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Supplementary Information

Structural Studies and Photovoltaic Investigation of Indolo[2,3-*b*]quinoxaline-Based Sensitizers/Co-Sensitizers Achieving Highly Efficient DSSCs

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1. Experimental section

1.1. Materials and equipment

The starting materials such as 1*H*-indole-2,3-dione, ethyl iodide, 4-bromobenzene-1,2-diamine, 5-formyl-2-thienylboronic acid, *N*-bromosuccinimide, triphenylamine, carbazole, phenothiazine, hexyl bromide, bis(pinacolato)diboron and cyanoacetic acid were purchased from Sigma-Aldrich, Alfa Aesar, Fisher Scientific or Ark Pharm and used as received. All the solvents and reagents used in the reactions were synthesis grade (Fisher Scientific) and used without further purification. All the reactions were performed under Argon atmosphere and the progress of the reactions was monitored using thin layer chromatography (TLC) technique. The synthesized compounds were purified using recrystallization or column chromatographic methods.

^{1}H NMR spectra were recorded in chloroform-*d* or DMSO-d_6 solvent using a Bruker Avance NEO 600 MHz spectrometer. Splitting patterns reported here are s (singlet), d (doublet), t (triplet), q (quartet), and m (multiplet). The chemical shift (δ) was expressed in ppm with tetramethylsilane (TMS) as an internal standard and coupling constant (*J*) was expressed in Hz. The mass spectrometry analysis was carried out on a high-resolution mass spectrometer, the Thermo Fisher Scientific Exactive Plus MS, a benchtop full-scan OrbitrapTM mass spectrometer using heated electrospray ionization (HESI). Samples were dissolved in the desired solvents (chloroform, methanol, etc.) and sonicated for 15 min. The mass spectrometer was operated in both positive and negative ion modes. Attenuated Total Reflectance-Fourier Transform Infra-Red (ATR/FT-IR) spectra were recorded on a Thermo Nicolet, Nexus 470 FTIR Spectrophotometer with Omnic 7.2 software. The compound under investigation was placed in its powder form on a germanium crystal and a pressure probe was placed in position to apply consistent pressure to the sample. An average of 32 scans was used at a resolution of 4 cm^{-1}.

1.2. UV-Visible and fluorescence spectra

UV-Visible spectra were recorded using a concentration of 2.0×10^{-5} M in dimethylformamide. The spectra were recorded at room temperature in a quartz cell (1.0 cm) on a Cary 3 Spectrophotometer. Fluorescence spectra were measured in a 1 cm path length quartz cell using 2.0×10^{-5} M solutions of dimethylformamide on Fluorolog-311. The emitted light was detected in the steady state mode using a Hamamatsu R2658 detector. The emission was measured in the steady state mode by exciting at the λ_{max} for each dye with exit and entrance slits set at 5 nm at an integration time of 0.2 sec.

1.3. Ground state oxidation potential (GSOP) and excited state oxidation potential (ESOP) measurements

The experimental HOMO and E_{0-0} energy values were calculated using a cyclic voltammetry (CV) and the UV-Vis absorption onset, respectively. The CV was carried in DMF with 0.1 M [TBA][PF_6] as an electrolyte at a scan rate of 50 mV s^{-1}. Glassy carbon was used as the working electrode (WE), Pt wire as counter electrode and Ag/Ag^+ in acetonitrile was used as the reference electrode. Fc/Fc^+ was used as internal reference, voltage measured was converted to NHE by addition of 0.63 V.

1.4. TiO_2 electrode preparation and device fabrication

A double-layer TiO_2 photoelectrode (10 + 5) mm in thickness with a 10 mm thick nanoporous layer and a 5 mm thick scattering layer (area: 0.18 cm^2) were prepared using a reported method [1]. Fluorine-doped tin oxide (FTO) coated glasses (2.2 mm thickness, sheet resistance of 8 Ω/cm^2, TEC 8, Pilkington) were washed with detergent, water, acetone and ethanol, sequentially. After this FTO glass plates were immersed into a 40 mM aqueous $TiCl_4$ solution at 70 °C for 30 min and washed with water and ethanol. Thin layer (8-12 μm thick) of TiO_2 (Solaronix, Ti-Nanoxide T/SP) was deposited on transparent conducting glass by squeegee printing. After drying the electrodes at 350 °C for 10 min and continuously at 500 °C for 30 min, scattering layer (5 μm thick) TiO_2 particles (Solaronix, Ti-Nanoxide R/SP) were printed. The TiO_2 electrodes were heated under an air flow at 350 °C for 10 min, followed by heating at 500 °C for 30 min. After cooling to room temperature, the TiO_2 electrodes were treated with 40 mM aqueous solution of $TiCl_4$ at 70 °C for 30 min and then washed with water and ethanol. The electrodes were heated again at 500 °C for 30 min and left to cool to 80 °C before dipping into the dye solution. The dye solutions were prepared in 1:1:1 acetonitrile, *tert*-butyl alcohol and DMSO. Deoxycholic acid was added to the dye solution as a co-adsorbate at a concentration of 20 mM. The working electrodes were immersed in the dye solutions and then kept at 25 °C in the darkroom for 20 h to adsorb the dye onto the TiO_2 surface. For preparing the counter electrode, pre-cut TCO glasses were washed with water followed by 0.1 M HCl in EtOH, and sonication in acetone bath for 10 min. These washed TCO were then dried at 400 °C for 15 min. Thin layer of Pt-paste (Solaronix, Platisol T/SP) on TCO was printed and the printed electrodes were then cured at 450 °C for 10 min.

Photovoltaic and incident photon-to-current efficiency (IPCE) measurements were launched on sandwich cells, in which TiO_2 coated working electrodes and platinum coated counter electrodes were sealed using a 40 μm Syrlyn spacer through heating of the polymer frame. The redox electrolyte consisted of a solution of 0.6 M DMPII, 0.05 M I_2, 0.1 M LiI and 0.5 M TBP in acetonitrile (Solaronix, Iodolyte HI-30).

1.5. Photovoltaic measurements

Photovoltaic measurements of sealed cells were made by illuminating the cell through the conducting glass from the anode side with a solar simulator (WXS-155S-10) at AM 1.5 illuminations (light intensity: 100 mW cm^{-2}).

1.6. Incident photon to current efficiency (IPCE) conversion

IPCE measurements were made on a CEP-2000 system (Bunkoh-Keiki Co. Ltd.). IPCE at each wavelength was calculated using Equation 1, where I_{SC} is the short-circuit photocurrent density (mA cm^{-2}) under monochromatic irradiation, q is the elementary charge, λ is the wavelength of incident radiation in nm and P_0 is the incident radiative flux in W/m^2 [2].

$$IPCE(\lambda) = 1240\left(\frac{I_{SC}}{q\lambda P_o}\right) \qquad (1)$$

1.7. Electrochemical impedance spectroscopy (EIS)

The electrochemical impedance spectra were measured with an impedance analyzer potentiostat (Bio-Logic SP-150) under illumination using a solar simulator (SOL3A, Oriel) equipped with a 450 W xenon lamp (91160, Oriel). EIS spectra were recorded over a frequency range of 100 mHz to 200 kHz at room temperature. The applied bias voltage was set at the Voc of the DSCs, with AC amplitude set at 10 mV. The electrical impedance spectra were fitted using Z-Fit software (Bio-Logic).

1.8. Molecular modeling

Equilibrium molecular geometries of novel molecules were calculated using the hybrid exchange–correlation functional CAM-B3LYP [3] and the valence double-zeta polarized basis set 6-31G(d). The geometry optimization calculations were followed by energy calculations using time-dependent density functional theory (TD-DFT) utilizing the functional CAM-B3LYP and the basis set 6-31G(d). The solvent (DMF) effect was accounted for by using the conductor-like polarizable continuum model (CPCM) [4], implemented in Gaussian 09, and the ground and excited states oxidation potentials were calculated. All DFT and TD-DFT jobs were submitted remotely at North Carolina State University's Supercomputer Jasta via HPC linkage.

2. The detailed synthetic procedures of the important intermediates

*2.1. 5-(6-Ethyl-6H-indolo[2,3-b]quinoxalin-2-yl)thiophene-2-carbaldehyde (**2**)*

Under an argon atmosphere, a mixture of compound **1** (3.91 g, 12.03 mmol), 5-formyl-2-thienylboronic acid (2.06 g, 13.23 mmol), $Pd(PPh_3)_4$ (1.39 g, 1.20 mmol), 2 M K_2CO_3 aqueous solution (30.1 mL), and tetrahydrofuran (150 mL)was stirred and heated at 75 °C for 18 h. When the reaction was completed, the mixture was extracted with ethyl acetate for three times. The combined organic solution was washed with sodium chloride solution and dried by anhydrous sodium sulfate. After the rotary evaporation of the solvent, the residue was purified by flash column chromatography (silica gel, hexane/ethyl acetate = 5:1 → 1:2) to obtain yellow solid **2** (3.05 g, 70%). HRMS-ESI (*m*/*z*): $[M + H]^+$ calcd for $C_{21}H_{16}N_3OS$, 358.10086; found, 358.10207 (error, 3.37674 ppm).

*2.2. 5-(9-Bromo-6-ethyl-6H-indolo[2,3-b]quinoxalin-2-yl)thiophene-2-carbaldehyde (**3**)*

Under an argon atmosphere, compound **2** (1.16 g, 3.24 mmol) and *N*-bromosuccinimide (605 mg, 3.40 mmol) were dissolved in anhydrous chloroform (75 mL). The reaction was stirred at the room temperature for 18 h. When the reaction was finished, the solvent was rotary evaporated and the residue was purified by flash column chromatography (silica gel, hexane/ethyl acetate = 5:1 → 1:2) to obtain yellow solid **3** (1.13 g, 80%). HRMS-ESI (*m*/*z*): $[M + H]^+$ calcd for $C_{21}H_{15}BrN_3OS$, 436.01137; found, 436.01190 (error, 1.21604 ppm).

*2.3. N,N-Diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (**4a**)*

Under an argon atmosphere, a mixture of 4-bromotriphenylamine (1.90 g, 5.86 mmol), bis(pinacolato)diboron (1.64 g, 6.45 mmol), $PdCl_2$(dppf) (43 mg, 0.059 mmol), potassium acetate (2.30 g, 23.4 mmol), and 1,4-dioxane (80 mL) was stirred and heated at 90 °C for 18 h. When the reaction was completed, the mixture was extracted with ethyl acetate for three times. The combined organic solution was washed with sodium chloride solution and dried by anhydrous sodium sulfate. After the rotary evaporation of the solvent, the residue was purified by flash column chromatography (silica gel, hexane/ethyl acetate = 10:1 → 4:1) to obtain white solid **4a** (1.44 g, 66%). HRMS-ESI (*m*/*z*): $[M + H]^+$ calcd for $C_{24}H_{27}BNO_2$, 372.21294; found, 372.21329 (error, 0.94452 ppm).

*2.4. 9-Hexyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-carbazole (**4b**)*

Compound **4b** (white oil, 1.68 g, 64%) was synthesized similar to compound **5a** by using compound 3-bromo-9-hexyl-9*H*-carbazole instead of 4-bromotriphenylamine. HRMS-ESI (*m*/*z*): $[M + H]^+$ calcd for $C_{24}H_{33}BNO_2$, 378.25989; found, 378.26022 (error, 0.87082 ppm).

*2.5. 10-Hexyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-10H-phenothiazine (**4c**)*

Compound **4c** (white oil, 1.50 g, 52%) was synthesized similar to compound **5a** by using compound 3-bromo-10-hexyl-10*H*-phenothiazine instead of 4-bromotriphenylamine. HRMS-ESI (*m*/*z*): $[M + H]^+$ calcd for $C_{24}H_{33}BNO_2S$, 410.23196; found, 410.23258 (error, 1.51416 ppm).

