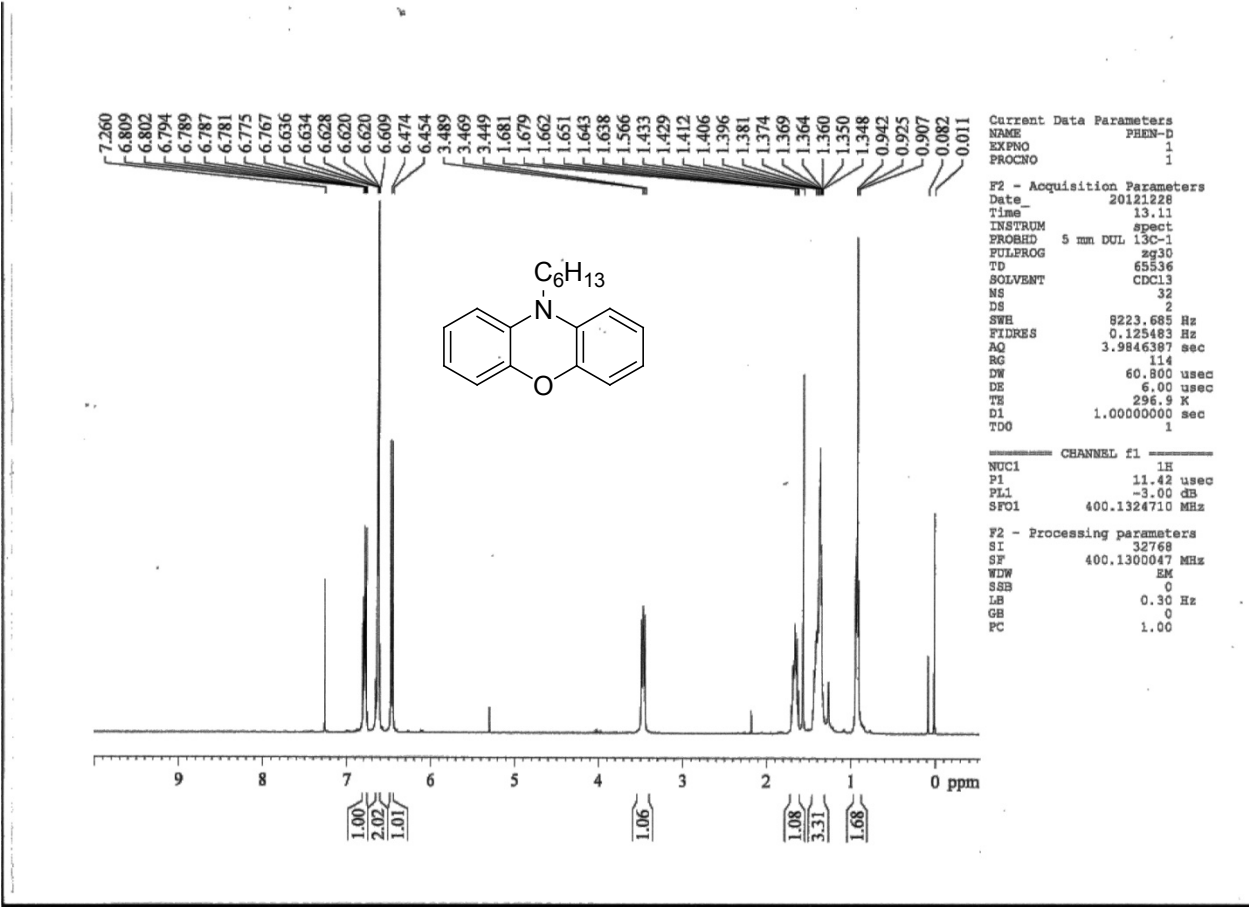
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C	1.13386300	2.51548000	-0.73677200
C	3.55616100	2.29821100	-0.53849200
C	3.46875600	0.89330900	-0.47966700
C	1.04677800	1.10934000	-0.66783500
H	4.51480900	2.79657600	-0.48725200
H	2.03677500	-0.75186300	-0.50240100
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C	-1.27110400	2.62553400	-0.74340000
