Electronic Supplementary Information (ESI)

Transport properties of single-component organic conductors, TED derivatives

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Preparation of materials

General

^{1}H nuclear magnetic resonance (NMR) spectrum for a solution was recorded on AVANCE system (600 MHz) (Bruker Corp.). ESI-TOF-MS was measured with Exactive (Thermo Fisher Scientific K. K.). ESR was measured with FA100 (JEOL Ltd.) NIR/MIR spectrum was measured with FT/IR-6700 adopting InGaAs and DLATGS detectors, respectively (JASCO Corp.). Transport properties were measured with PPMS-9 and MPMS-7 systems (Quantum Design Jpn. Inc). Toluene, DMF, and tetrahydrofuran (THF) (KANTO CHEMICAL), 1,4-dioxane (stabilizer free) (Nacalai tesque Inc.), and MeOH (water free) (WAKO Pure Chemical Industries, Ltd.) were used.

Sample preparation

Preparation of **1**

Precursor of **1** (100.0 mg, 0.17 mmol) was suspended by a mixture of 1,4-dioxane/THF/MeOH/toluene/DMF (4/2/2/2/1) (25 ml), and then 1N LiOH (254 μl) was added to the mixture at 0°C. After vigorously stirring at room temperature for 3 days, the precipitate was separated from the solution by filtration and added CH_3CN (140 ml) and 1N HCl (3 ml) slowly. After vigorously stirring at room temperature for 2 days, the precipitate was collected by filtration using membrane filter, H010A025A (ADVANTEC) and washed with deionized water (4 ml), MeOH (4 ml) and chloroform (8 ml). The resulting polycrystalline solid was dried in vacuo to afford dark brown crystals **1** (74.8 mg, 0.13 mmol, 78 %). ^{1}H NMR (600 MHz, DMSO-d_6): δ 3.40 (m, 4H).

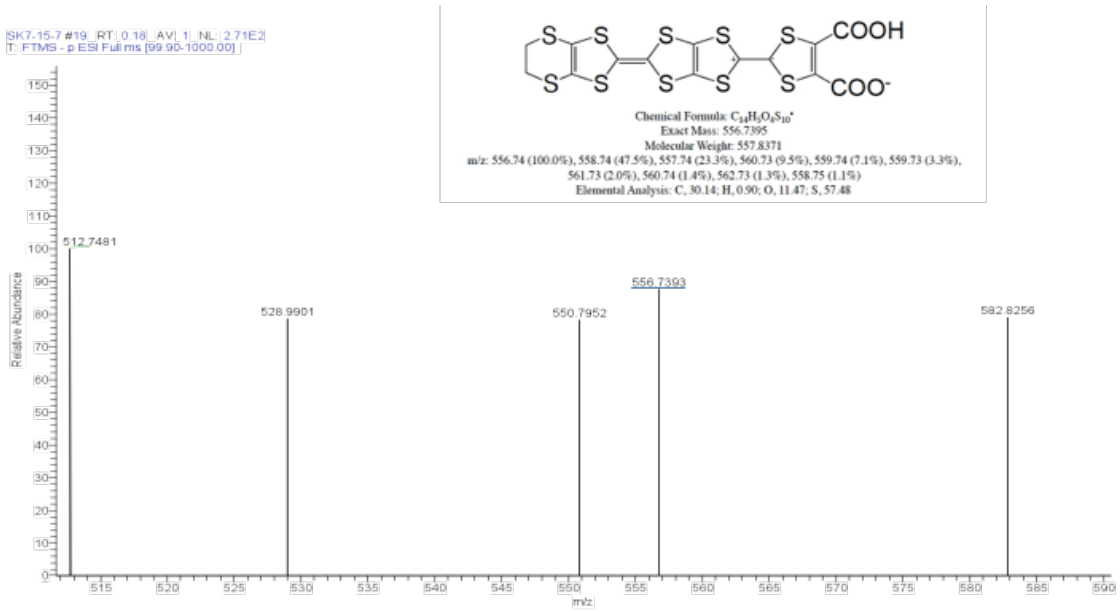

Fig. S1. ESI-TOF-MS spectrum of **1**.

Preparation of **2**

Precursor of **2** (50.0 mg, 0.085 mmol) was suspended by a mixture of 1,4-dioxane/THF/MeOH/toluene/DMF (4/2/2/2/1) (13 ml), and then 1N LiOH (127 μl, 0.25 mmol) was added to the mixture at 0°C. After vigorously stirring at room temperature for 3 days, the precipitate was separated from the solution by filtration and added CH_3CN (83 ml) and 1N HCl (1.7 ml) slowly. After vigorously stirring at room temperature for 2 days, the precipitate was collected by filtration using membrane filter, H010A025A (ADVANTEC) and washed with deionized water (2 ml), MeOH (2 ml) and chloroform (5 ml). The resulting polycrystalline solid was dried in vacuo to afford dark brown crystals **2** (34.5 mg, 0.062 mmol, 78 %). ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.43 (s, 6H).