3. Additional results of analytical measurements

*3.1. Figure 1S: UV-Vis absorption and emission spectra of **HD-2***

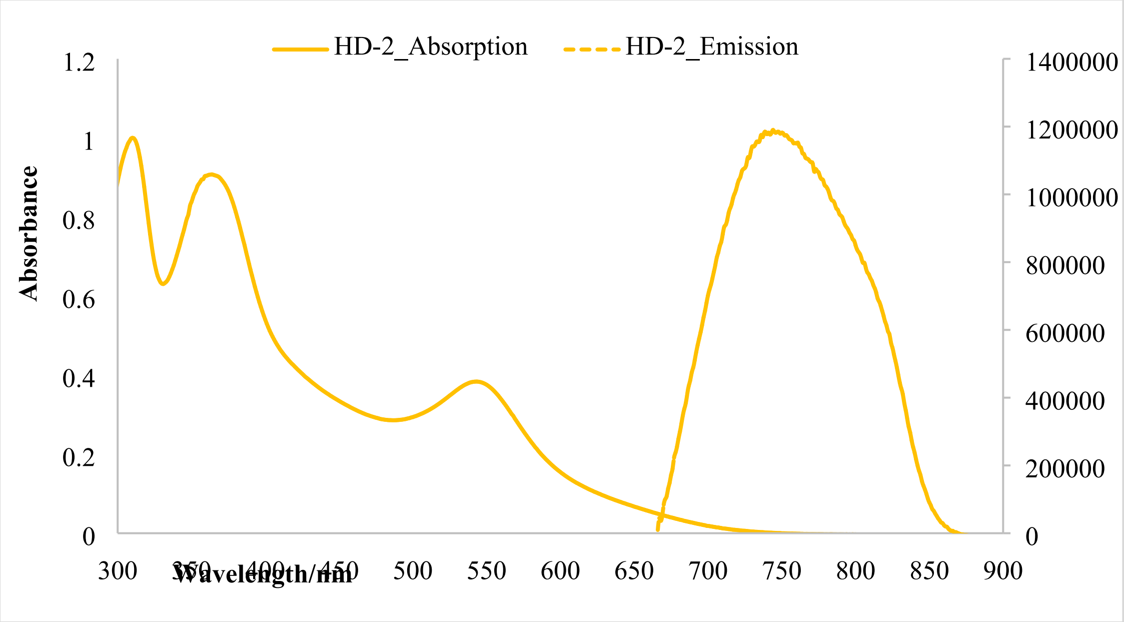

Figure 1S UV-Vis absorption (solid-line) and emission spectra (dashed-line) of **HD-2** in DMF (2×10^{-5} M).

3.2. Figure 2S-4S: Attenuated Total Reflectance Fourier-transform Infra-Red Spectroscopy of ***FS10****,* ***FS11*** *and* ***FS12***

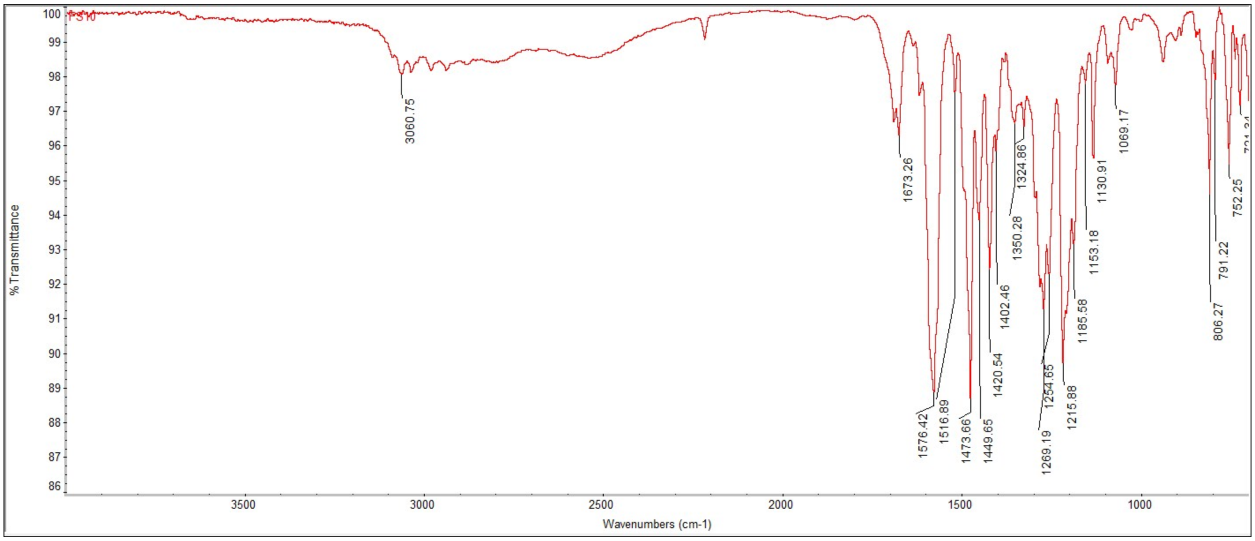

Figure 2S ATR/FT-IR spectrum of **FS10**.

FS10: 3060.75 cm^{-1} ($-CH_3$ stretch), 1673.26 (-conjugated C=O stretch of -COOH).

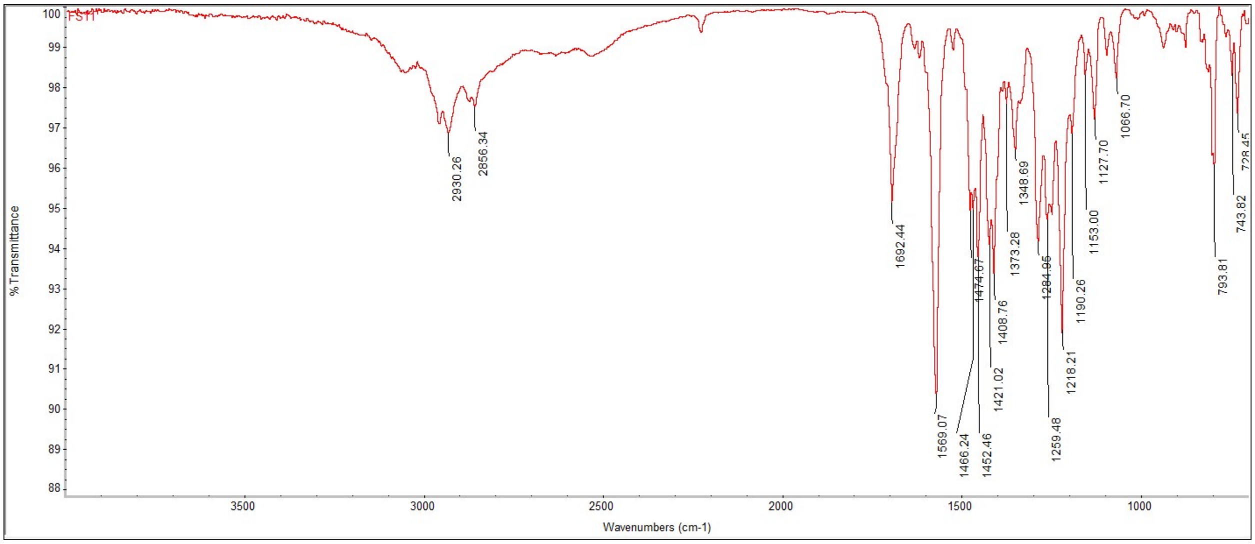

Figure 3S ATR/FT-IR spectrum of **FS11**.

FS11: 2930.26, 2856.34 cm^{-1} (-CH$_3$ stretch), 1692.44 (-conjugated C=O stretch of -COOH).

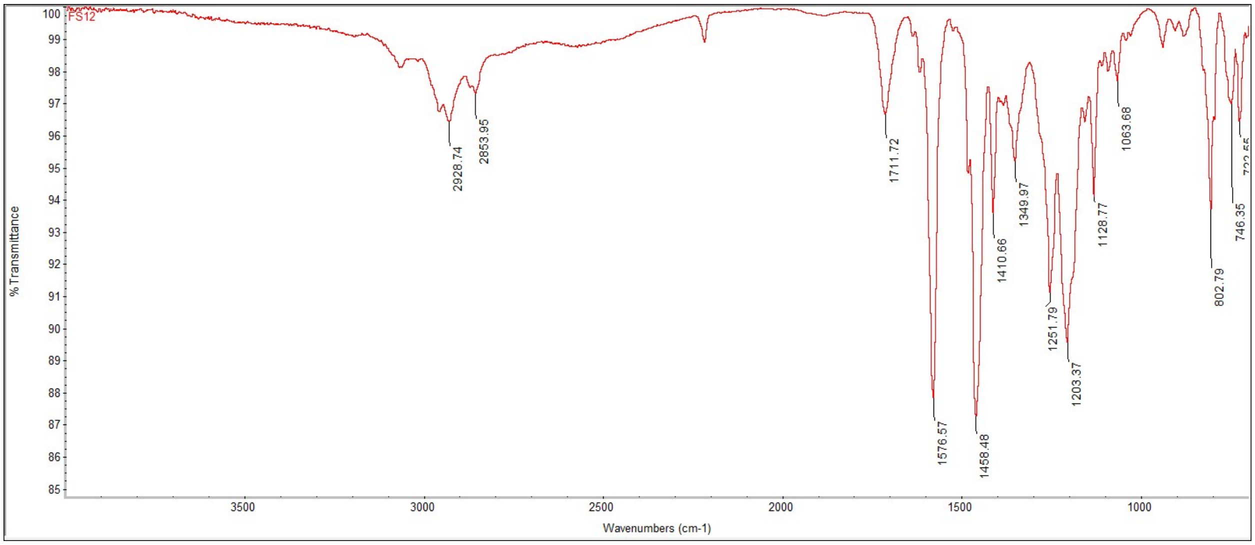

Figure 4S ATR/FT-IR spectrum of **FS12**.

FS12: 2928.74, 2853.95 cm^{-1} (-CH$_3$ stretch), 1711.72 (-conjugated C=O stretch of -COOH).

