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Supporting Information

High Efficiently Halogen-Free Solvent Processed Small-Molecule Organic Solar Cells Enabled by Material Design and Device Engineering

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1. Materials and Characterization

2-Tributylstannyl-3,4'''-dioctylterthienyl (1), 4,9-dibromonaphtho[1,2-c:5,6-c']bis[1,2,5]thiadiazole
(2), 2,6-bis(tributyltin)-4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene (6a),
(4,8-bis(5-((2-ethylhexyl)thio)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene-2,6-

diyl)bis(trimethylstannane) (**6b**) were synthesized according to previously reportedprocedures.¹⁻⁴ PC₇₁BM was purchased from Solenne BV (Netherlands) with 99% purity. All the other chemicals were purchased as reagent grade from Aladdin, Adamas, Sigma-Aldrich, and Alfa Asear Chemical Co., and used without further purification. All solvents were freshly distilled immediately prior to use.

¹H and ¹³C NMR spectra were recorded on a Bruker Avance-400 spectrometer with d-chloroform (CDCl₃) as the solvent and tetramethylsilane (TMS) as an internal standard. The molecular mass was confirmed by using an Autoflex III matrix-assisted laser desorption ionization mass spectrometer (MADI-TOF-MS). The elemental analysis was performed on a Thermo Electron SPA Flash EA 1112 series analyzer. Thermogravimetric analysis (TGA) was conducted on a TA Instrument Model SDT Q500 and differential scanning calorimetry (DSC) was conducted on a Netzsch Instrument Model DSC200 at a heating rate of 10 °C min⁻¹ and under a N₂ flow rate of 90 mL min⁻¹. UV-vis spectra were obtained on a Hitachi U2910 spectrophotometer. XRD patterns of the polymers were recorded on a Philips X'Pert X-ray diffractometer operated in reflection geometry mode at 30 mA, 40 kV with Cu K α radiation. AFM images were obtained by using a Bruker Inova atomic force microscope in tapping mode. TEM images were obtained by using a ZEISS LIBRA 200 FE transmission electron microscope. Cyclic voltammetry (CV) measurements were carried out on a CHI660

potentiostat/galvanostat electrochemical workstation at a scan rate of 50 mV s⁻¹ according to our previously reported methods.⁵

2. Synthesis of the Small Molecules

2.1. Synthetic routes of the small molecules



Scheme S1. Synthetic routes of the small molecules.

2.2. Detail Synthetic procedures

Compound 3: Compound **1** (0.76 g, 1 mmol) and compound **2** (0.1 g, 0.25 mmol) were added into 30 mL of toluene in a flask. The reaction mixture was degassed twice with argon. After that, the catalyst $Pd(PPh_3)_4$ (4.3 mg, 1.5%) was added and the solution was degassed twice again with argon.