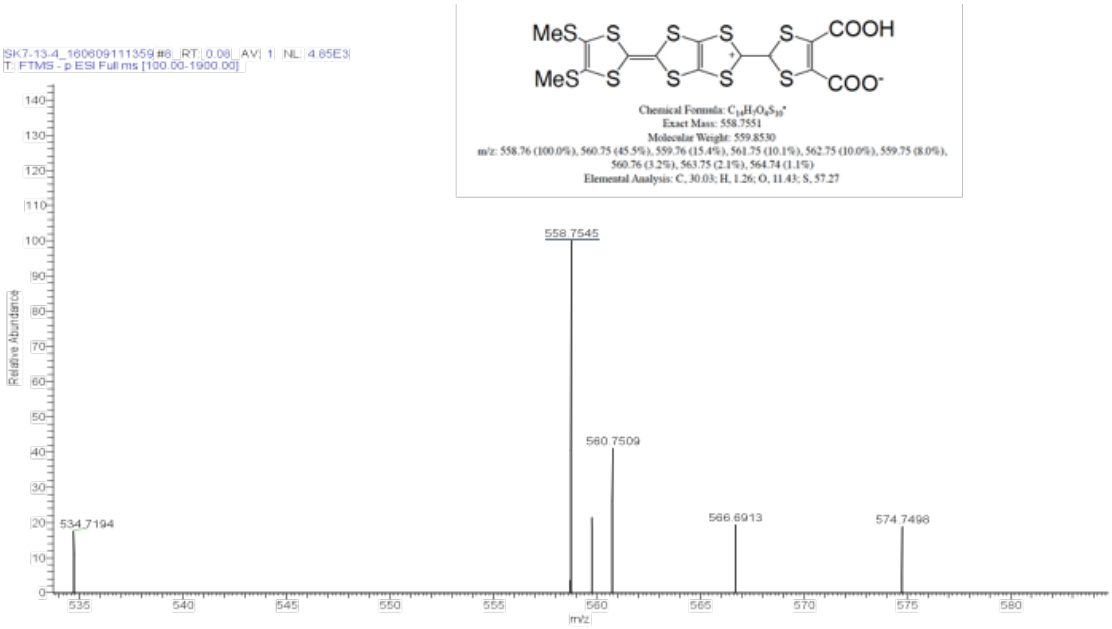

Fig. S2. ESI-TOF-MS spectrum of **2**.

Preparation of **3**

Precursor of **3** (100 mg, 0.31 mmol) was solved in a mixture of 1,4-dioxane /MeOH (2/1) (5 ml), and then 1N LiOH (3.1 ml) was added to the mixture at 0°C. After stirring at room temperature for 45 min, the solution was washed by toluene (10 ml x 2), then 2N HCl (3.2 ml) was added and stirred to afford precipitate for 5min at room temperature. The suspension was cooled to 5°C, and the precipitate was collected by filtration using membrane filter, H010A025A (ADVANTEC) and washed with deionized water (200 μl) and 1,4-dioxane (100 μl). The resulting polycrystalline solid was dried in vacuo to afford dark brown crystals **3** (79.2 mg, 0.27 mmol, 87 %). ^{1}H NMR (600 MHz, DMSO-d_6): δ 6.44 (s, 2H).

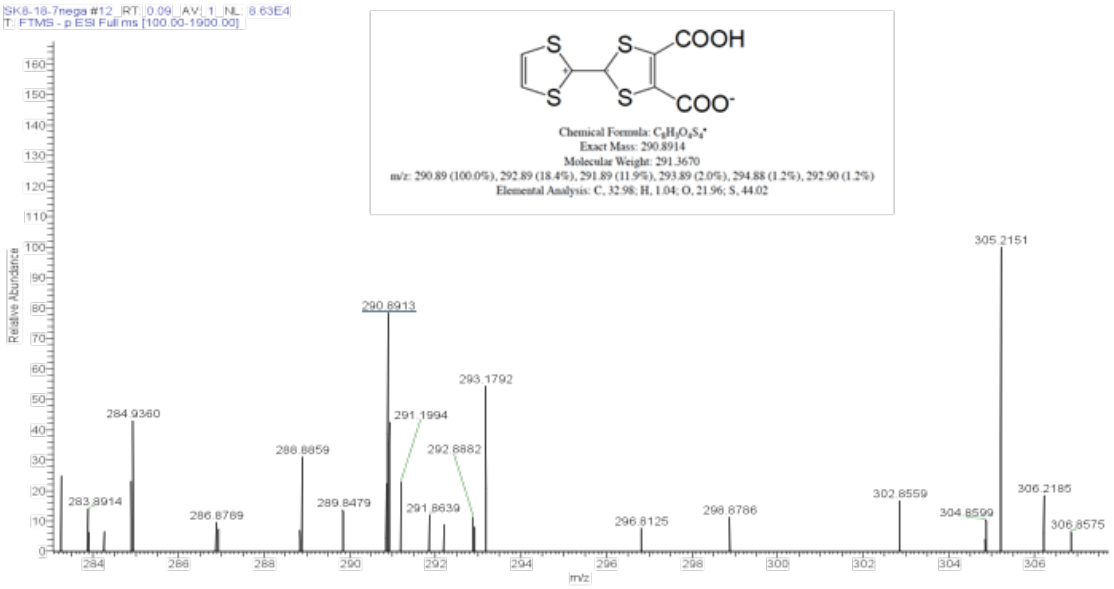

Fig. S3. ESI-TOF-MS spectrum of **3**.