*3.3. Figure 5S-10S: ^{1}H NMR spectra of **FS10**, **FS11** and **FS12** and other important intermediates*

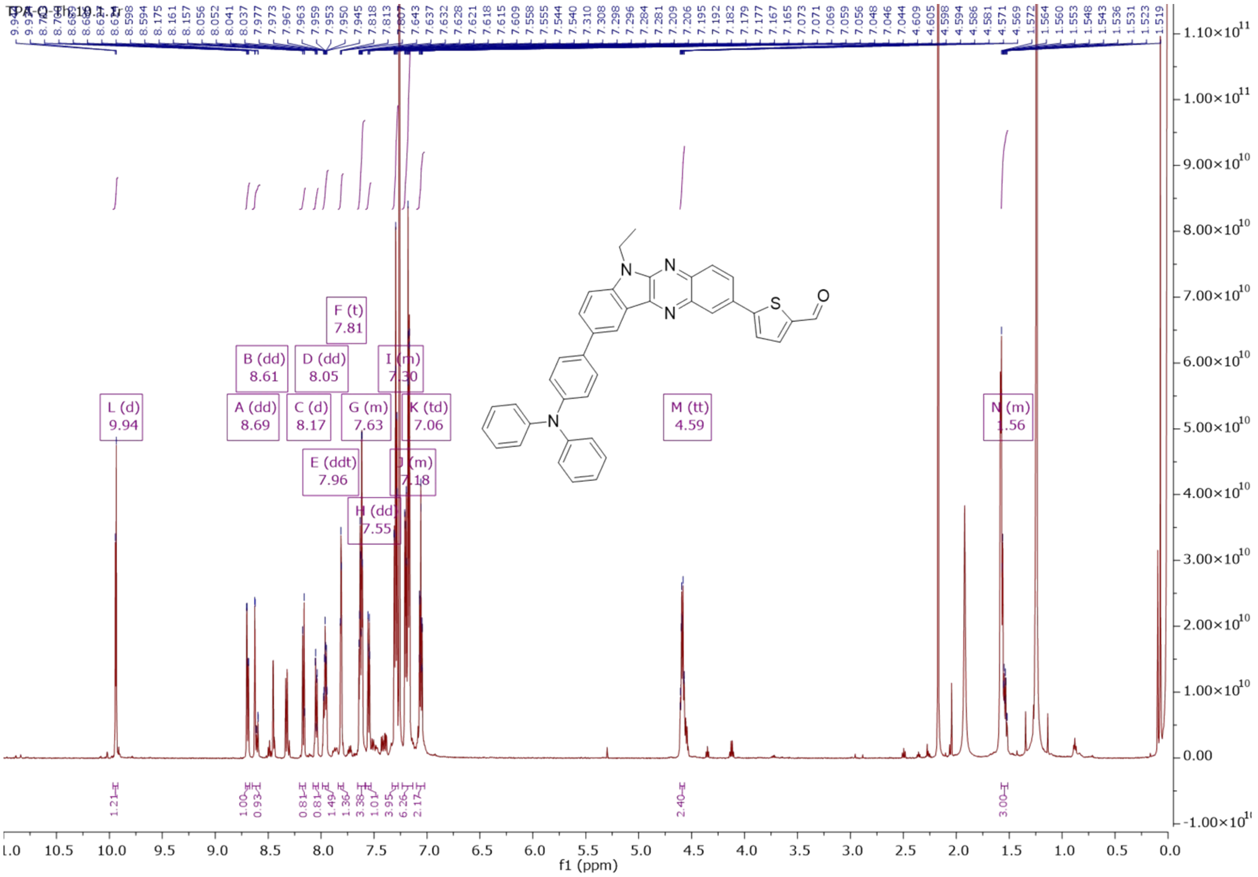

Figure 5S ^{1}H NMR spectra of compound **5a**.

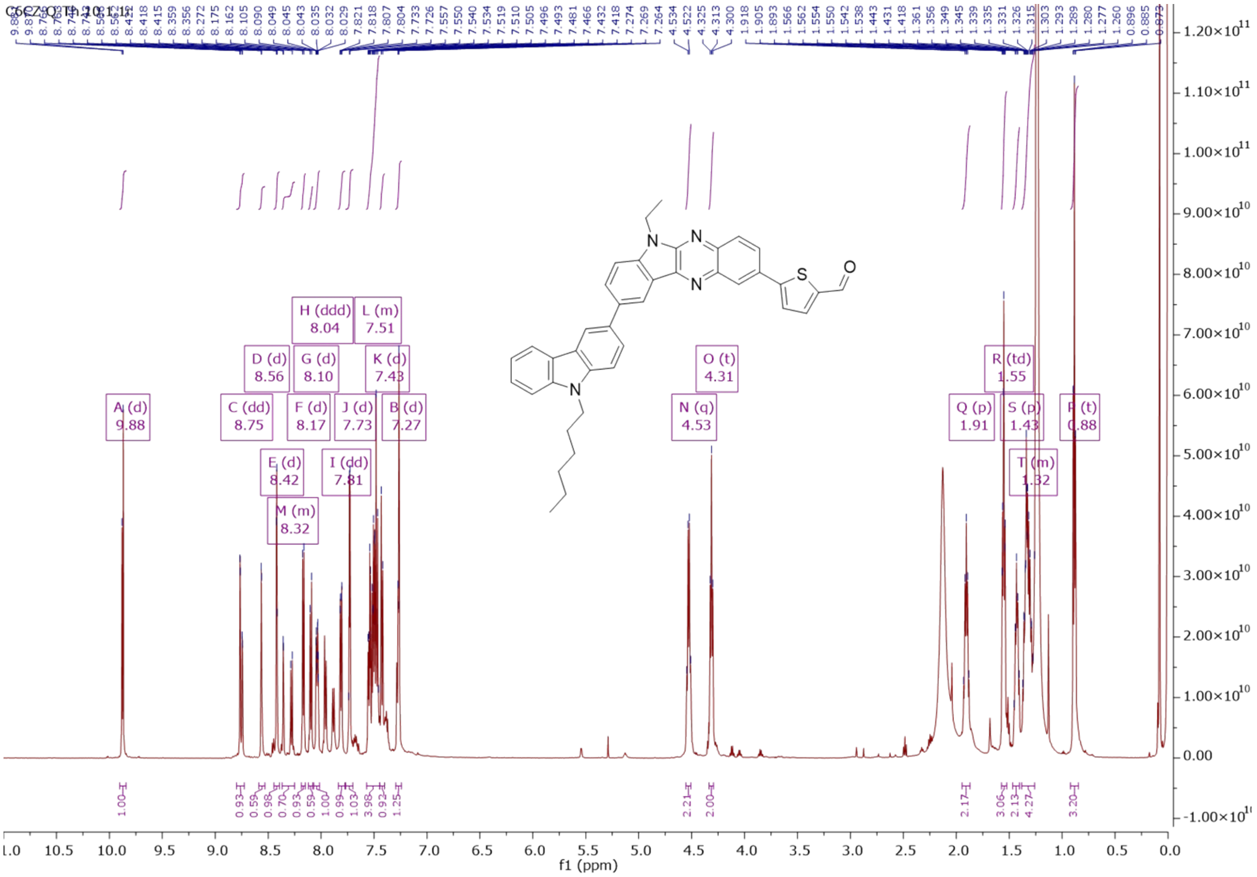

Figure 6S ^{1}H NMR spectra of compound **5b**.

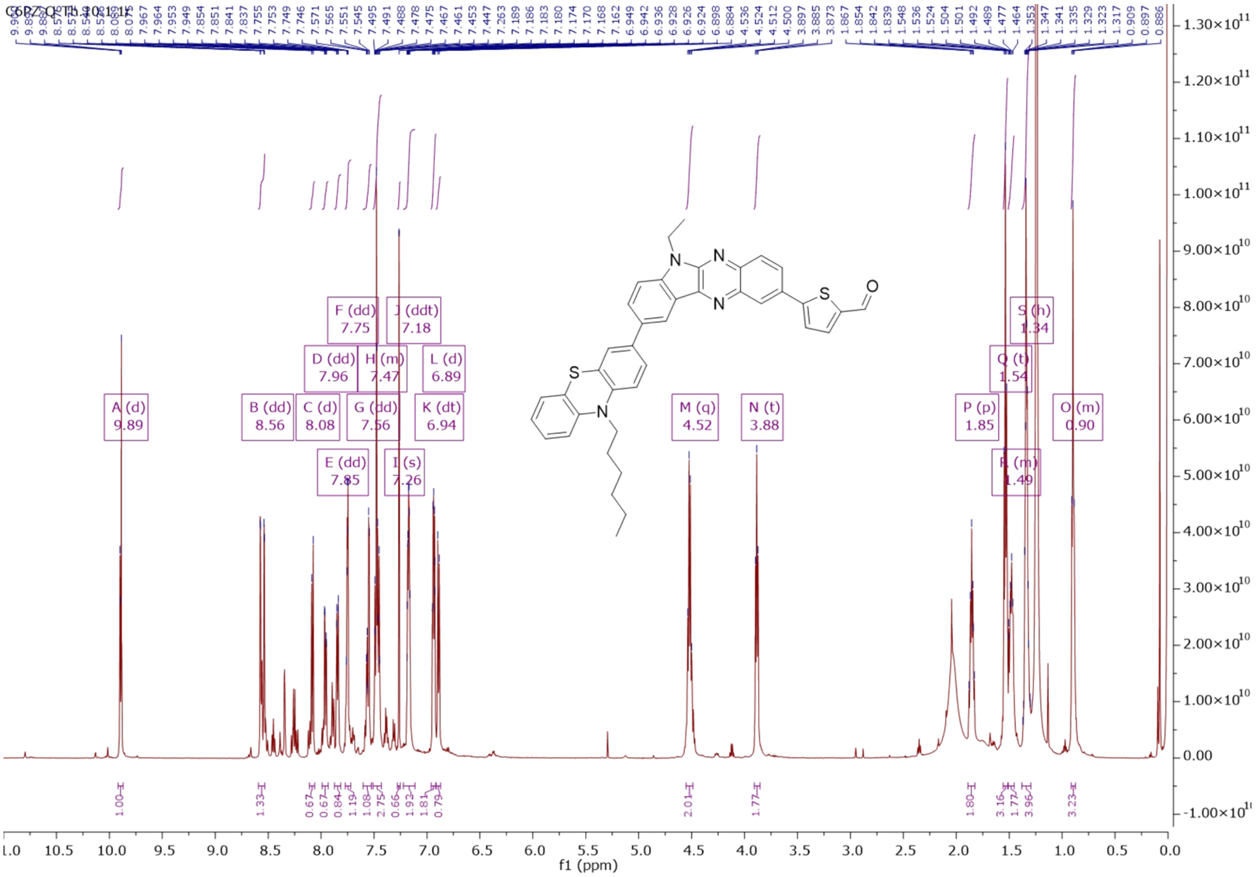

Figure 7S ^{1}H NMR spectra of compound **5c**.

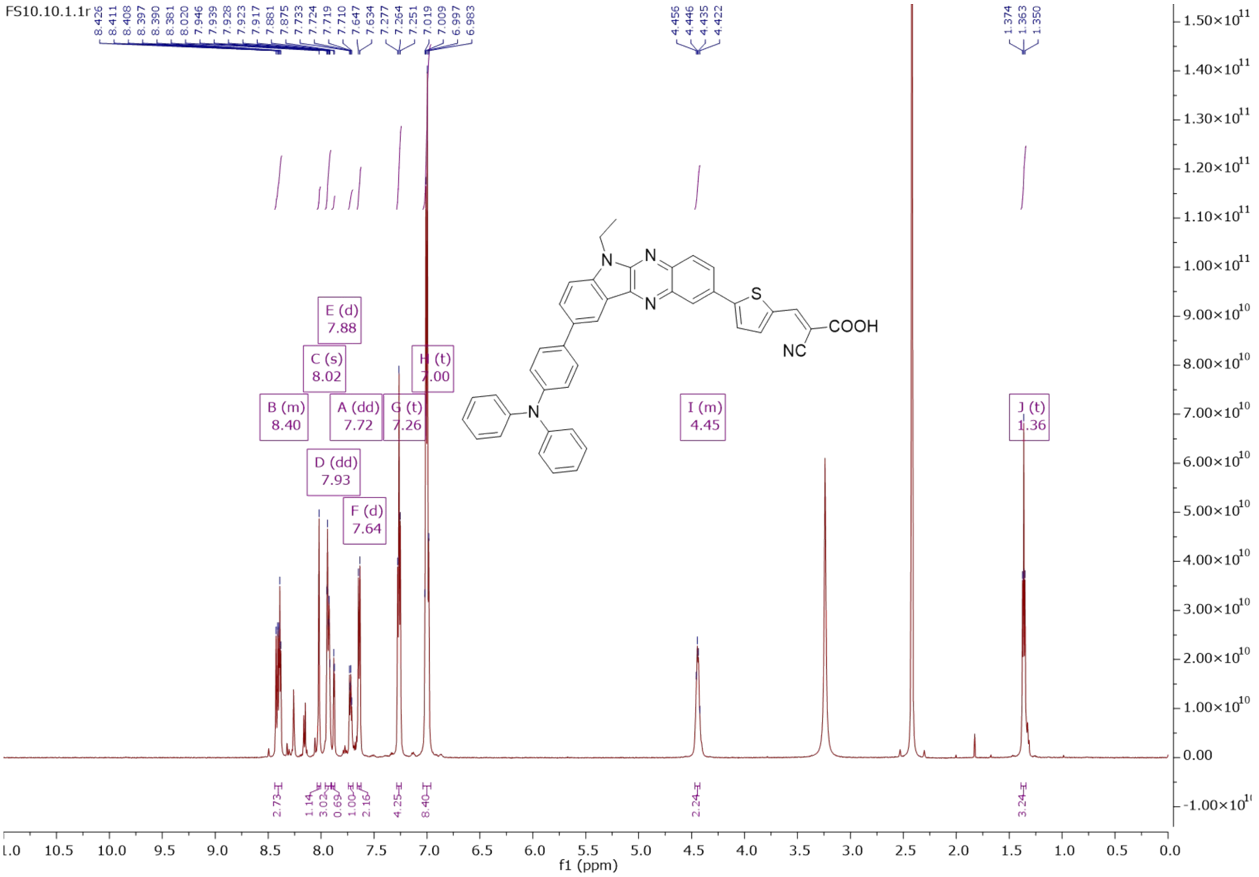

Figure 8S ^{1}H NMR spectra of **FS10**.