The reaction mixture was heated to 110 °C with stirring for 24 hours. After the reaction was finished, the reaction mixture was poured into water (50 mL) and extracted with CH₂Cl₂. The organic layer was washed with water for three times, and then dried over anhydrous MgSO₄. After evaporation of the solvent, the crude product was purified by column chromatography on silica gel using a mixture of CH_2Cl_2 and petroleum ether (3:2, v:v) as eluent to afford compound **3** as ablack solid (0.1 g, 33.78%). ¹H NMR (400 MHz, CDCl₃, δ/ppm): δ 8.99 (s, 2H, *J* = 9.1 Hz, ArH), 8.14(s, 2H, ArH), 7.19-7.23(d, 4H, J = 19.2 Hz, ArH), 7.12(d, 2H, J = 9.1 Hz, ArH), 6.96-6.97 (d, 2H, J = 9.1 Hz, ArH), 2.80-2.89 (t, 8H, CH₂), 1.65-1.81 (m, 8H, CH₂), 1.30(m, 40H, CH₂), 0.89(m, 12H, CH₃). ¹³C NMR (100 MHz, CDCl₃, δ/ppm): δ 147.59, 147.11, 143.45, 136.03, 131.46, 122.92, 121.23, 114.09, 38.25, 34.01, 33.08, 31.62, 29.72, 29.39, 29.37, 29.36, 29.33, 29.05, 26.23, 22.36, 13.78. Anal. Calcd for C₆₆H₈₀N₄S₈: C, 66.76; H, 6.78; N, 4.68; S, 21.59. Found: C, 66.84; H, 6.80; N, 4.72; S, 21.63 Compound 4: A solution of compound 3 (0.10 g, 0.084 mmol) in 25 mL dry 1,2-dichloroethane was cooled to 0 °C, anhydrous DMF (0.0617 g, 0.844 mmol) and POCl₃ (0.128 g, 0.844 mmol) were added dropwise slowly in turn under nitrogen atmosphere. The mixture was stirred at 85 °C for 24 h. After that, the mixture was cooled to room temperature, and 30 mL of saturated NH₄Cl solution was added. The mixture was extracted with CH₂Cl₂ for several times, and the combined organic layers were dried over anhydrous MgSO₄. After the solvent was removed, the crude product was purified by column chromatography on silica gel using a mixture of CH_2Cl_2 and petroleum ether (3:2, v:v) as eluent to afford compound 4 as a black solid (0.04 g, 39.41%). ¹H NMR (400 MHz, CDCl₃, δ/ppm): 9.89 (s, 1H, ArH), 8.98 (s, 1H, ArH), 8.88 (s, 1H, ArH) 8.14 (s, 2H, ArH), 7.17-7.21 (d, 4H, J = 9.1 Hz, ArH), 7.12 (s, 1H, ArH), 6.96-6.98 (d, 2H, J = 28.9 Hz, ArH), 2.79-2.85 (t, 8H, CH₂), 1.64-1.81 (m, 8H, CH₂), 1.30 (m, 40H, CH₂), 0.89 (m, 12H, CH₃). ¹³C NMR (100 MHz, CDCl₃, δ/ppm):

181.75, 147.71, 147.24, 143.58, 136.16, 131.60, 123.08, 121.39, 114.26, 38.55, 34.32, 33.38, 31.92,
30.03, 29.70, 29.68, 29.67, 29.64, 29.36, 26.55, 22.69, 14.11. Calcd for C₆₇H₈₀N₄OS₈: C, 66.29; H,
6.65; N, 4.57; O, 1.33; S, 21.09. Found: C, 66.29; H, 6.64; N, 4.62; O, 1.32; S, 21.13.

Compound 5: N-bromosuccinimide (NBS, 0.016 g, 0.0902 mmol) was added in small portions to a solution of compound **4** (0.1 g, 0.082 mmol) in chloroform and acetic acid (100 mL, 1:1, v/v) at 0 °C. After being stirred for 4 h at room temperature, the reaction mixture was poured into water (100 ml) and extracted with CH₂Cl₂. The organic layer was washed in turn with water, aqueous sodium bicarbonate, brine and water, and then dried over anhydrous MgSO₄. After the solvent was removed, the crude product was purified by column chromatography on silica gel using a mixture of CH₂Cl₂ and petroleum ether (1:1, v:v) as eluent to afford compound **5** as a black solid. (0.072 g, 68%). ¹H NMR (400 MHz, CDCl₃, δ /ppm): 9.92 (s, 1H, ArH), 9.00 (s, 1H, ArH), 8.92 (s, 1H, ArH) 8.18 (s, 2H, ArH), 7.23-7.24 (d, 4H, *J* = 9.1 Hz, ArH), 6.95-6.97 (d, 2H, *J* = 16.8 Hz, ArH), 2.80-2.86 (t, 8H, CH₂), 1.65-1.82 (m, 8H, CH₂), 1.30 (m, 40H, CH₂), 0.88 (m, 12H, CH₃). ¹³C NMR (100 MHz, CDCl₃, δ /ppm): 181.75, 147.71, 147.23, 143.58, 136.16, 131.60, 123.08, 121.39, 114.26, 38.55, 34.32, 33.38, 31.92, 30.03, 29.70, 29.67, 29.64, 29.36, 26.55, 22.68, 14.11. Anal. Calcd for C₆₇H₇₉BrN₄OS₈: C, 62.23; H, 6.19; Br, 6.21; N, 4.32; O, 1.28; S, 19.89. Found: C, 62.25; H, 6.16; Br, 6.18; N, 4.33; O, 1.24; S, 19.84.