C	-3.73717400	1.20726400	-0.48924600
C	-2.49593400	3.30836900	-0.67515600
C	-1.31526400	1.21282800	-0.66999700
C	-2.49990300	0.51996800	-0.54490200
C	-3.69329900	2.61369400	-0.55816600
H	-2.52152500	4.39020700	-0.70347200
H	-2.43992100	-0.55952400	-0.50208700
H	-4.62038200	3.17825100	-0.51128700
O	-0.16478600	0.45990800	-0.75386400
C	0.02791600	4.71380800	-1.10331300
H	-0.82695400	4.99385600	-1.72588100
H	0.91485000	4.91705600	-1.71007300
C	0.05406100	5.54812800	0.18656400
H	0.91287000	5.24267400	0.79795300
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H	-0.68087500	10.08951300	2.77541200
H	0.27738700	11.32924700	1.95162900
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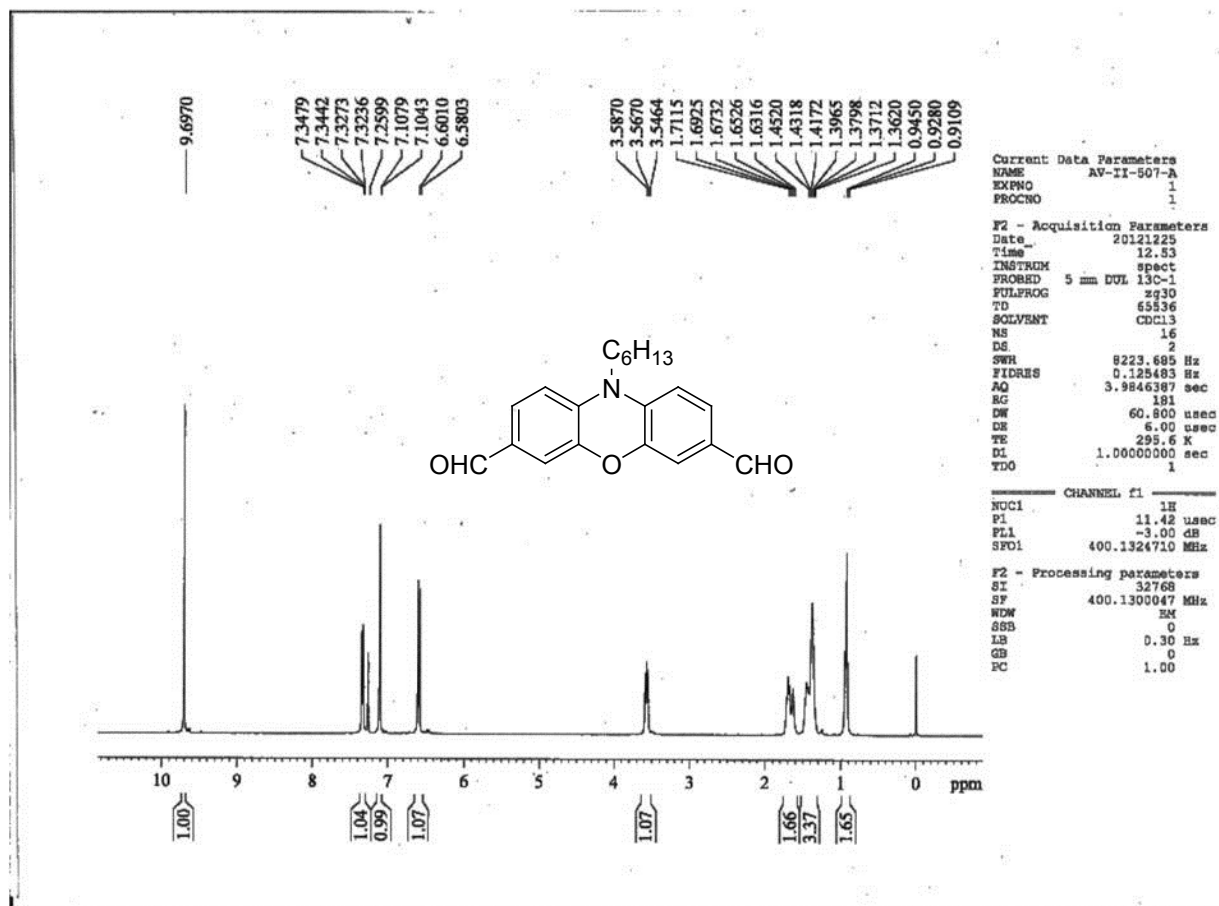