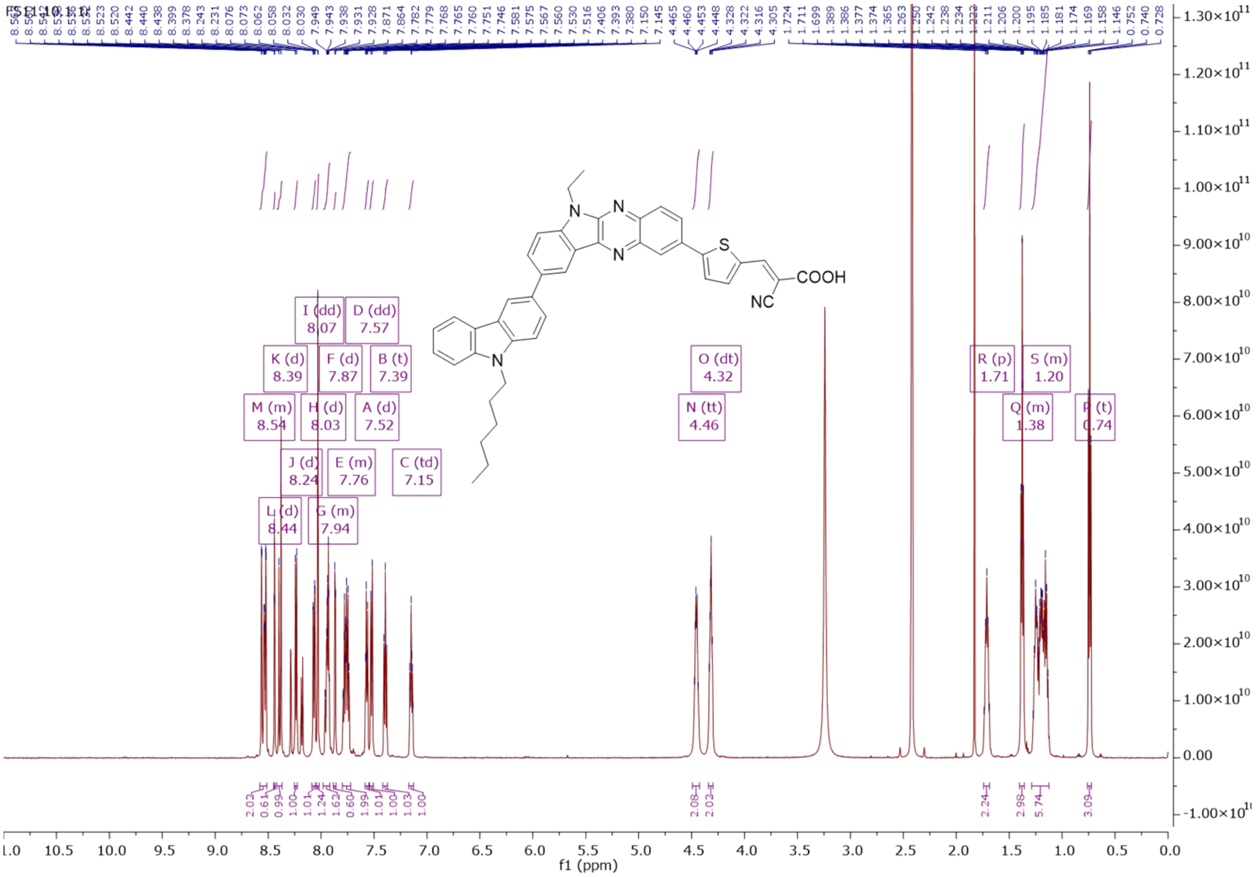

Figure 9S ^{1}H NMR spectra of **FS11**.

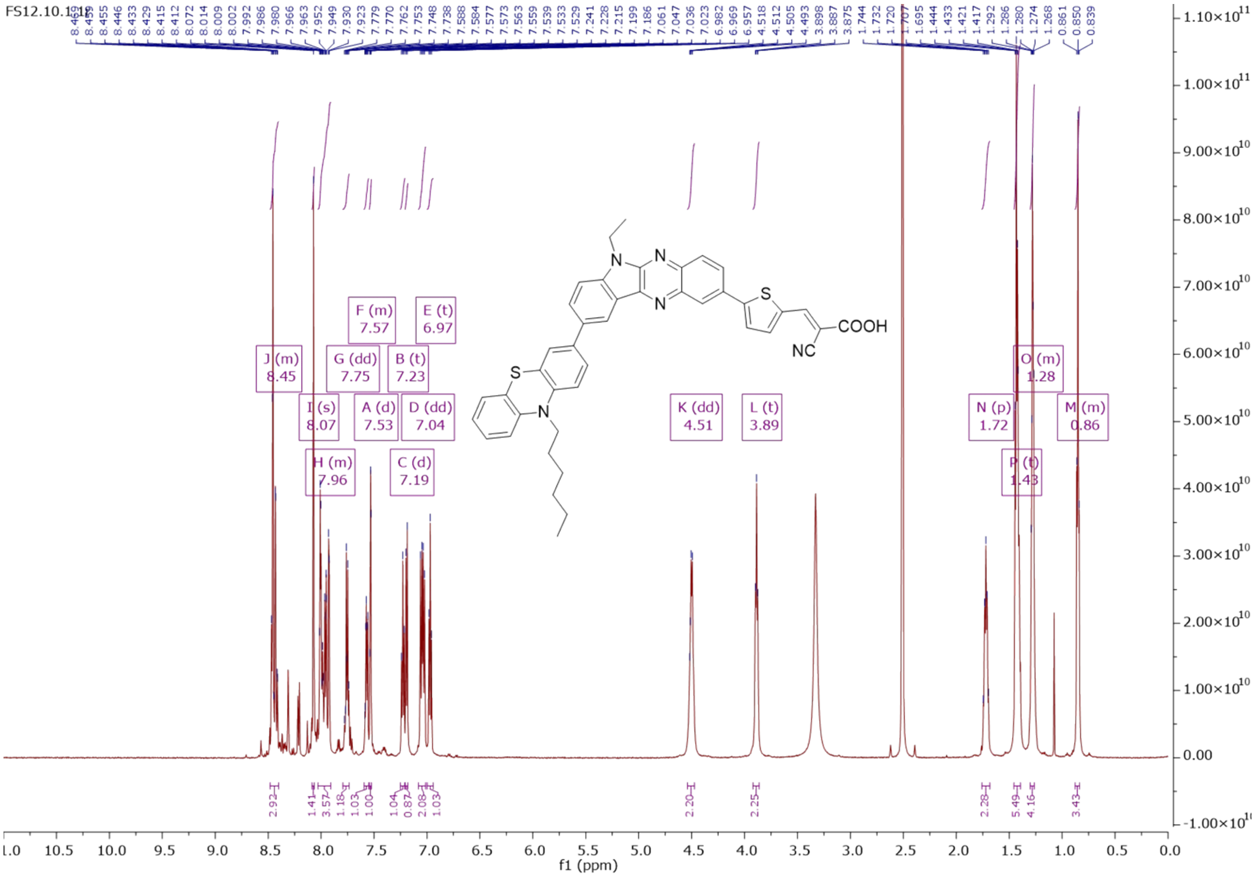

Figure 10S ^{1}H NMR spectra of **FS12**.

*3.4. Figure 11S-21S: High resolution mass spectrometry of **FS10**, **FS11** and **FS12** and other important intermediates*

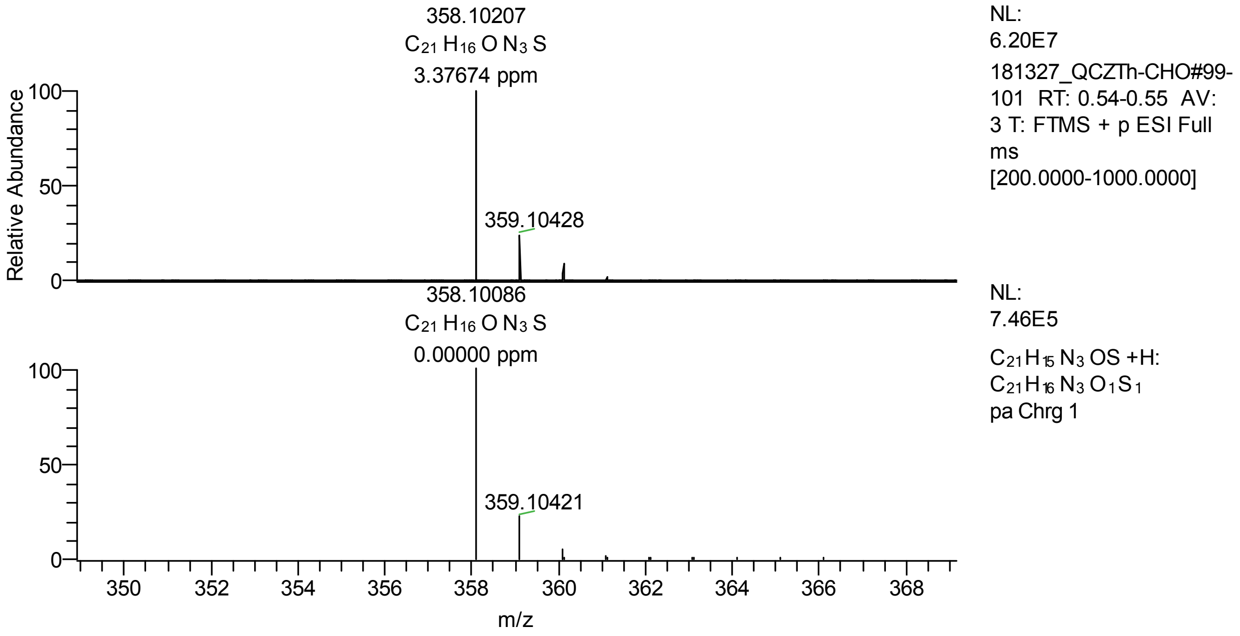

Figure 11S ESI mass spectrum of compound **2**.