Compound 7a: A mixture of compound **5** (0.3 g, 0.2325 mmol) and compound **6a** (0.12 g, 0.1056 mmol) in dry toluene (30 mL) was degassed twice with argon followed by the addition of $Pd(PPh_3)_4$ (1.83 mg, 1.5%). After being stirred at 100 °C for 24 h under argon, the reaction mixture was poured into water (50 mL) and extracted with CH_2Cl_2 . The organic layer was washed with water for three times, and then dried over anhydrous MgSO₄. After evaporation of the solvent, the crude product

was purified by column chromatography on silica gel using a mixture of CH₂Cl₂ and petroleum ether (3:1, v:v) as eluent to afford compound **7a** as a black solid (0.15 g, 48.83%). ¹H NMR (400 MHz, CDCl₃, δ /ppm): 9.90 (s, 2H, ArH), 8.5-8.73 (s, 4H, ArH), 8.14 (s, 4H, ArH), 7.89 (s, 4H, ArH), 7.39-7.58 (d, 4H, *J* = 16.8 Hz, ArH), 6.87-7.12 (d, 8H, *J* =19.4 Hz, ArH), 6.48-6.49 (d, 2H, *J* = 9.1 Hz, ArH), 3.0 (t, 16H, CH₂), 2.79 (d, 4H, CH₂), 1.63 (m, 18H, CH₂), 1.30 (m, 96H, CH₂), 0.88 (m, 36H, CH₃). ¹³C NMR (100 MHz, CDCl₃, δ /ppm): 190.75, 162.21, 161.43, 160.21, 159.43, 158.87, 155.10, 154.30, 149.69, 147.55, 145.98, 145.46, 145.32, 143.60, 141.71, 140.04, 135.81, 134.97, 133.29, 132.32, 132.15, 130.96, 130.26, 129.49, 127.70, 127.34, 44.18, 42.79, 40.91, 36.97, 36.73, 35.51, 35.33, 35.18, 34.83, 34.17, 34.00, 31.97, 31.67, 30.96, 30.64, 30.44, 28.29, 28.03, 27.45, 24.86, 24.78, 24.76, 24.63, 24.37, 24.25, 15.37, 15.33, 15.22, 15.20, 15.16, 11.85. Anal. Calcd for C₁₆₈H₁₉₈N₈O₂S₂₀: 67.18; H, 6.66; N, 3.71; O, 1.05; S, 21.28. Found: C, 67.20; H, 6.65; N, 3.73; O, 1.07; S, 21.36.

Compound 7b: Compound **7b** was synthesized as a black solid similar to the synthetic procedure of compound **7a** with a yield of 46.65%. ¹H NMR (400 MHz, CDCl₃, δ/ppm): 9.99 (s, 2H, ArH), 8.82 (s, 4H, ArH), 8.65 (s, 4H, ArH), 8.22 (s, 4H, ArH), 7.97-7.66 (d, 4H, *J* = 9.1 Hz ArH), 6.94-7.19 (d, 8H, *J* = 9.1 Hz, ArH), 6.54-6.71 (d, 2H, *J* = 19.4 Hz, ArH), 3.06 (d, 4H, *J* = 9.1 Hz, CH₂), 2.84 (t, 16H, CH₂), 1.83 (m, 18H, CH₂), 1.28 (m, 96H, CH₂), 0.88 (m, 36H, CH₃). ¹³C NMR (100 MHz, CDCl, δ/ppm): δ 181.96, 153.03, 152.29, 151.76, 146.32, 145.57, 140.55, 138.54, 137.05, 136.68, 136.56, 136.43, 134.81, 133.03, 131.45, 128.12, 126.54, 125.62, 125.45, 124.33, 123.67, 122.95, 121.26, 120.92, 41.52, 40.21, 38.44, 34.72, 34.50, 33.35, 33.18, 33.03, 32.71, 32.08, 31.92, 30.01, 29.73, 29.06, 28.76, 28.56, 26.53, 26.29, 25.74, 23.30, 23.23, 23.21, 23.09, 22.84, 22.73. Anal. Calcd

