# Modulating nonlinear optical properties of TIDC-Cl by varying the terminal units

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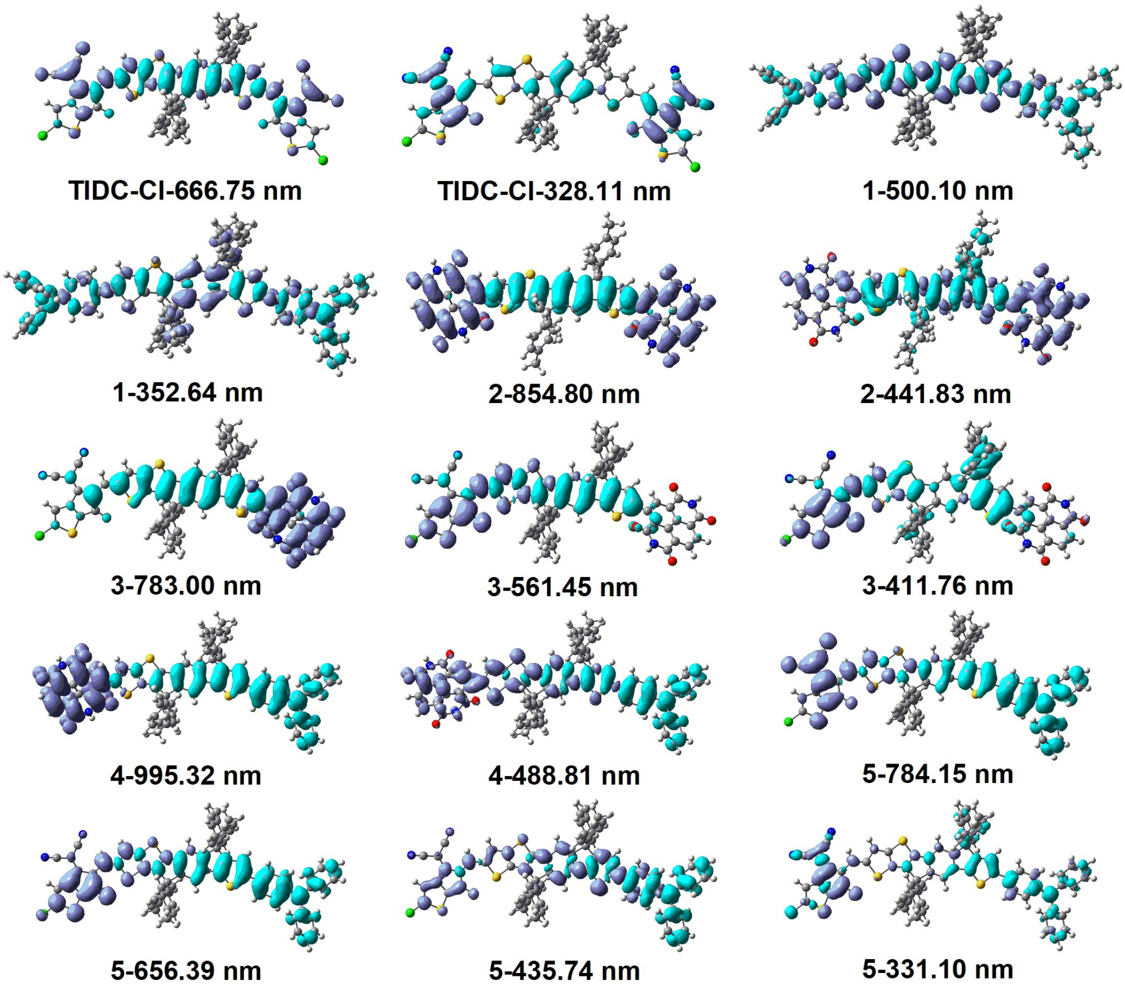

TIDC-Cl-666.75 nm

TIDC-Cl-328.11 nm

1-500.10 nm

1-352.64 nm

2-854.80 nm

2-441.83 nm

3-783.00 nm

3-561.45 nm

3-411.76 nm

4-995.32 nm

4-488.81 nm

5-784.15 nm

5-656.39 nm

5-435.74 nm

5-331.10 nm

**Fig. S1.** Electron density difference maps of the studied molecules. Blue and purple colors represent depletion and accumulation of electron density, respectively.

**Table S1**. The computed absorption peak (*λ*, nm) using the different functionals at 6-31G**(**d,p**)** basis set level for TIDC-Cl along with the experimental value. The data in parentheses is the oscillator strength corresponding to the main electronic transition.

| Functional | B3LYP | CAM-B3LYP | M062X | BH&HLYP | wB97XD | Exp |
|---|---|---|---|---|---|---|
| $\lambda_1$ | 666.75(1.994) | 537.14(2.940) | 541.09(2.905) | 545.46(2.978) | 519.51(3.000) | 643 |
| $\lambda_2$ | 567.23(0.726) | 402.53(0.184) | 401.49(0.183) | 400.24(0.198) | 393.46(0.164) | 597 |
| $\lambda_3$ | 328.11(0.414) | 290.13(0.427) | 295.81(0.333) | 297.20(0.487) | 316.32(0.495) | 335 |

**Table S2.** The calculated isotropic polarizability $\alpha_{iso}$ values (×$10^{-23}$ esu) in the zero-frequency limit and frequency-dependent case ($\lambda$ = 1907, 1460, 1340, and 1180 nm) of the studied derivatives at CAM-B3LYP/6-31+G(d) level.

| Derivatives | $\alpha_{iso,\infty}$ | $\alpha_{iso,1907}$ | $\alpha_{iso,1460}$ | $\alpha_{iso,1340}$ | $\alpha_{iso,1180}$ |
|---|---|---|---|---|---|
| TIDC-Cl | 19.0 | 19.5 | 19.9 | 20.1 | 20.5 |
| 1 | 17.8 | 18.1 | 18.2 | 18.3 | 18.5 |
| 2 | 17.2 | 17.5 | 17.8 | 17.9 | 18.1 |
| 3 | 18.2 | 18.6 | 18.9 | 19.1 | 19.4 |
| 4 | 17.8 | 18.1 | 18.3 | 18.4 | 18.7 |

| | | | | | |
|---|---|---|---|---|---|
| 5 | 18.3 | 19.3 | 19.6 | 19.7 | 20.1 |

**Table S3.** The calculated $\beta_{HRS}$ values ($\times10^{-30}$ esu) in the zero-frequency limit and frequency-dependent case ($\lambda$ = 1907, 1460, 1340, and 1180 nm) of the studied derivatives at CAM-B3LYP/6-31+G(d) level.

| Derivatives | $\beta_{HRS,\infty}$ | $\beta_{HRS,1907}$ | $\beta_{HRS,1460}$ | $\beta_{HRS,1340}$ | $\beta_{HRS,1180}$ |
|---|---|---|---|---|---|
| TIDC-Cl | 37.6 | 61.7 | 96.0 | 122.8 | 227.9 |
| 1 | 10.5 | 13.1 | 15.6 | 17.1 | 20.5 |
| 2 | 68.6 | 123.6 | 218.0 | 305.8 | 822.0 |
| 3 | 85.9 | 123.1 | 167.2 | 201.4 | 448.3 |
| 4 | 242.2 | 447.4 | 841.0 | 1259.7 | 5197.5 |
| 5 | 300.5 | 493.5 | 780.9 | 1011.6 | 1913.3 |