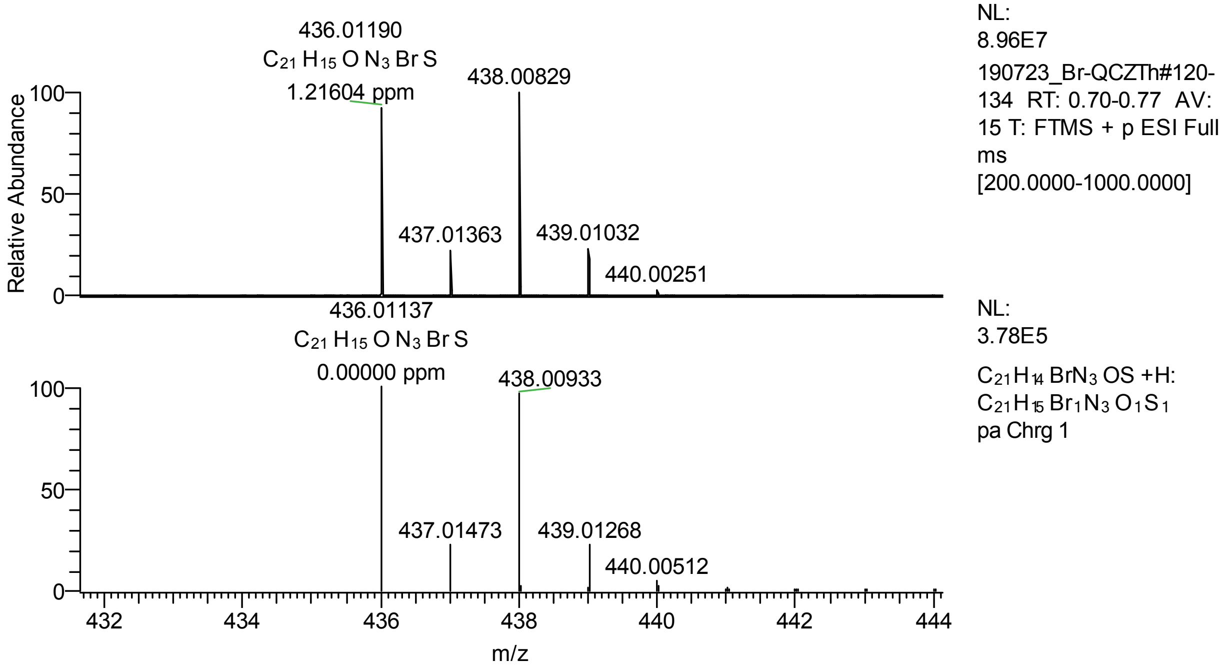

Figure 12S ESI mass spectrum of compound **3**.

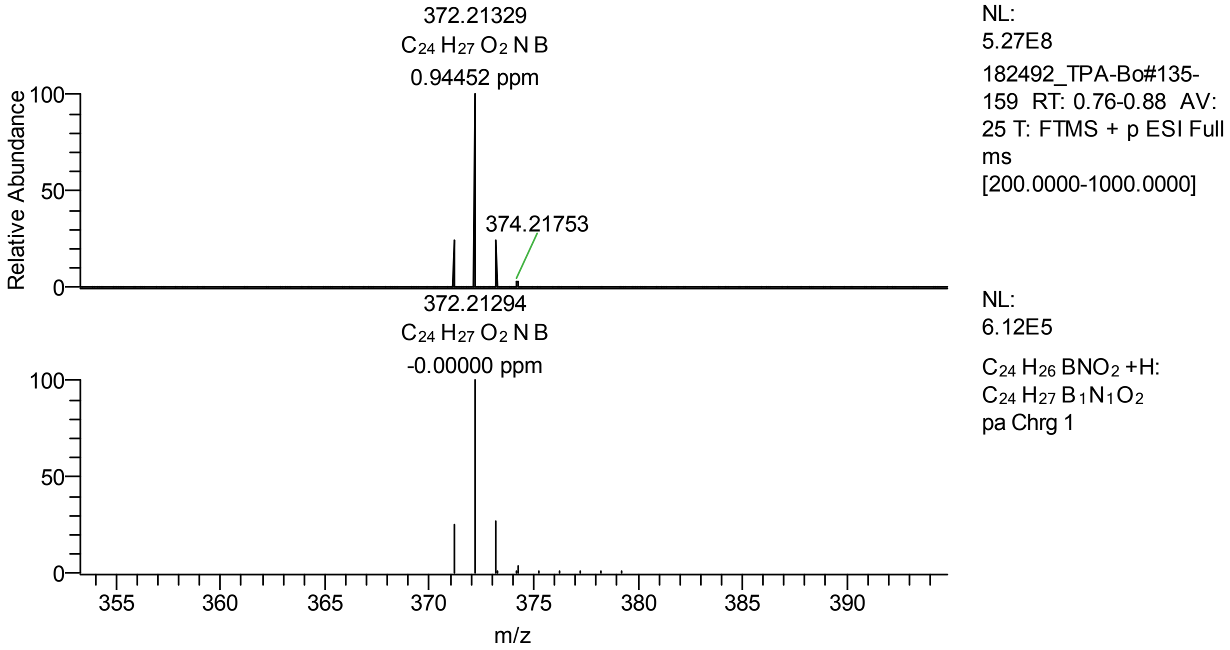

Figure 13S ESI mass spectrum of compound **4a**.

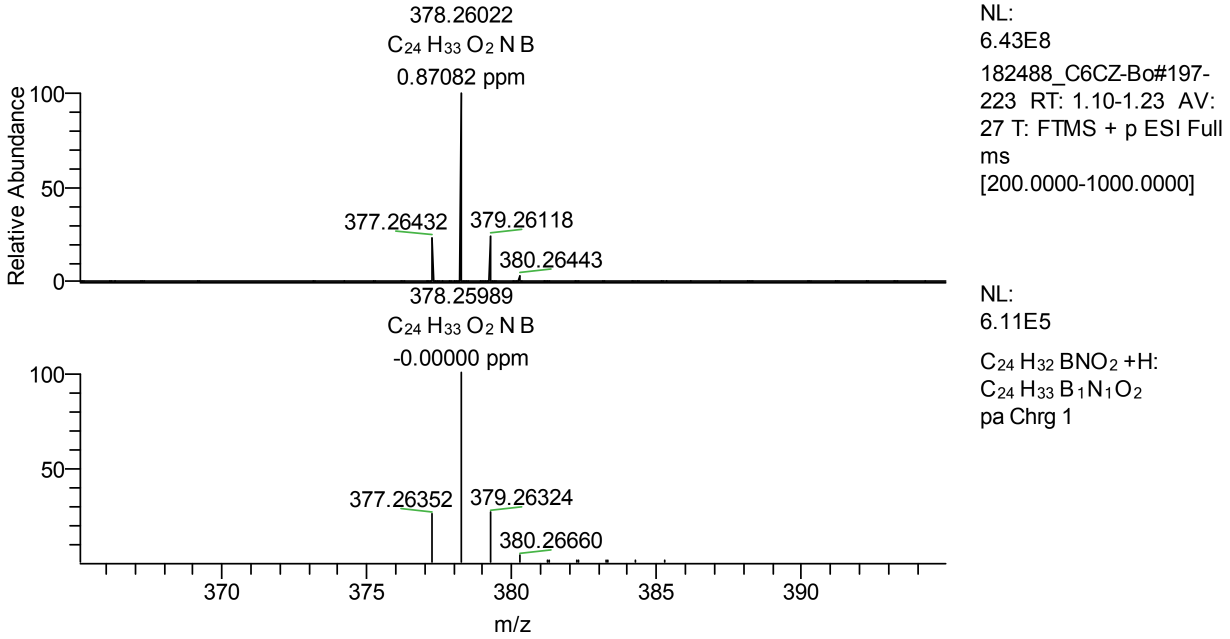

Figure 14S ESI mass spectrum of compound **4b**.

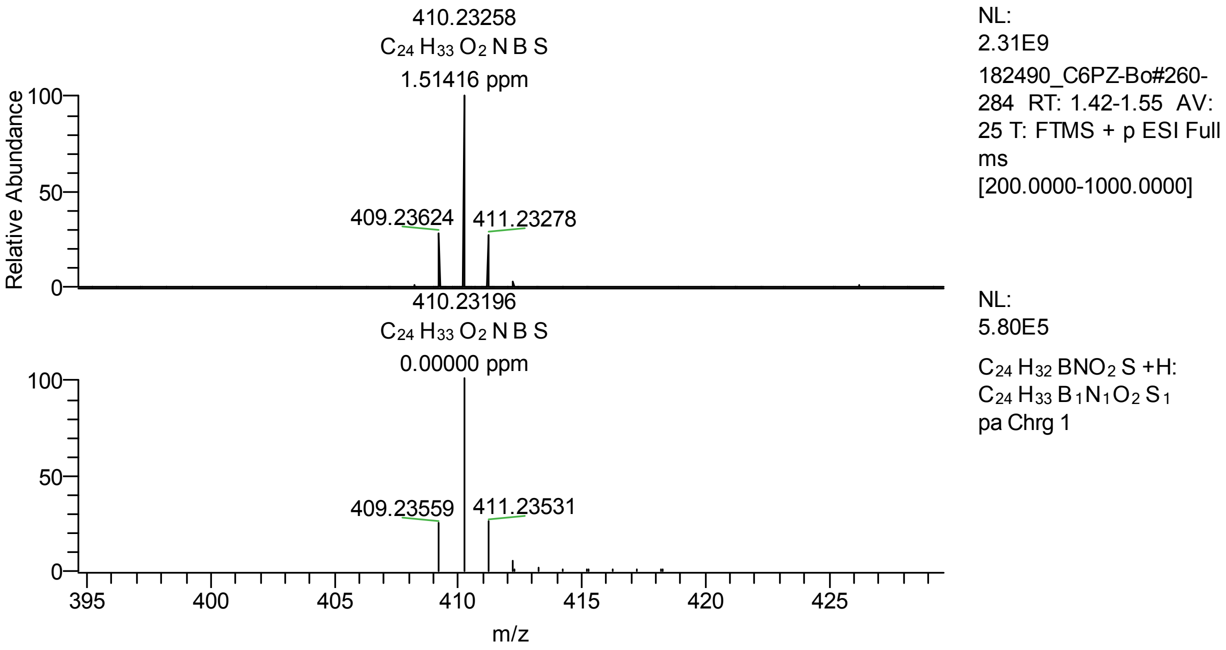

Figure 15S ESI mass spectrum of compound **4c**.

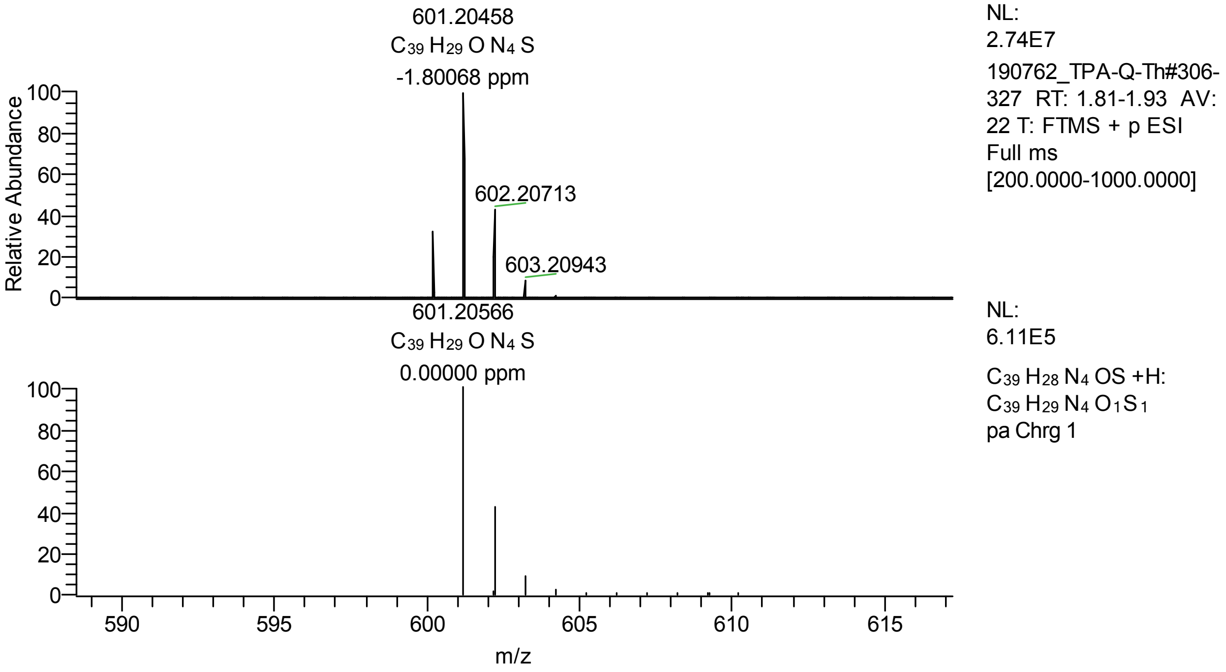

Figure 16S ESI mass spectrum of compound **5a**.