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C	7.77506000	-3.10484100	-0.21690600
C	8.91956000	-2.38863400	0.12508600
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H	7.76811000	-4.17927200	-0.34955400
C	-9.96539100	-3.37229100	0.38508800
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C	-11.33245400	-3.31709600	0.40712900
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C	-12.08094800	-4.59134600	0.68863800
O	-13.43023600	-4.51139900	0.70484500
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O	-11.52195200	-5.64373000	0.89272000
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H	10.98196600	-2.02221300	0.61640600
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C	12.25607800	-4.18106600	0.66870300
O	12.68087500	-5.46326800	0.62797600
H	13.63282800	-5.44122900	0.83877800
O	12.98811800	-3.24655300	0.92676200
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N	9.41432200	-6.17969000	-0.16466900

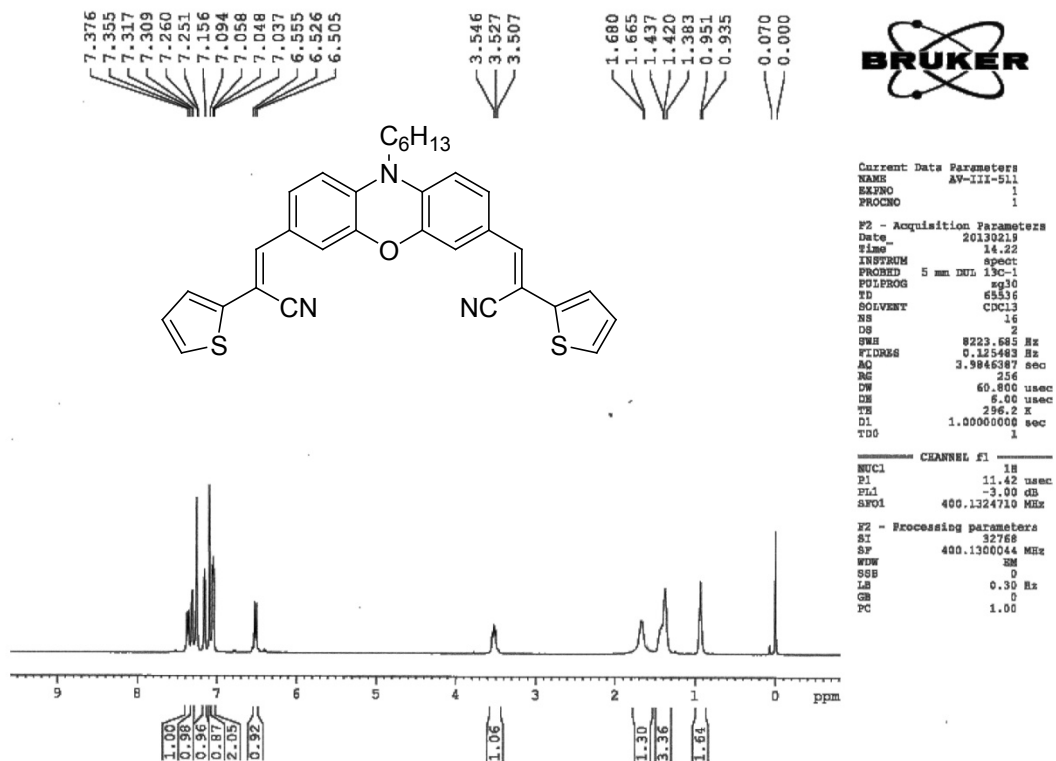
Cartesian Coordinates of (2E,2'E)-3,3'-(5,5'-(1E,1'E)-2,2'-(4,4'-(phenylazanediy)bis(4,1-phenylene))bis(1-cyanoethene-2,1-diyl)bis(thiophene-5,2-diyl))bis(2-cyanoacrylic acid) (TPA-th-CN)

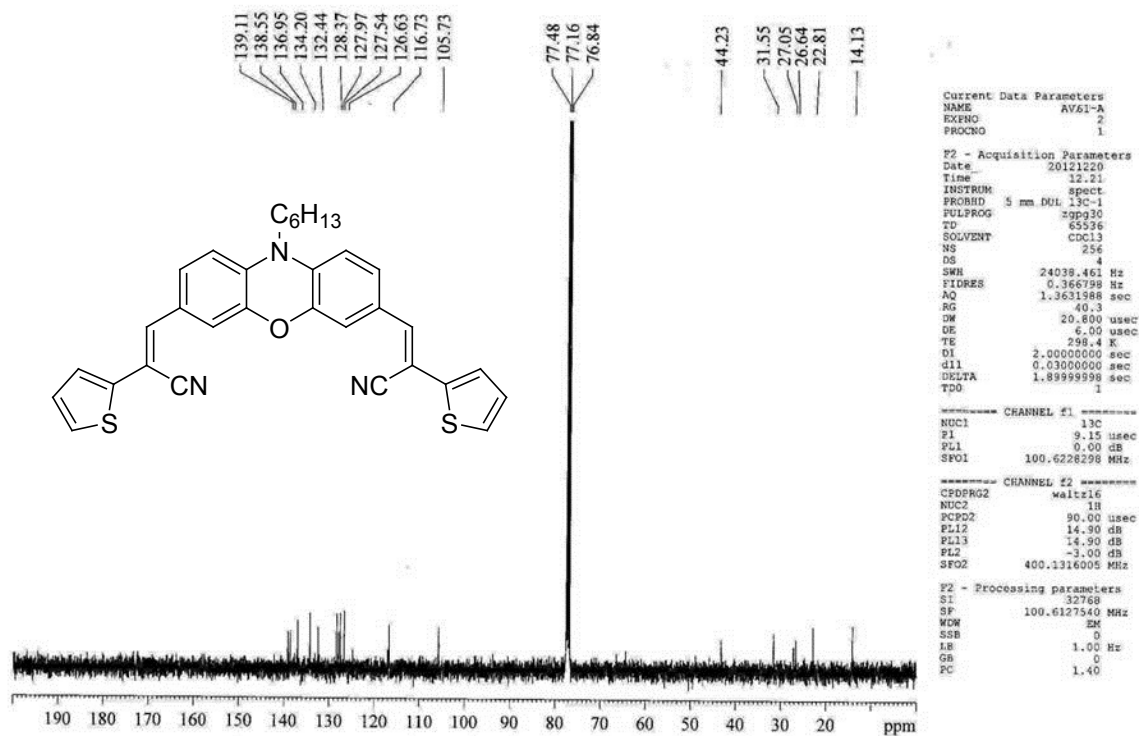
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C	2.33458100	3.24276500	-0.55615800
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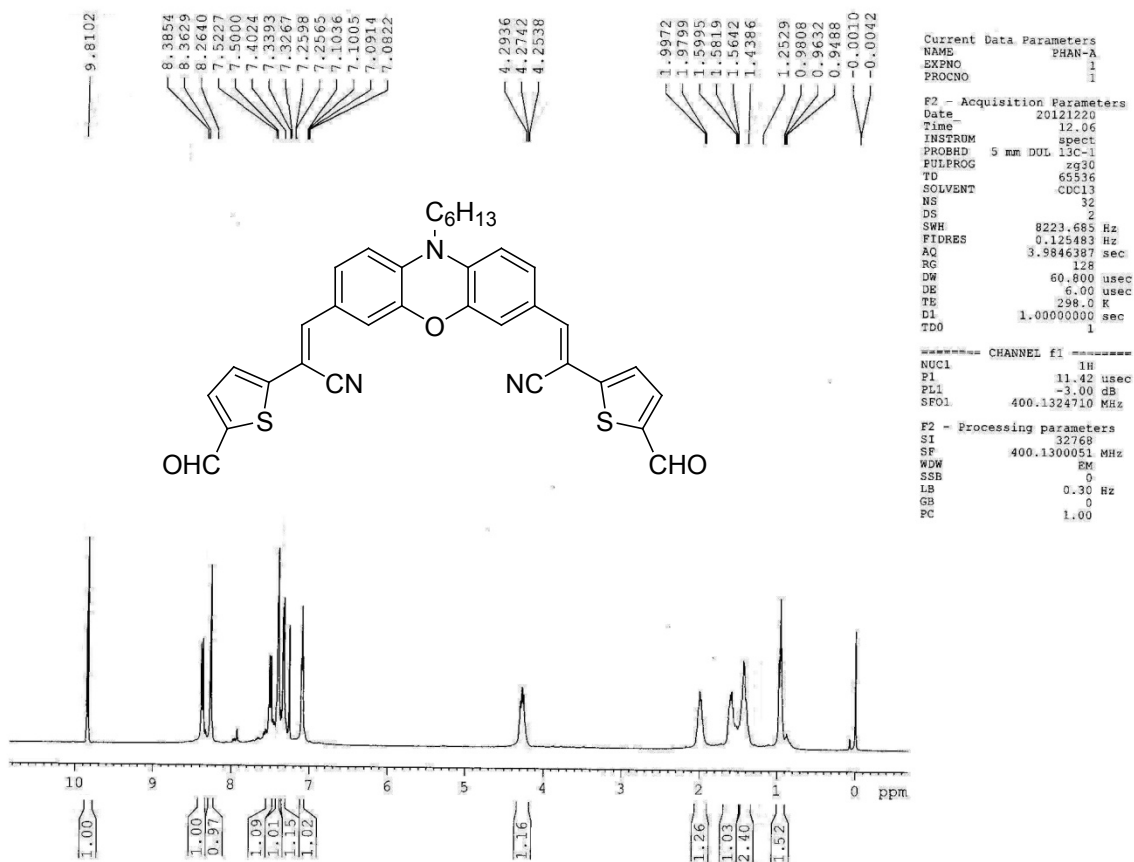