for C₁₆₈H₁₉₈N₈O₂S₂₂: C, 65.73; H, 6.46; N, 3.60; O, 1.05; S, 22.93. Found: C, 65.79; H, 6.51; N, 3.65; O, 1.04; S, 23.00.

BDTTNTTR: Compound 7a (0.15 g, 0.05 mmol) was first dissolved in dry CHCl₃ (25 mL), three drops of piperidine and then 3-ethylrhodanine (0.042 g, 0.5 mmol) were added into above solution. The resulting solution was then refluxed for 24 under argon. After the reaction mixture was cooled to room temperature, it was extracted with CHCl₃ for three times. The combined organic phase was washed with water for three times and dried over anhydrous MgSO₄. After evaporation of the solvent, it was purified by column chromatography on a silica gel column using a mixture of dichloromethane and petroleum ether (3:1, v:v) as eluent to afford BDTTNTTR as a black solid (0.11 g, 71%). ¹H NMR (400 MHz, CDCl₃, δ /ppm): 8.57-8.74 (d, 4H, J = 9.1 Hz, ArH), 8.14 (s, 4H, ArH), 7.89 (s, 4H, ArH), 7.39-7.59 (d, 4H, J = 9.1 Hz, ArH), 7.12 (d, 8H, J = 19.4 Hz, ArH), 6.88, (s, 2H, ArH), 6.48-6.65 (d, 2H, J = 9.1 Hz, ArH), 4.15 (m, 4H, CH₂), 3.00 (t, 16H, CH₂), 2.55 (d, 4H, J = 19.4 Hz), 1.81 (m, 18H), 1.30 (m, 96H), 0.86 (m, 42H). ¹³C NMR (100 MHz, CDCl₃, δ/ppm): 190.74, 152.08, 151.03, 150.88, 144.53, 141.93, 139.58, 137.79, 137.20, 144.88, 144.75, 144.61, 142.89, 141.01, 139.33, 135.80,134.13, 133.15, 132.97, 136.11, 136.01, 135.88, 135.70, 133.04, 131.37, 129.15, 126.98, 125.20, 124.43, 123.30, 122.26, 122.07, 120.52, 40.44, 37.88, 37.63, 34.02, 33.53, 33.42, 32.31, 32.23, 32.06, 31.99, 31.61, 31.00, 30.95, 28.94, 28.78, 28.70, 27.97, 27.84, 27.59, 25.59, 25.31, 24.69, 22.23, 22.13, 21.77, 21.73, 21.68, 13.26, 13.24, 13.21, 13.14, 13.10, 9.94. Anal. Calcd for C₁₇₈H₂₀₈N₁₀O₂S₂₄: C, 65.09; H, 6.34; N, 4.29; O, 0.97; S, 23.35. Found: C, 65.00; H, 6.37; N, 4.26; O, 0.97; S, 23.40. MALDI-TOF-MS: [M+1]+: Calcd: 3284.978. Found: 3284.968 BDTSTNTTR: BDTSTNTTR was synthesized as a red solid similar to the synthetic procedure of **BDTTNTTR** with a yield of 70.24%. ¹H NMR (400 MHz, CDCl₃, δ /ppm): 8.59-8.77 (d, 4H, J = 9.1