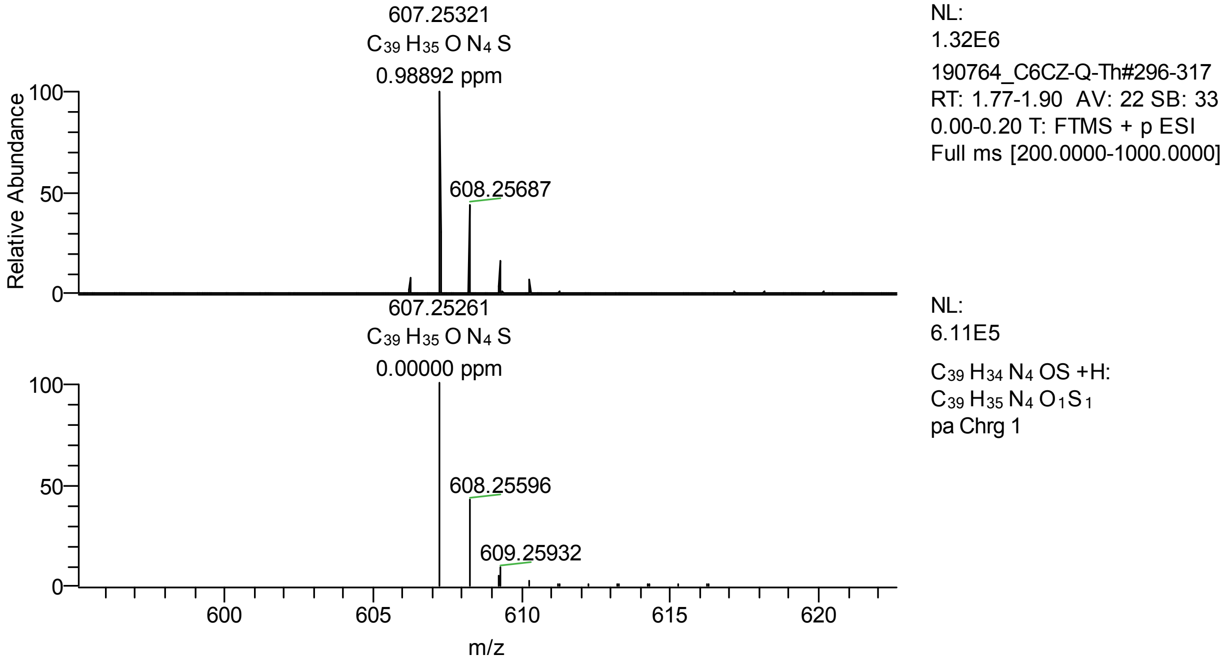

Figure 17S ESI mass spectrum of compound **5b**.

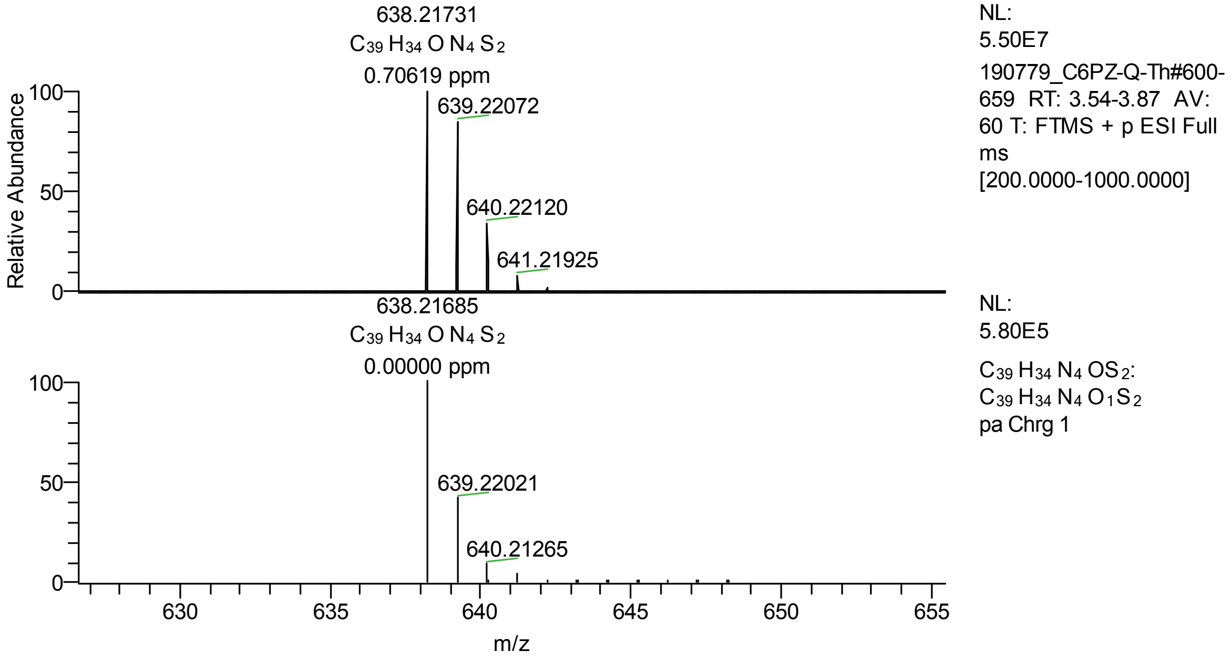

Figure 18S ESI mass spectrum of compound **5c**.

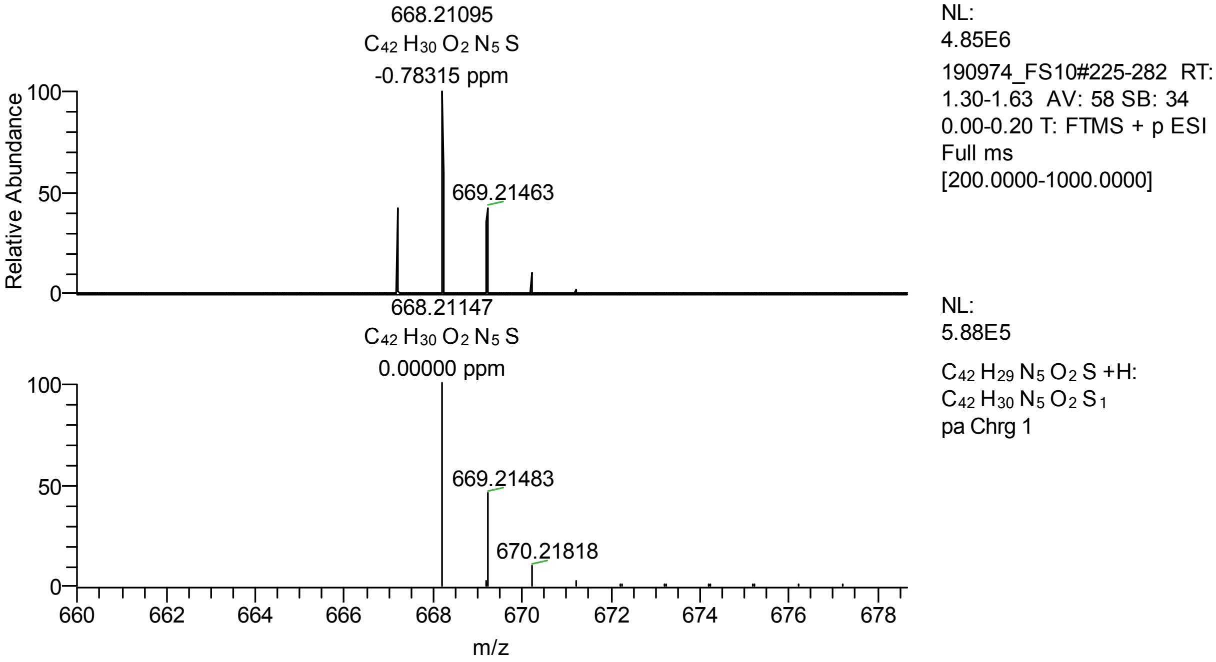

Figure 19S ESI mass spectrum of **FS10**.

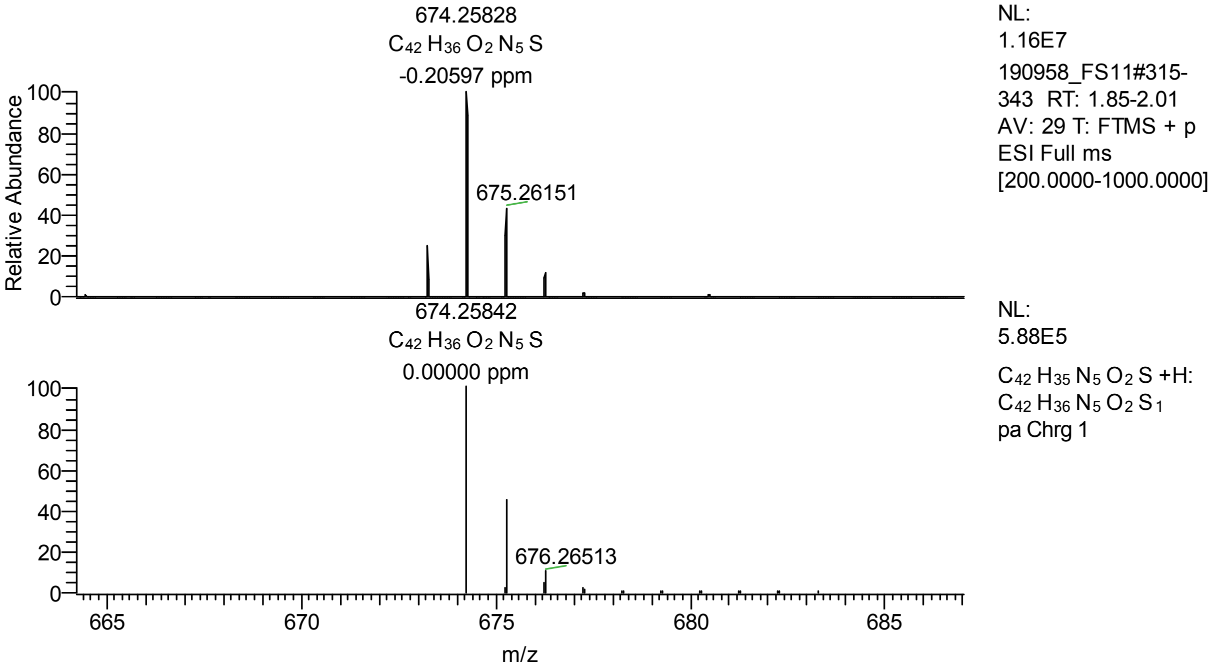

Figure 20S ESI mass spectrum of **FS11**.