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H	-11.19168400	-0.61576400	-0.14328600
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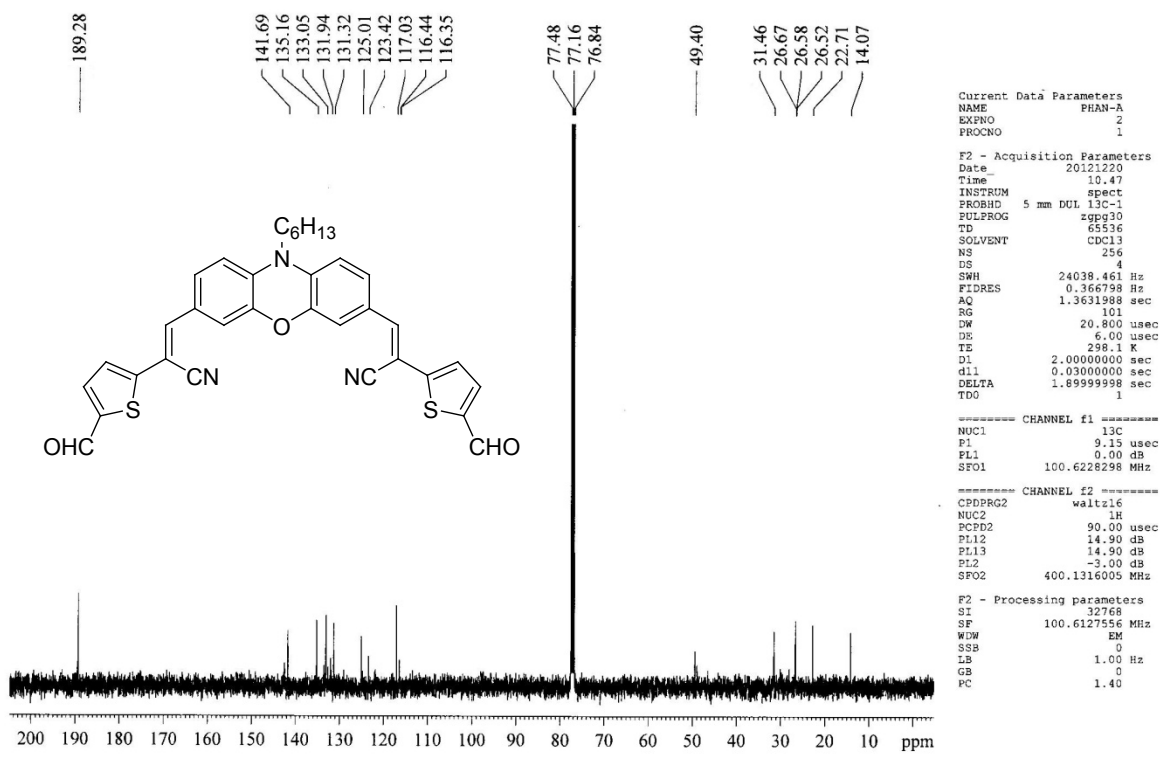


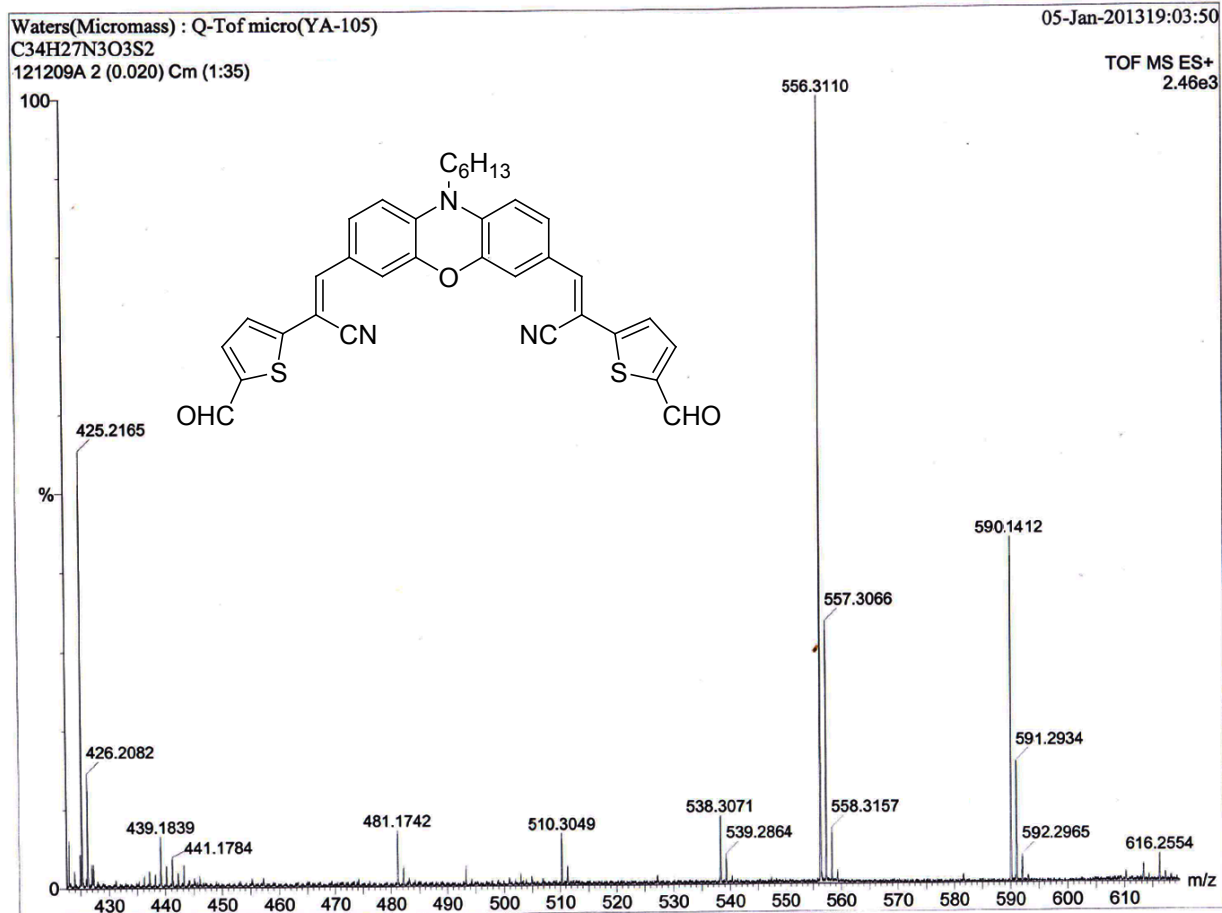


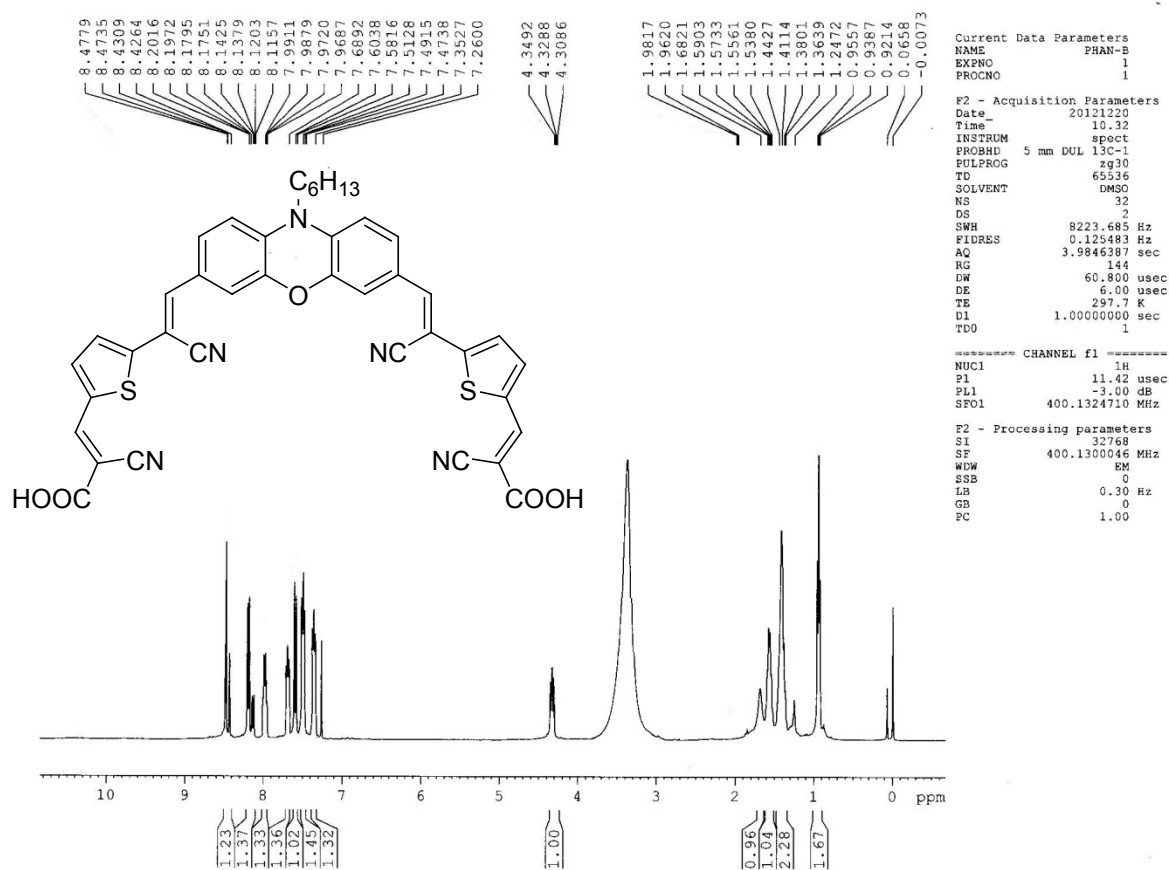


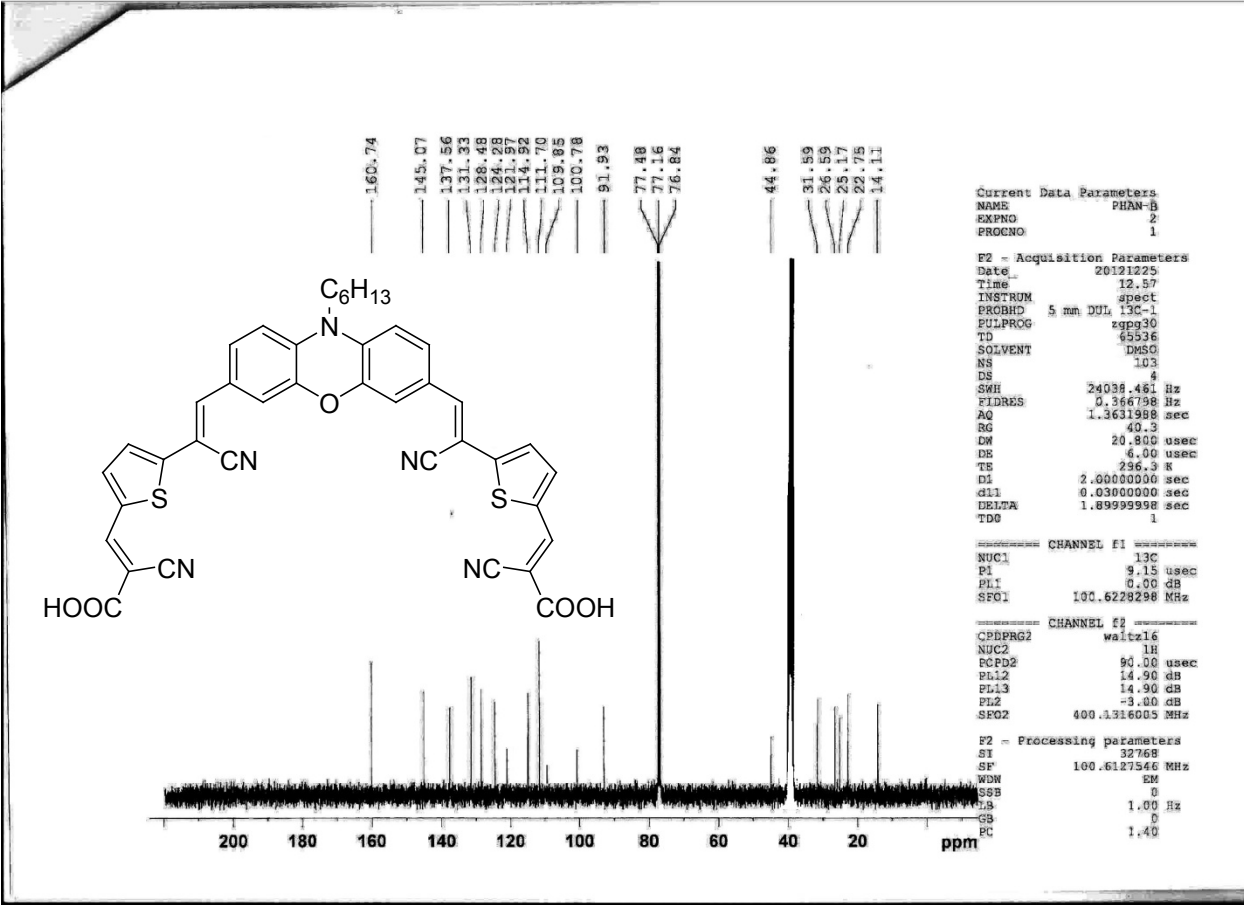












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