Hz ArH), 8.16 (s, 4H, ArH), 7.91 (s, 4H, ArH), 7.40-7.60 (d, 4H, J = 9.1 Hz, ArH), 7.13 (d, 8H, J = 19.4 Hz, ArH), 6.88 (s, 2H, ArH), 6.48-6.67 (d, 2H, J = 9.1 Hz, ArH), 4.15 (m, 4H, CH₂), 3.06 (d, 4H, J = 19.4 Hz, CH₂), 2.83 (t, 16H, CH₂), 1.80 (m, 18H, CH₂), 1.31 (m, 96H, CH₂), 0.89 (m, 42H, CH₃). ¹³C NMR (100 MHz, CDCl₃, δ /ppm): 191.75, 166.77, 152.87, 151.62, 151.48, 149.59, 145.17, 144.71, 139.99, 137.88, 137.03, 136.45, 136.15, 136.09, 134.63, 134.54, 133.04, 130.72, 128.23, 125.86, 125.28, 125.10, 123.87, 123.54, 122.59, 122.40, 122.12, 120.71, 120.36, 119.93, 41.53, 39.87, 39.73, 38.02, 34.94, 34.54, 33.65, 33.36, 33.07, 32.80, 32.21, 31.95, 30.15, 29.81, 29.13, 14.16, 14.12, 12.31, 11.07. Anal. Calcd for C₁₇₈H₂₀₈N₁₀O₂S₂₆: C, 63.59; H, 6.23; N, 4.15; O, 0.96; S, 24.96. Found: C, 63.76; H, 6.25; N, 4.18; O, 0.95; S, 24.86. MALDI-TOF-MS: [M+1]⁺: Calcd: 3348.922. Found: 3348.892.

3. Device Fabrication and Characterization

The device structure is ITO/CuSCN/SM:PC₇₁BM/ZrAcac/Al. A glass substrate with a pre-patterned ITO (sheet resistance = 15Ω sq⁻¹) was sequentially ultrasonicated in detergent, deionized water, acetone, and isopropanol, and then UV-cleaned in a UV-Ozone chamber for 20 min. The CuSCN solution (6 mg mL⁻¹ in ethyl sulfide) was spin-coated onto the surface of the ITO substrate at a rate of 5000 rpm for 30 s, and then baked on a hot plate at 100 °C for 10 min to form a thin anode buffer layer of about 30 nm. A blend films of **BDTTNTTR**:PC₇₁BM and **BDTSTNTTR**:PC₇₁BM (1:1, w/w) were prepared by spin-coating their CF or CS₂ solutions (adding 0.4 wt% of PDMS) at 2000 rpm for 60 s, and the total concentration was controlled at 12 mg mL⁻¹. The ZrAcac solution (1.0 mg mL⁻¹) was subsequently spin-coated on the top surface of the blend to form a thin electron

transporting layer (10 nm). Al layer (100 nm) was deposited finally in a high vacuum chamber (~10⁻⁶ mbar). Hole- and electron-only devices were fabricated similar to the typical fabrication conditions of **SM-OSCs** with the architectures ITO/PEDOT:PSS/SM:PC71BM/MoO3/Au of and Al/SM:PC₇₁BM/Al, respectively. The thickness of the each layer was screened by using a Dektak 6 M surface profilometer. The device area was fixed at 4.0 mm². The J-V characterization of the devices was carried out on a computer-controlled Keithley 2400 source meter with an Air Mass 1.5 Global (AM 1.5 G) solar simulator (XES-70S1, SAN EI Co., Ltd.) as the light source with an irradiation intensity of 100 mW cm⁻², which was calibrated by using a standard silicon solar cell. The EQE values were tested with a Newport Model 77890 (Newport Co. Ltd.) during the illumination with a monochromatic light from a xenon lamp. All fabrication and characterization processes, except for the EQE measurements, were conducted in a glove box filled with argon atmosphere (< 0.1 ppm O_2 and H_2O).