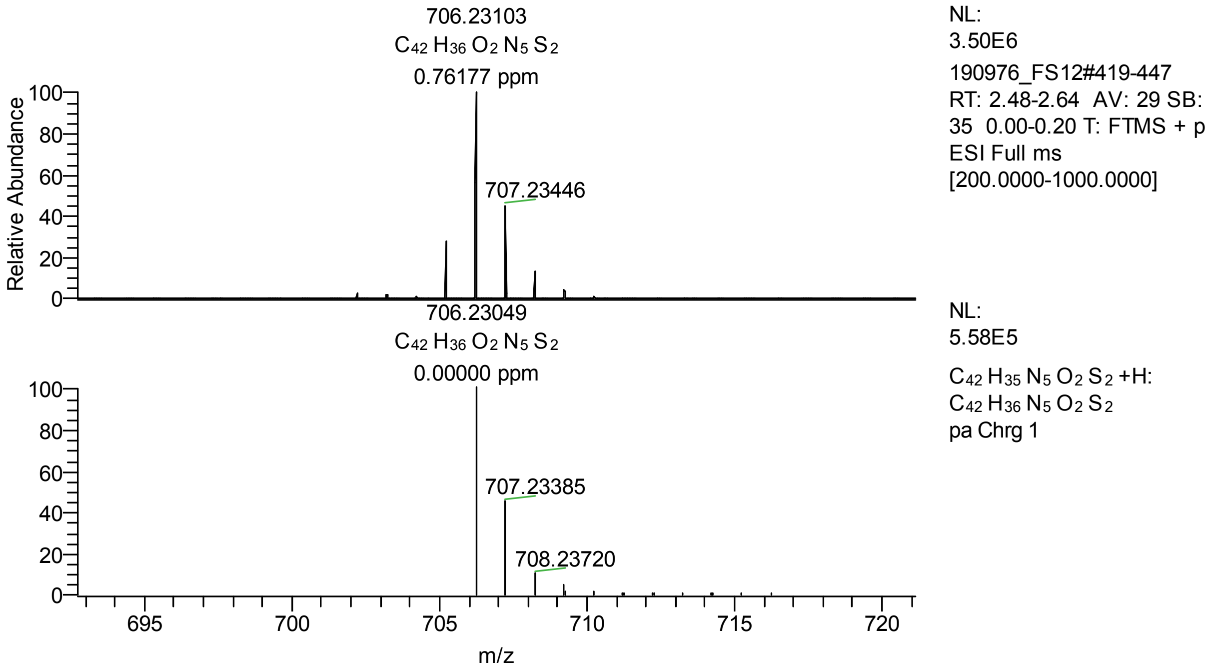

Figure 21S ESI mass spectrum of **FS12**.

*3.5. Figure 22S-24S: Cyclic voltammetry graphs of **FS10**, **FS11** and **FS12***

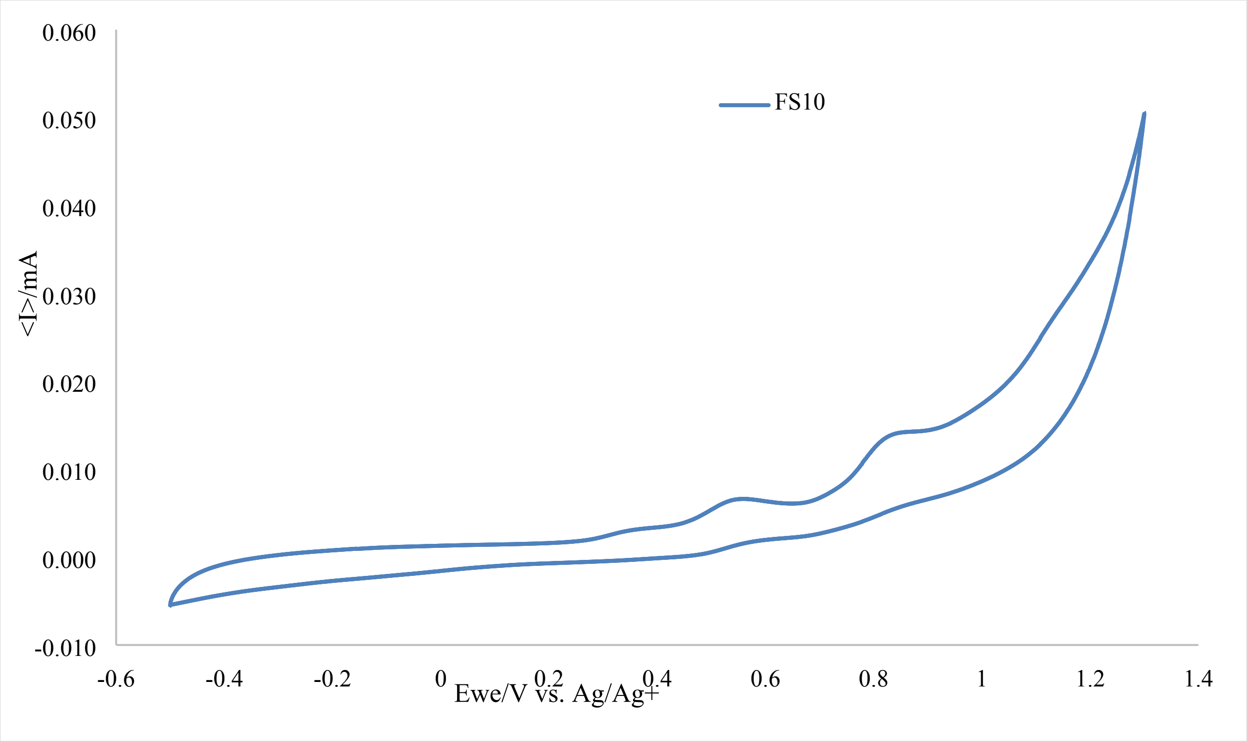

Figure 22S CV graph of **FS10** (-5.54eV).

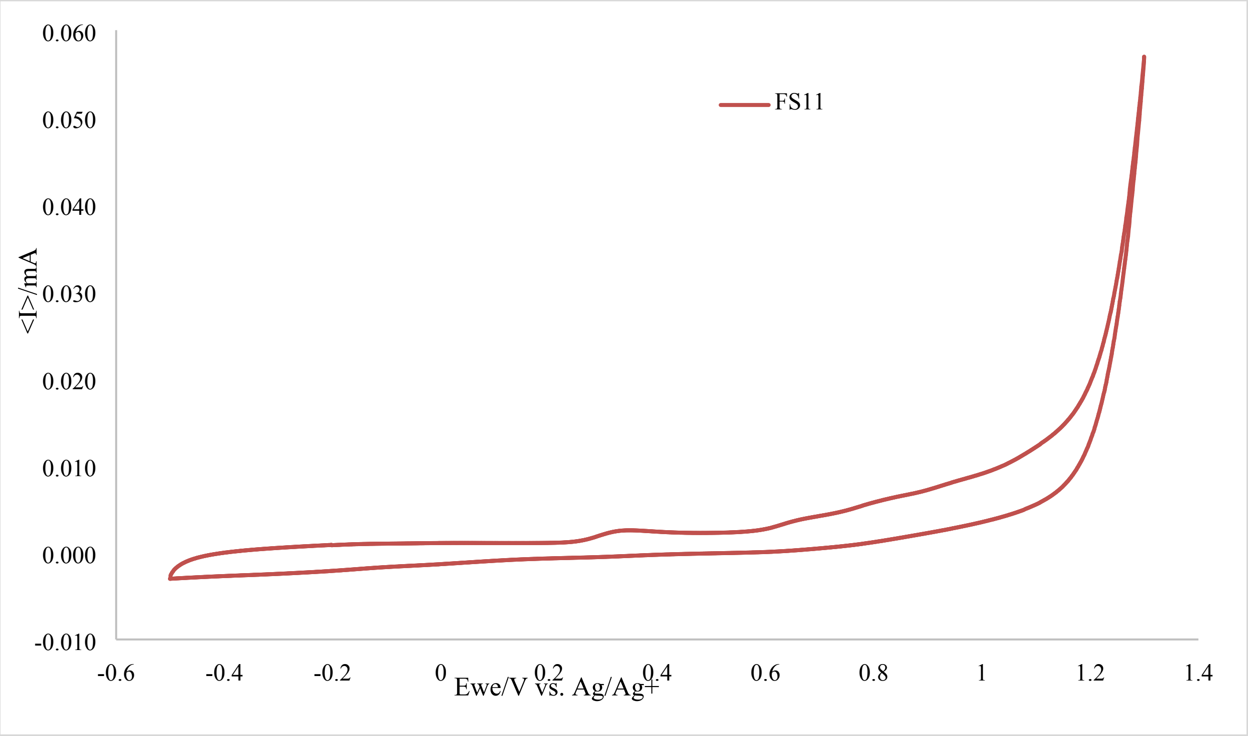

Figure 23S CV graph of **FS11** (-5.54eV).

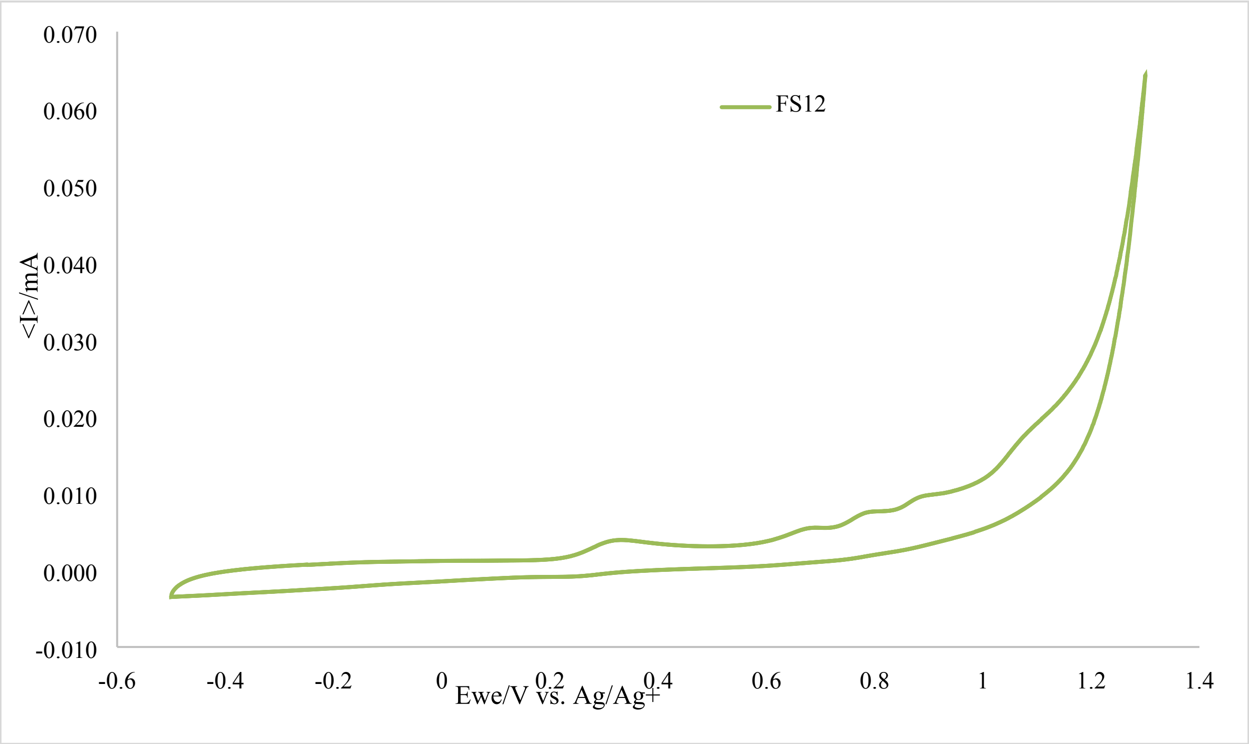

Figure 24S CV graph of **FS12** (-5.53eV).

4. Theoretical calculations: Table 1S-3S: Cartesian coordinates for the optimized geometry of FS10, FS11 and FS12

Table 1S Cartesian coordinates for the optimized geometry of **FS10**.

