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Supporting Information

Isomerization of Two-Dimensional Non-Fullerene Electron Acceptor Materials for Developing High-Performance Organic Solar Cells

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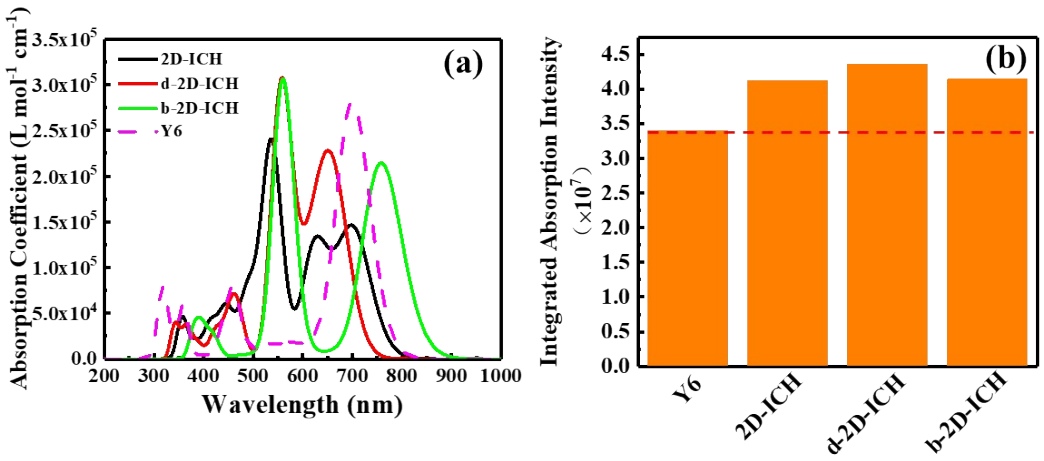

Figure S1. TDDFT calculated absorption spectra (a) and integrated absorption intensity (b) of Y6, **2D-ICH**, **d-2D-ICH** and **b-2D-ICH** in chloroform based on PBE0/def2-SVPD.

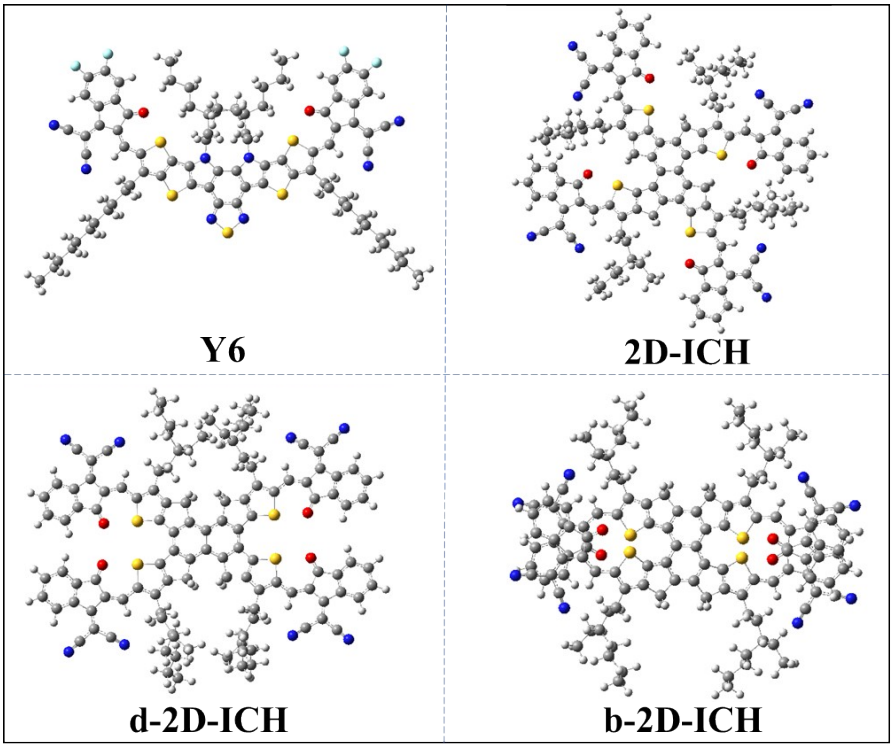

Figure S2. Molecular structures of Y6, 2D-ICH, d-2D-ICH and b-2D-ICH linked with four 4-ethyloctane as side chain.

Table S1. Molecular surface descriptors (Area, σ^2_+ and σ^2_-) of Y6, 2D-ICH, d-2D-ICH and b-2D-ICH used to predict the solubility.

	Area ($Å^2$)	**σ^2_+ (kcal/mol)2**	**σ^2_- (kcal/mol)2**
Y6	1436.10	31.35	60.39
2D-ICH	1722.35	34.60	73.27
d-2D-ICH	1764.93	51.85	87.21
b-2D-ICH	1618.45	47.55	79.39