4. TGA and DSC Measurements



Figure S1. a) Thermogravimetric analysis (TGA) curves of **BDTTNTTR** and **BDTSTNTTR** with a heating rate of 10 °C/min under nitrogen atmosphere. b) Differential scanning calorimetry (DSC) curves of **BDTTNTTR** and

BDTSTNTTR with a heating rate of 10 °C/min under nitrogen atmosphere.



5. Cyclic Voltammetry (CV) Measurements

Figure S2. CV curves of BDTTNTTR, BDTSTNTTR and PC71BM with a scan rate of 50 mV s⁻¹.

6. Density Functional Theory (DFT) Studies



Figure S3. Molecular orbital surfaces of the HOMO-1, HOMO, LUMO and LUMO+1 for BDTTNTTR (a) and

7. Performance of the SM-OSCs Fabricated by Using High Boiling Point Solvents

To investigate the boiling point of the solvents effect on the phase separation behavior and the resulting device performance, SM-OSCs were also fabricated by using high boiling point solvents, chlorobenzene (CB) and *o*-dichlorobenzene (DCB). For CB processed devices, the total concentration was controlled at 20 mg mL⁻¹ and which was 28 mg mL⁻¹ for DCB based devices. The spin-coating speed was controlled at 2000 r.p.m for all the devices. The other conditions were similar to those CF and CS₂ processed devices.



Figure S4. J-V curves (a) and EQE cures (b) of the SM-OSCs processed by CB and DCB solvents. **Table S1.** Device parameters of the optimized SM-OSCs under the illumination of AM 1.5G, 100 mW cm⁻².

SMs	Sol.	V _{oc}	J _{sc}	J _{cal} ^a	FF	PCE ^b
		[V]	[mA cm ⁻²]	[mA cm ⁻²]	[%]	[%]
BDTTNTTR	CB	0.88	9.62	9.40	42.0	3.54 (3.21±0.33)
	DCB	0.87	7.80	7.63	35.8	2.43 (2.04±0.39)
BDTSTNTTR	CB	0.92	11.05	10.87	49.2	5.00 (4.75±0.25)
	DCB	0.91	8.97	8.88	41.2	3.36 (3.02±0.34)

^aThe calculated Jsc values were obtained from the EQE measurements. ^bThe average PCE values were obtained from more than 20 devices.

8. Atomic Force Microscopy (AFM) and transmission electron microscopy (TEM) measurements



Figure S5. AFM height images (a, b, c, d) and phase images (e, f, g, h) and TEM images (i, j, k, l) of the active

blend films. **BDTTNTTR:PC**₇₁**BM** film spin-coated from CF solution (a, e, i) and CS₂ solution (b, f, j);

BDTSTNTTR:PC71BM film spin-coated from CF solution (c, g, k) and CS2 solution (d, h, l).

AFM image size: $5 \times 5 \ \mu m^2$.



Figure S6. AFM height images (a, b, c, d) and phase images (e, f, g, h) and TEM images (i, j, k, l) of the active blend films. BDTTNTTR:PC₇₁BM film spin-coated from CB solution (a, e, i) and DCB solution (b, f, j);
BDTSTNTTR:PC₇₁BM film spin-coated from CB solution (c, g, k) and DCB solution (d, h, l).

AFM image size: $5\times5~\mu m^2.$

9. Charge Carrier Mobility Measurements

The carrier mobilities are measured *via* the SCLC method, which is described by $J = 9\varepsilon_0\varepsilon_r\mu V^2/8L^3$, where J is the current density, L is the film thickness of the active layer, μ is the hole or electron mobility, ε_r is the relative dielectric constant of the transport medium, ε_0 is the permittivity of free space (8.85×10⁻¹² F m⁻¹), V is the internal voltage in the device and $V = V_{appl} - V_{bi} - V_a$, where V_{appl} is the applied voltage to the device, V_{bi} is the built-in voltage due to the relative work function difference of the two electrodes and V_a is the voltage drop due to contact resistance and series resistance across the electrodes.