Atoms	Cartesian Coordinates		
0 1			
C	-2.98037	3.678245	0.042914
C	-2.64429	2.312158	-0.02531
C	-1.29576	1.95961	-0.08237
C	-0.32649	2.954621	-0.06905
C	-0.68947	4.314204	-0.00413
C	-2.02777	4.687219	0.053588
C	1.120212	2.930054	-0.12339
C	1.551048	4.311927	-0.08197
N	0.448517	5.120513	-0.02044
N	1.964508	1.940467	-0.19396
C	3.283832	2.303871	-0.22391

C	3.692147	3.668375	-0.18308
N	2.796804	4.695705	-0.10611
C	4.260454	1.289616	-0.30388
C	5.605633	1.591055	-0.34001
C	6.002789	2.956718	-0.29539
C	5.076477	3.959371	-0.22081
C	0.481157	6.571135	0.081966
C	0.390706	7.064475	1.521556
H	-4.02702	3.956526	0.111134
H	-0.99802	0.918863	-0.15717
H	-2.32853	5.72696	0.115841
H	3.905874	0.265239	-0.35488
H	7.058458	3.203993	-0.30092
H	5.378679	5.000251	-0.18049
H	1.41578	6.896727	-0.37841
H	-0.33811	6.970152	-0.52206
H	0.414769	8.157632	1.54368
H	1.231816	6.689288	2.110943
H	-0.5375	6.733487	1.995876
C	-3.70332	1.27447	-0.03435
C	-3.524	0.050747	0.61927
C	-4.91748	1.479645	-0.69808
C	-4.51144	-0.92231	0.617976
H	-2.60722	-0.13405	1.170593
C	-5.90543	0.507145	-0.71696
H	-5.08338	2.404344	-1.24211
C	-5.71865	-0.70989	-0.05465
H	-4.35218	-1.85303	1.151298
H	-6.82812	0.686282	-1.25789
N	-6.72606	-1.7018	-0.06466
C	-8.09045	-1.3322	0.05115
C	-6.37565	-3.07052	-0.19007
C	-8.48575	-0.35439	0.96852
C	-9.05977	-1.94402	-0.74875
C	-7.00735	-4.03786	0.596583
C	-5.3969	-3.47168	-1.10384
C	-9.82252	0.008757	1.073331
H	-7.74052	0.119147	1.598525
C	-10.3971	-1.5889	-0.62464
H	-8.75987	-2.69939	-1.46711
C	-6.67079	-5.37903	0.462886

H	-7.76358	-3.73338	1.312129
C	-5.05242	-4.81259	-1.21819
H	-4.90793	-2.7277	-1.72347
C	-10.787	-0.60808	0.282245
H	-10.1119	0.770826	1.790453
H	-11.137	-2.07514	-1.25302
C	-5.68907	-5.77501	-0.4404
H	-7.17232	-6.11743	1.08096
H	-4.28929	-5.10666	-1.93228
H	-11.8314	-0.3276	0.371765
H	-5.42312	-6.82257	-0.53737
C	6.627617	0.54339	-0.42748
C	7.906459	0.656839	-0.92494
S	6.313627	-1.06537	0.133362
C	8.627409	-0.54859	-0.86727
H	8.303815	1.573243	-1.3421
C	7.91241	-1.59726	-0.32235
H	9.645354	-0.66377	-1.22129
C	8.44404	-2.91118	-0.16775
H	9.469522	-3.02523	-0.51087
C	7.892972	-4.04664	0.333963
C	6.562411	-4.12148	0.840235
N	5.480414	-4.17537	1.250922
C	8.724105	-5.27257	0.353155
O	9.86642	-5.33185	-0.04677
O	8.06817	-6.32175	0.865727
H	8.672986	-7.08583	0.844486

Table 2S Cartesian coordinates for the optimized geometry of **FS11**.

Atoms	Cartesian Coordinates		
0 1			
C	2.586956	-3.64887	0.665075
C	2.28766	-2.33229	0.264302
C	0.948615	-1.95034	0.181776
C	-0.04682	-2.86769	0.495212
C	0.279999	-4.17905	0.891708
C	1.607943	-4.58192	0.977081
C	-1.49281	-2.79566	0.508248
C	-1.96048	-4.10098	0.926844

N	-0.87977	-4.90721	1.159997
N	-2.31078	-1.82214	0.224991
C	-3.63967	-2.12414	0.353528
C	-4.08453	-3.41455	0.762445
N	-3.21654	-4.42671	1.05432
C	-4.58932	-1.12335	0.061525
C	-5.94256	-1.36603	0.16893
C	-6.37615	-2.65636	0.583296
C	-5.47661	-3.64587	0.867448
C	-0.94953	-6.30749	1.547129
C	-0.83464	-7.25682	0.359884
H	3.627819	-3.94371	0.750542
H	0.677492	-0.95079	-0.14206
H	1.881465	-5.58487	1.284981
H	-4.20881	-0.16224	-0.26893
H	-7.4371	-2.85081	0.693427
H	-5.80599	-4.62812	1.18858
H	-0.15797	-6.49543	2.277669
H	-1.90478	-6.44334	2.057475
H	-0.88811	-8.29329	0.704765
H	0.114494	-7.12065	-0.16619
H	-1.64921	-7.08725	-0.3496
C	3.37603	-1.3768	-0.06287
C	3.267645	-0.0213	0.309252
C	4.518981	-1.79948	-0.73968
C	4.254956	0.906993	0.023866
H	2.390227	0.303768	0.859329
C	5.52879	-0.88713	-1.03608
H	4.614289	-2.83496	-1.05307
C	5.38977	0.465861	-0.65707
H	4.144478	1.939558	0.336996
C	6.805996	-0.99419	-1.70908
N	6.501473	1.176689	-1.07189
C	7.372938	0.299756	-1.69715
C	7.49981	-2.0487	-2.30359
C	6.756834	2.580358	-0.80649
C	8.624198	0.55061	-2.26189
C	8.74147	-1.80341	-2.87042
H	7.073536	-3.04754	-2.3203
H	5.797351	3.105933	-0.81879
H	7.340396	2.981327	-1.64061

C	7.480635	2.825898	0.516903
C	9.293818	-0.51453	-2.84639
H	9.065779	1.541264	-2.24566
H	9.293208	-2.61403	-3.3353
H	6.885751	2.398273	1.333253
H	8.43554	2.286348	0.507713
C	7.725367	4.310559	0.775614
H	10.26881	-0.34439	-3.29263
H	8.30813	4.734058	-0.05362
H	6.764555	4.842828	0.778337
C	8.453591	4.575953	2.091643
H	7.873704	4.14744	2.920479
H	9.416451	4.047162	2.086941
C	8.69503	6.06005	2.360468
H	9.272438	6.48795	1.530763
H	7.732082	6.586877	2.366116
C	9.425256	6.315286	3.676063
H	10.40493	5.824891	3.683764
H	9.585993	7.384718	3.844613
H	8.853777	5.925423	4.525649
C	-6.93692	-0.33339	-0.13837
C	-8.24416	-0.51662	-0.52994
S	-6.54536	1.350672	-0.02942
C	-8.92516	0.692523	-0.75436
H	-8.69052	-1.49186	-0.67652
C	-8.1504	1.814791	-0.53458
H	-9.95732	0.755968	-1.07909
C	-8.63327	3.145341	-0.70528
H	-9.67238	3.210112	-1.01889
C	-8.02195	4.347561	-0.54514
C	-6.66328	4.494794	-0.13948
N	-5.55864	4.607653	0.191198
C	-8.8151	5.570292	-0.80934
O	-9.97614	5.571511	-1.15632
O	-8.10176	6.688177	-0.62156
H	-8.68533	7.445048	-0.81295

Table 3S Cartesian coordinates for the optimized geometry of **FS12**.

Atoms Cartesian Coordinates

0 1

C	-2.81946	-3.81221	-0.32058
C	-2.46138	-2.45212	-0.25065
C	-1.10912	-2.12055	-0.16873
C	-0.15639	-3.13142	-0.15868
C	-0.54058	-4.48502	-0.22799
C	-1.88357	-4.83652	-0.30803
C	1.289224	-3.13079	-0.07701
C	1.697501	-4.51961	-0.10648
N	0.584067	-5.30924	-0.20861
N	2.148296	-2.15518	0.008579
C	3.460289	-2.54043	0.067835
C	3.846169	-3.9119	0.043501
N	2.935264	-4.9244	-0.04524
C	4.451985	-1.54228	0.1641
C	5.790725	-1.86611	0.23062
C	6.165482	-3.23857	0.20246
C	5.224155	-4.22597	0.114065
C	0.588919	-6.76398	-0.21258
C	0.359213	-7.36084	1.171252
H	-3.86917	-4.07384	-0.40616
H	-0.79635	-1.08433	-0.09227
H	-2.20018	-5.87162	-0.36751
H	4.11379	-0.51183	0.202101
H	7.216435	-3.5036	0.232117
H	5.5095	-5.27201	0.086466
H	-0.17571	-7.1014	-0.9174
H	1.558071	-7.07262	-0.60871
H	0.367508	-8.45285	1.112135
H	-0.60482	-7.04849	1.582579
H	1.146647	-7.04726	1.86206
C	6.828357	-0.83535	0.333711
C	8.09347	-0.96691	0.860861
S	6.554965	0.774078	-0.24592
C	8.836428	0.225396	0.810357
H	8.465173	-1.88675	1.293816
C	8.152305	1.281873	0.241352
H	9.84798	0.326003	1.186424
C	8.710145	2.585097	0.088582
H	9.729832	2.683968	0.453056
C	8.190279	3.72619	-0.43332

C	6.872594	3.820728	-0.96912
N	5.800991	3.890473	-1.40395
C	9.043244	4.937083	-0.44302
O	10.17748	4.979325	-0.01871
O	8.417278	5.993842	-0.97719
H	9.034943	6.747302	-0.94798
C	-3.50251	-1.39591	-0.26422
C	-4.72508	-1.57947	0.387865
C	-3.30008	-0.18527	-0.93084
C	-5.68838	-0.58118	0.397869
H	-4.92012	-2.50062	0.927736
C	-4.27267	0.804931	-0.94918
H	-2.37691	-0.02033	-1.47701
S	-7.18763	-0.78313	1.329495
C	-5.48324	0.631836	-0.27349
H	-4.08377	1.716938	-1.50237
C	-8.28349	0.035507	0.195518
N	-6.49471	1.614776	-0.25318
C	-9.58143	-0.42506	0.009966
C	-7.8223	1.180945	-0.46932
C	-6.14194	3.004243	-0.54069
C	-10.4575	0.266724	-0.81916
H	-9.90649	-1.32114	0.529186
C	-8.6999	1.842118	-1.33322
C	-5.17681	3.592639	0.487203
H	-5.74413	3.120657	-1.55905
H	-7.06623	3.581583	-0.50111
C	-10.0088	1.398403	-1.48873
H	-11.476	-0.08381	-0.94691
H	-8.36256	2.704688	-1.89515
C	-4.83235	5.047991	0.176442
H	-4.25516	3.003341	0.531032
H	-5.64208	3.520412	1.477389
H	-10.6741	1.937651	-2.15545
C	-3.89371	5.670932	1.207743
H	-4.36983	5.109273	-0.81796
H	-5.75578	5.640385	0.122075
C	-3.53404	7.12308	0.899824
H	-2.97284	5.074785	1.267698
H	-4.35847	5.615666	2.201613
C	-2.59921	7.737776	1.937805

H	-3.06731	7.176644	-0.09224
H	-4.45457	7.717681	0.836731
H	-1.65783	7.180568	1.998796
H	-2.3567	8.776804	1.69374
H	-3.05518	7.726376	2.933973

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