Figure S7. J^{1/2}-V cures of the hole-only devices (a) and electron-only devices (b) for the blend films of

BDTTNTTR:PC71BM and BDTSTNTTR:PC71BM processed with CF or CS2.

10. Summarized Performance Data of the SM-OSCs Reported so far

SMs	Band gap	V_{oc}	J _{sc}	FF	PCE	E_{Loss}	Daf
	[eV]	[V]	[mA cm ⁻²]	[%]	[%]	[eV]	Rei.
DR3TBDT	1.74	0.93	12.21	65.0	7.38	0.81	6
DR3TBDT2T	1.78	0.92	12.09	72.1	8.02	0.86	7
DR3TCz	1.88	0.94	8.02	54	4.08	0.94	8
DR2TDTCz	1.82	0.90	10.34	75	7.03	0.92	8
DR3TDTS	1.66	0.82	13.67	69	8.02	0.84	9
BDTT-S-TR	1.73	0.97	13.45	70.5	9.20	0.76	10
DRCN5	1.60	0.93	15.66	68	10.08	0.67	11
DRBDT-TT	1.78	0.92	13.12	72	8.70	0.86	12
DRBDT-STT	1.80	0.91	12.40	71	8.01	0.87	13
DINI-IND	1.68	0.85	12.18	68	7.04	0.83	13

Table S2. Summarized performance data of the SM-OSCs reported so far

BDT3SCNCOO	1.84	0.89	9.98	72	6.21	0.95	14
BDT3SCNCO	1.76	0.92	10.2	68	6.34	0.84	14
BDT2	1.76	0.90	13.17	73	8.56	0.86	15
BDT3	1.82	0.90	11.34	70	7.14	0.92	15
DCA3T(T-BDT)	1.80	0.95	11.86	70	7.93	0.85	16
BDTTOTR	1.74	0.90	11.03	65.5	6.26	0.84	17
TTH-D3TRh	1.74	0.86	10.26	66.8	5.89	0.88	18
TTF-D3TRh	1.73	0.93	11.03	69.6	7.14	0.80	18
DR3TBDTTF	1.73	0.93	14.1	74.7	9.80	0.80	19
STB-3	1.69	0.928	14.24	70	9.26	0.762	20
BTID-2F	1.68	0.95	15.7	76	11.3	0.73	21
O-BDTdFBT	1.83	0.98	11.48	70	8.10	0.85	22
BDT(dFBT-ON) ₂	1.68	0.86	9.19	65.9	5.55	0.82	23
BDT(dFBT-TT) ₂	1.75	0.95	7.48	49.6	3.54	0.80	23
BIT-4F-T	1.76	0.90	11.9	76	8.1	0.86	24
BIT4FFu	1.85	0.89	11.73	60	6.01	0.96	25
BIT4FSe	1.77	0.87	13.4	72	8.41	0.90	25
IDTTFBT3T	1.69	0.95	12.4	55	6.54	0.74	26
X2	1.41	0.66	15.2	65	6.5	0.75	27
1	1.50	0.78	14.4	59.3	6.7	0.72	28
DTSi(FBTTh ₂) ₂	1.66	0.767	14.3	59.7	6.53	0.893	29
Th6FSe	1.68	0.87	11.78	67	7.17	0.81	30
Se6FTh	1.75	0.87	14.3	72	9.26	0.88	30
DR3TBDD	1.93	0.97	14.59	66	9.53	0.96	31
DPPEZnP-TEH	1.37	0.78	16.76	61.8	8.08	0.59	32
DPPEZnP-TBO	1.37	0.73	19.58	63.38	8.96	0.60	33
NDPPFBT	1.56	0.88	10.71	71.16	7.0	0.68	34

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